



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:45 PM UTC

PDB ID : 1C7O / pdb_00001c7o
Title : CRYSTAL STRUCTURE OF CYSTALYSIN FROM TREPONEMA DENTICOLOA CONTAINS A PYRIDOXAL 5'-PHOSPHATE-L-AMINOETHOXYVINYLGLYCINE COMPLEX
Authors : Krupka, H.I.; Huber, R.; Holt, S.C.; Clausen, T.
Deposited on : 2000-03-16
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

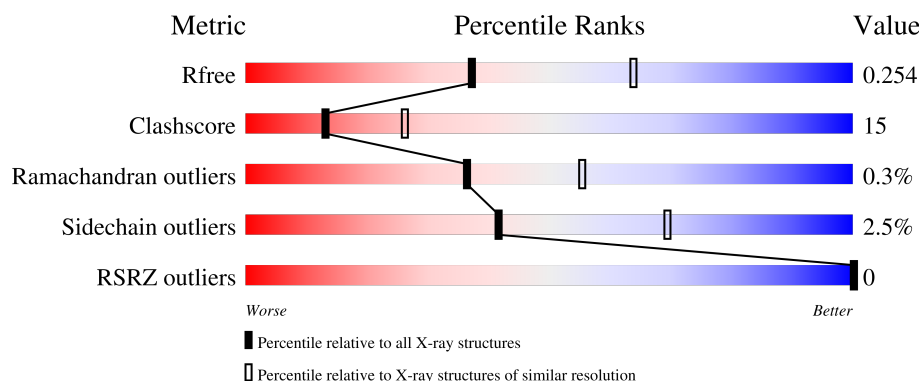
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	399	 65% 31% ..
1	B	399	 70% 26% ..
1	C	399	 69% 27% ..
1	D	399	 66% 31% ...

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Mol	Chain	Length	Quality of chain
1	E	399	63%32% ••
1	F	399	70%26% ••
1	G	399	61%34% ••
1	H	399	64%32% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27138 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRYSTALYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	B	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	C	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	D	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	E	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	F	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	G	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	H	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			

There are 24 discrepancies between the modelled and reference sequences:

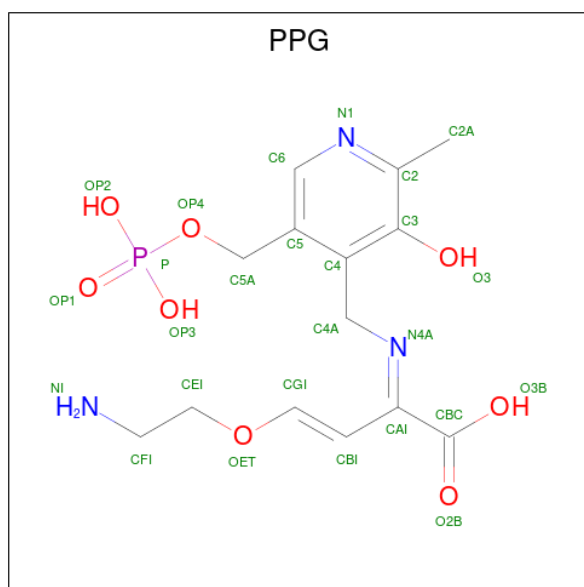
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLN	GLU	conflict	UNP Q56257
A	154	GLN	GLU	conflict	UNP Q56257
A	267	ALA	ILE	conflict	UNP Q56257
B	88	GLN	GLU	conflict	UNP Q56257
B	154	GLN	GLU	conflict	UNP Q56257
B	267	ALA	ILE	conflict	UNP Q56257
C	88	GLN	GLU	conflict	UNP Q56257
C	154	GLN	GLU	conflict	UNP Q56257
C	267	ALA	ILE	conflict	UNP Q56257
D	88	GLN	GLU	conflict	UNP Q56257
D	154	GLN	GLU	conflict	UNP Q56257
D	267	ALA	ILE	conflict	UNP Q56257
E	88	GLN	GLU	conflict	UNP Q56257

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Chain	Residue	Modelled	Actual	Comment	Reference
E	154	GLN	GLU	conflict	UNP Q56257
E	267	ALA	ILE	conflict	UNP Q56257
F	88	GLN	GLU	conflict	UNP Q56257
F	154	GLN	GLU	conflict	UNP Q56257
F	267	ALA	ILE	conflict	UNP Q56257
G	88	GLN	GLU	conflict	UNP Q56257
G	154	GLN	GLU	conflict	UNP Q56257
G	267	ALA	ILE	conflict	UNP Q56257
H	88	GLN	GLU	conflict	UNP Q56257
H	154	GLN	GLU	conflict	UNP Q56257
H	267	ALA	ILE	conflict	UNP Q56257

- Molecule 2 is (2E,3E)-4-(2-aminoethoxy)-2-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]imino]but-3-enoic acid (CCD ID: PPG) (formula: C₁₄H₂₀N₃O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	B	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	C	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	D	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	E	1	Total	C	N	O	P	0	0
			26	14	3	8	1		

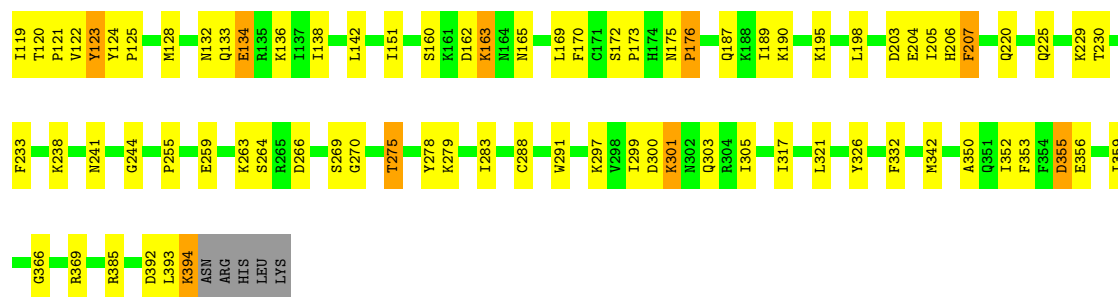
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	G	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	H	1	Total	C	N	O	P	0	0
			26	14	3	8	1		

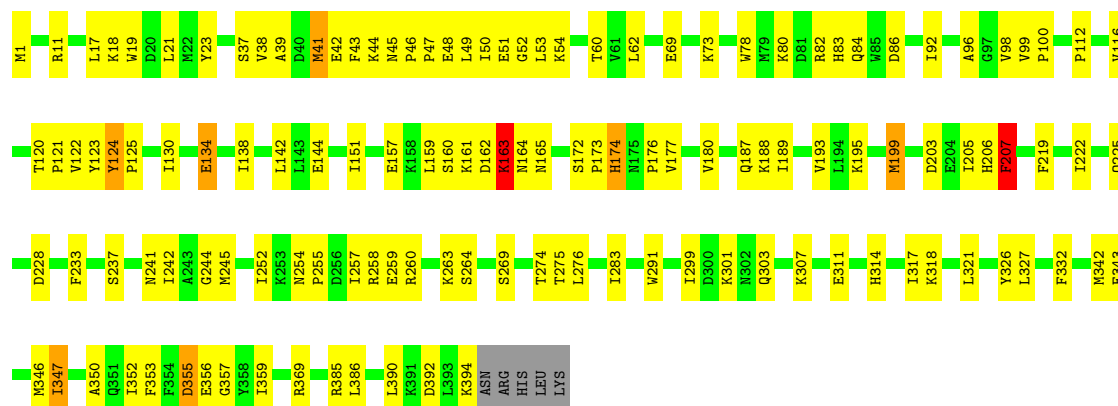
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	175	Total	O	0	0
			175	175		
3	B	181	Total	O	0	0
			181	181		
3	C	167	Total	O	0	0
			167	167		
3	D	139	Total	O	0	0
			139	139		
3	E	142	Total	O	0	0
			142	142		
3	F	180	Total	O	0	0
			180	180		
3	G	161	Total	O	0	0
			161	161		
3	H	129	Total	O	0	0
			129	129		



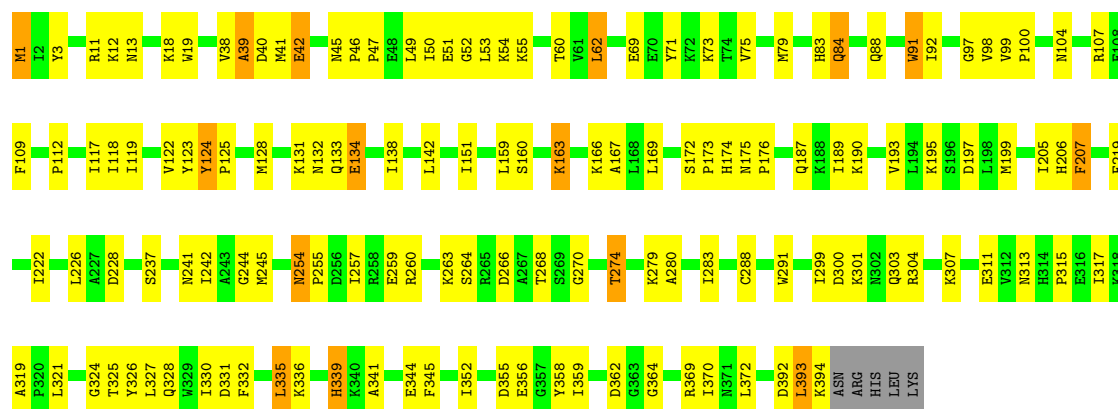
• Molecule 1: CYSTALYSIN

Chain D: 66% 31%



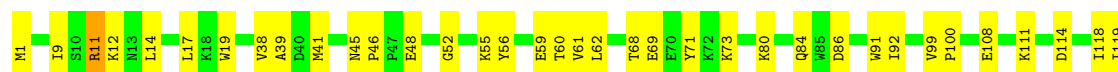
• Molecule 1: CYSTALYSIN

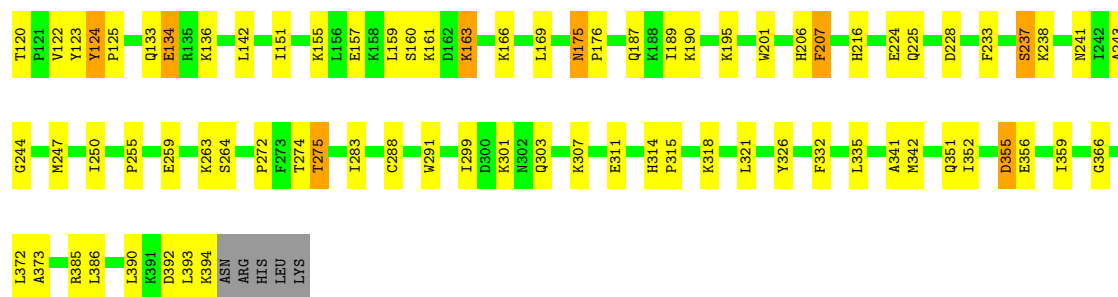
Chain E: 63% 32%



• Molecule 1: CYSTALYSIN

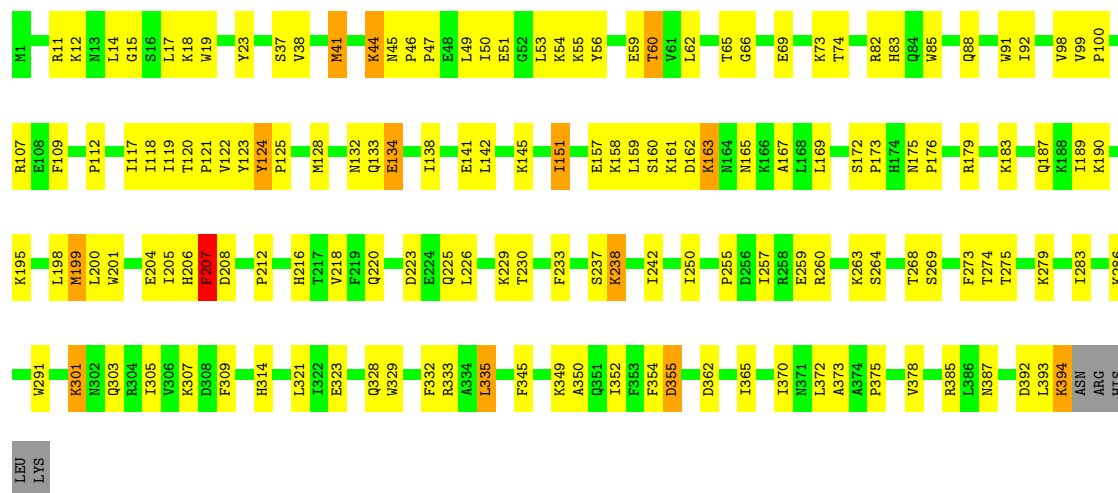
Chain F: 70% 26%





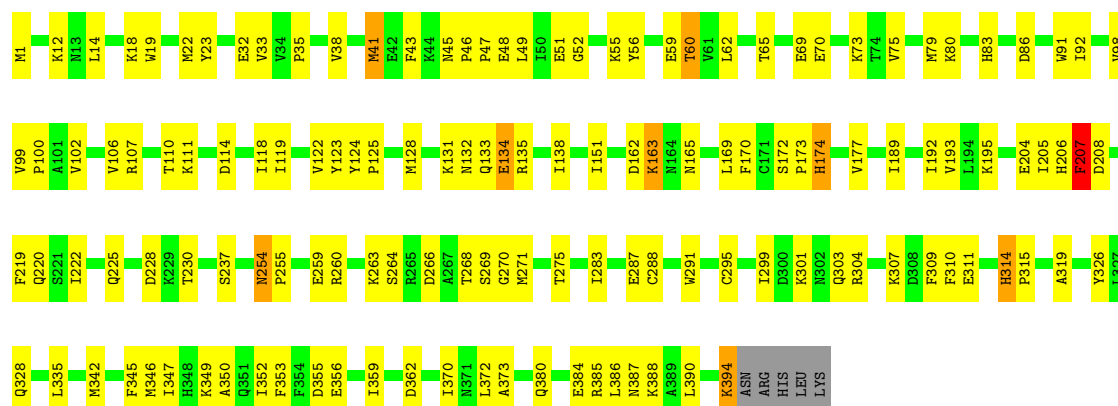
• Molecule 1: CYSTALYSIN

Chain G: 61% 34%



• Molecule 1: CYSTALYSIN

Chain H: 64% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.37Å 107.93Å 176.16Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-2.50) 91.9 (20.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.50Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.193 , 0.260 0.197 , 0.254	Depositor DCC
R_{free} test set	5379 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27138	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PPG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/3283	0.96	19/4429 (0.4%)
1	B	0.42	0/3283	0.98	14/4429 (0.3%)
1	C	0.42	0/3283	0.95	10/4429 (0.2%)
1	D	0.39	0/3283	0.96	18/4429 (0.4%)
1	E	0.39	0/3283	0.96	17/4429 (0.4%)
1	F	0.43	0/3283	0.98	18/4429 (0.4%)
1	G	0.42	0/3283	0.96	16/4429 (0.4%)
1	H	0.40	0/3283	0.94	16/4429 (0.4%)
All	All	0.41	0/26264	0.96	128/35432 (0.4%)

There are no bond length outliers.

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	THR	N-CA-C	8.39	121.93	110.35
1	F	355	ASP	N-CA-C	-7.79	94.20	107.99
1	B	207	PHE	N-CA-C	7.73	122.14	112.87
1	C	92	ILE	N-CA-C	7.20	118.85	107.98
1	E	288	CYS	N-CA-C	7.11	120.82	112.72
1	D	60	THR	N-CA-C	7.09	120.87	110.59
1	E	39	ALA	N-CA-C	6.86	120.45	108.52
1	D	42	GLU	N-CA-C	-6.84	105.71	112.97
1	B	174	HIS	N-CA-C	6.83	120.01	107.99
1	E	60	THR	N-CA-C	6.79	120.44	110.59
1	H	237	SER	N-CA-C	6.78	119.25	111.11
1	B	91	TRP	N-CA-C	-6.69	104.93	113.23
1	F	92	ILE	N-CA-C	6.50	117.42	108.84
1	C	91	TRP	N-CA-C	-6.50	105.17	113.23
1	H	41	MET	N-CA-C	6.49	120.46	110.20
1	C	41	MET	N-CA-C	6.48	120.44	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	339	HIS	N-CA-C	6.48	119.17	111.33
1	D	41	MET	N-CA-C	6.47	119.85	110.28
1	G	314	HIS	CA-C-N	6.40	126.89	119.47
1	G	314	HIS	C-N-CA	6.40	126.89	119.47
1	B	314	HIS	CA-C-N	6.34	126.83	119.47
1	B	314	HIS	C-N-CA	6.34	126.83	119.47
1	F	237	SER	N-CA-C	6.32	117.83	111.07
1	E	92	ILE	N-CA-C	6.30	117.87	108.54
1	D	207	PHE	N-CA-C	6.29	120.67	113.19
1	A	393	LEU	N-CA-C	-6.26	104.90	112.54
1	D	92	ILE	N-CA-C	6.21	117.36	107.98
1	G	207	PHE	N-CA-C	6.11	120.20	112.87
1	F	124	TYR	CA-C-N	-6.10	113.34	119.56
1	F	124	TYR	C-N-CA	-6.10	113.34	119.56
1	E	40	ASP	N-CA-C	-6.05	99.50	108.99
1	H	32	GLU	N-CA-C	-6.04	105.94	113.38
1	B	39	ALA	N-CA-C	6.02	118.97	109.39
1	F	39	ALA	N-CA-C	6.01	119.01	108.56
1	C	355	ASP	N-CA-C	-5.97	95.34	107.41
1	C	393	LEU	N-CA-C	-5.97	105.70	112.87
1	F	207	PHE	N-CA-C	5.97	120.29	113.19
1	A	175	ASN	N-CA-C	-5.95	102.55	109.93
1	B	393	LEU	N-CA-C	-5.94	104.88	111.71
1	G	44	LYS	N-CA-C	-5.94	102.69	110.53
1	E	42	GLU	N-CA-C	-5.92	104.20	112.25
1	D	39	ALA	N-CA-C	5.89	118.75	109.39
1	G	41	MET	N-CA-C	5.87	118.33	110.35
1	D	318	LYS	N-CA-C	5.86	118.46	108.90
1	E	207	PHE	N-CA-C	5.84	120.14	113.19
1	G	37	SER	N-CA-C	5.84	118.11	108.48
1	E	393	LEU	N-CA-C	-5.82	106.02	113.01
1	G	393	LEU	N-CA-C	-5.82	105.28	112.38
1	H	91	TRP	N-CA-C	-5.80	106.20	113.28
1	A	174	HIS	N-CA-C	5.76	118.12	107.99
1	H	92	ILE	N-CA-C	5.74	117.04	108.54
1	A	91	TRP	N-CA-C	-5.73	105.78	112.89
1	H	207	PHE	N-CA-C	5.73	120.01	113.19
1	A	287	GLU	N-CA-C	5.72	121.69	114.31
1	H	314	HIS	CA-C-N	5.71	125.57	119.28
1	H	314	HIS	C-N-CA	5.71	125.57	119.28
1	D	314	HIS	CA-C-N	5.71	126.98	119.84
1	D	314	HIS	C-N-CA	5.71	126.98	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	287	GLU	N-CA-C	5.70	121.66	114.31
1	A	243	ALA	N-CA-C	-5.68	106.20	113.01
1	B	37	SER	N-CA-C	5.65	117.80	108.48
1	H	347	ILE	N-CA-C	5.65	115.73	110.42
1	B	92	ILE	N-CA-C	5.64	116.89	108.54
1	F	166	LYS	N-CA-C	5.63	120.21	113.23
1	G	275	THR	N-CA-C	5.62	117.08	111.07
1	A	92	ILE	N-CA-C	5.56	116.77	108.54
1	H	254	ASN	CA-C-N	5.55	125.01	119.24
1	H	254	ASN	C-N-CA	5.55	125.01	119.24
1	G	92	ILE	N-CA-C	5.53	116.36	107.73
1	C	353	PHE	N-CA-C	5.53	118.30	107.57
1	D	180	VAL	N-CA-C	-5.53	99.00	106.85
1	G	60	THR	N-CA-C	5.51	118.58	110.59
1	A	39	ALA	N-CA-C	5.50	119.22	110.70
1	H	288	CYS	N-CA-C	5.47	118.96	112.72
1	G	124	TYR	N-CA-C	5.47	121.89	109.81
1	A	318	LYS	N-CA-C	5.46	117.80	108.90
1	A	314	HIS	CA-C-N	5.41	126.61	119.84
1	A	314	HIS	C-N-CA	5.41	126.61	119.84
1	E	174	HIS	N-CA-C	5.41	117.12	108.41
1	G	355	ASP	N-CA-C	-5.41	96.96	107.62
1	A	348	HIS	N-CA-C	5.41	119.99	112.90
1	A	199	MET	N-CA-C	-5.41	102.52	110.52
1	D	357	GLY	N-CA-C	5.41	119.18	112.64
1	C	37	SER	N-CA-C	5.40	117.39	108.48
1	D	347	ILE	N-CA-C	5.40	116.18	110.72
1	D	237	SER	N-CA-C	5.40	117.86	111.33
1	A	41	MET	N-CA-C	5.39	118.89	110.32
1	F	91	TRP	N-CA-C	-5.39	106.55	113.23
1	F	314	HIS	CA-C-N	5.38	126.57	119.84
1	F	314	HIS	C-N-CA	5.38	126.57	119.84
1	E	91	TRP	N-CA-C	-5.36	106.75	113.28
1	E	124	TYR	N-CA-C	5.36	120.90	113.45
1	B	41	MET	N-CA-C	5.34	118.38	110.48
1	H	174	HIS	N-CA-C	5.29	116.87	108.67
1	A	207	PHE	N-CA-C	5.29	119.22	112.87
1	B	120	THR	N-CA-C	5.27	117.31	110.40
1	D	174	HIS	N-CA-C	5.27	116.84	108.67
1	B	175	ASN	N-CA-C	-5.25	103.04	109.65
1	F	175	ASN	N-CA-C	-5.23	103.48	110.07
1	E	254	ASN	CA-C-N	5.22	124.85	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	254	ASN	C-N-CA	5.22	124.85	119.05
1	D	124	TYR	N-CA-C	5.21	120.70	113.45
1	C	42	GLU	N-CA-C	-5.20	104.32	111.81
1	E	55	LYS	N-CA-C	-5.19	105.51	111.07
1	A	40	ASP	N-CA-C	-5.18	101.50	109.52
1	C	44	LYS	N-CA-C	-5.16	103.22	110.50
1	F	318	LYS	N-CA-C	5.16	117.49	108.76
1	F	124	TYR	N-CA-C	5.16	121.20	109.81
1	F	393	LEU	N-CA-C	-5.15	105.64	112.34
1	A	124	TYR	N-CA-C	5.15	121.19	109.81
1	G	151	ILE	N-CA-C	5.14	116.21	109.21
1	H	33	VAL	N-CA-C	5.12	115.64	108.89
1	E	41	MET	N-CA-C	5.11	118.05	110.48
1	A	237	SER	N-CA-C	5.11	117.25	111.02
1	D	355	ASP	N-CA-C	-5.11	98.25	107.75
1	F	108	GLU	N-CA-C	5.11	117.97	111.69
1	D	193	VAL	N-CA-C	5.10	115.77	110.82
1	G	82	ARG	N-CA-C	5.09	119.55	113.23
1	C	175	ASN	N-CA-C	-5.09	103.66	110.07
1	H	60	THR	N-CA-C	5.08	117.40	109.52
1	B	219	PHE	N-CA-C	5.07	117.20	111.11
1	D	44	LYS	N-CA-C	-5.07	103.36	110.50
1	G	167	ALA	N-CA-C	5.07	115.84	108.14
1	F	120	THR	N-CA-C	5.06	116.97	110.39
1	E	175	ASN	N-CA-C	-5.03	103.43	109.72
1	B	355	ASP	N-CA-C	-5.02	97.72	107.62
1	F	288	CYS	N-CA-C	5.02	118.88	112.26
1	G	333	ARG	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3207	0	3223	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3207	0	3223	88	0
1	C	3207	0	3223	96	0
1	D	3207	0	3223	96	0
1	E	3207	0	3223	111	0
1	F	3207	0	3223	80	0
1	G	3207	0	3223	112	0
1	H	3207	0	3223	107	0
2	A	26	0	17	7	0
2	B	26	0	16	4	0
2	C	26	0	16	4	0
2	D	26	0	16	4	0
2	E	26	0	17	3	0
2	F	26	0	16	3	0
2	G	26	0	16	4	0
2	H	26	0	16	3	0
3	A	175	0	0	12	0
3	B	181	0	0	10	0
3	C	167	0	0	6	0
3	D	139	0	0	3	0
3	E	142	0	0	7	0
3	F	180	0	0	8	0
3	G	161	0	0	5	0
3	H	129	0	0	9	0
All	All	27138	0	25914	772	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (772) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:LYS:H	1:F:163:LYS:HD3	1.03	1.17
1:H:163:LYS:H	1:H:163:LYS:HD3	1.06	1.14
1:G:163:LYS:H	1:G:163:LYS:HD3	1.00	1.13
1:C:163:LYS:H	1:C:163:LYS:HD3	1.01	1.12
1:D:163:LYS:H	1:D:163:LYS:HD3	1.11	1.10
1:E:163:LYS:HD3	1:E:163:LYS:H	1.10	1.08
1:A:163:LYS:H	1:A:163:LYS:HD3	1.18	1.08
1:B:163:LYS:H	1:B:163:LYS:HD3	1.20	1.04
1:H:151:ILE:HD13	1:H:189:ILE:HD11	1.41	1.01
1:A:45:ASN:HD21	1:B:62:LEU:H	1.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LYS:HD3	1:D:163:LYS:N	1.81	0.94
1:G:199:MET:HE3	1:G:257:ILE:HD13	1.52	0.92
1:C:163:LYS:HD3	1:C:163:LYS:N	1.86	0.91
1:F:163:LYS:HD3	1:F:163:LYS:N	1.88	0.89
1:G:163:LYS:HD3	1:G:163:LYS:N	1.86	0.89
1:G:62:LEU:H	1:H:45:ASN:HD21	1.21	0.89
1:B:1:MET:HE3	1:B:48:GLU:HG3	1.55	0.88
1:C:45:ASN:HD21	1:D:62:LEU:H	1.24	0.85
1:G:11:ARG:HA	1:G:14:LEU:HD12	1.58	0.85
1:G:163:LYS:H	1:G:163:LYS:CD	1.86	0.84
1:H:163:LYS:HD3	1:H:163:LYS:N	1.90	0.84
1:E:45:ASN:HD21	1:F:62:LEU:H	1.25	0.84
1:A:62:LEU:H	1:B:45:ASN:HD21	1.23	0.84
1:D:1:MET:HE3	1:D:48:GLU:HG3	1.58	0.84
1:C:151:ILE:HD13	1:C:189:ILE:HD11	1.60	0.83
1:F:151:ILE:HD13	1:F:189:ILE:HD11	1.57	0.83
1:E:47:PRO:O	1:E:51:GLU:HG2	1.76	0.83
1:F:11:ARG:HA	1:F:14:LEU:HD12	1.61	0.82
1:C:163:LYS:H	1:C:163:LYS:CD	1.86	0.81
1:F:163:LYS:H	1:F:163:LYS:CD	1.84	0.80
1:E:163:LYS:HD3	1:E:163:LYS:N	1.94	0.80
1:D:18:LYS:HD3	1:D:38:VAL:HB	1.64	0.79
1:A:163:LYS:H	1:A:163:LYS:CD	1.93	0.79
1:E:163:LYS:H	1:E:163:LYS:CD	1.95	0.78
1:C:1:MET:HE3	1:C:48:GLU:HG3	1.66	0.77
1:H:163:LYS:H	1:H:163:LYS:CD	1.90	0.77
1:D:299:ILE:HD13	1:D:326:TYR:HB3	1.66	0.77
1:C:394:LYS:HZ2	1:C:394:LYS:HB2	1.50	0.76
1:B:151:ILE:CD1	1:B:189:ILE:HD11	2.15	0.76
1:E:51:GLU:HG3	3:E:5503:HOH:O	1.85	0.76
1:G:45:ASN:HD21	1:H:62:LEU:H	1.33	0.76
1:H:299:ILE:HD13	1:H:326:TYR:HB3	1.67	0.75
1:A:1:MET:HE3	1:A:48:GLU:HG3	1.69	0.74
1:D:99:VAL:HB	1:D:100:PRO:HD3	1.69	0.74
1:A:107:ARG:HD2	3:B:2539:HOH:O	1.86	0.74
1:D:356:GLU:O	1:D:359:ILE:HG12	1.88	0.74
1:C:299:ILE:HD13	1:C:326:TYR:HB3	1.69	0.73
1:E:62:LEU:H	1:F:45:ASN:HD21	1.37	0.73
1:C:62:LEU:H	1:D:45:ASN:HD21	1.36	0.73
1:C:269:SER:HB3	1:D:269:SER:HB3	1.71	0.72
1:G:260:ARG:O	1:G:263:LYS:HG2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:GLN:O	1:H:134:GLU:HB2	1.89	0.72
1:A:38:VAL:HG13	2:A:1500:PPG:HGI	1.72	0.72
1:F:255:PRO:O	1:F:259:GLU:HG3	1.90	0.72
1:B:255:PRO:O	1:B:259:GLU:HG3	1.89	0.71
1:F:1:MET:HE3	1:F:48:GLU:HG3	1.72	0.71
1:G:190:LYS:HG3	1:G:226:LEU:HD22	1.72	0.71
1:A:2:ILE:HA	3:A:1592:HOH:O	1.91	0.70
1:E:187:GLN:HE22	1:E:190:LYS:NZ	1.89	0.70
1:E:255:PRO:O	1:E:259:GLU:HG3	1.92	0.70
1:F:41:MET:HG2	1:F:373:ALA:HB1	1.74	0.69
1:G:151:ILE:HD12	1:G:189:ILE:HD11	1.72	0.69
1:G:118:ILE:HG22	1:G:169:LEU:HB3	1.73	0.69
1:C:98:VAL:HG21	1:C:205:ILE:HD12	1.75	0.69
1:C:151:ILE:CD1	1:C:189:ILE:HD11	2.23	0.69
1:E:128:MET:O	1:E:132:ASN:HB2	1.92	0.69
1:B:163:LYS:H	1:B:163:LYS:CD	2.02	0.69
1:B:17:LEU:HD23	2:B:2500:PPG:HNI2	1.59	0.68
1:B:350:ALA:O	1:B:385:ARG:HD2	1.93	0.68
1:F:224:GLU:HG2	3:F:6566:HOH:O	1.94	0.67
1:E:187:GLN:HE22	1:E:190:LYS:HZ3	1.39	0.67
1:G:255:PRO:O	1:G:259:GLU:HG3	1.94	0.67
1:D:255:PRO:O	1:D:259:GLU:HG3	1.94	0.67
1:A:107:ARG:NE	1:A:268:THR:HG21	2.10	0.67
1:B:195:LYS:HD2	1:B:195:LYS:C	2.20	0.67
1:B:162:ASP:HB3	1:B:165:ASN:ND2	2.09	0.67
1:G:123:TYR:CZ	1:G:125:PRO:HG2	2.29	0.67
1:E:197:ASP:HA	3:E:5617:HOH:O	1.94	0.66
1:D:195:LYS:HG2	1:G:88:GLN:CD	2.20	0.66
1:H:356:GLU:O	1:H:359:ILE:HG12	1.94	0.66
1:H:163:LYS:HB3	3:H:8518:HOH:O	1.96	0.66
1:D:124:TYR:CD1	1:D:125:PRO:HD3	2.30	0.66
1:G:47:PRO:O	1:G:51:GLU:HG2	1.95	0.66
1:E:119:ILE:HG22	1:E:142:LEU:HG	1.77	0.66
1:H:255:PRO:O	1:H:259:GLU:HG3	1.96	0.66
1:H:122:VAL:HG22	1:H:123:TYR:N	2.11	0.65
1:B:11:ARG:HA	1:B:14:LEU:HD12	1.78	0.65
1:C:124:TYR:CG	1:C:125:PRO:HD3	2.31	0.65
1:C:88:GLN:HB2	1:C:91:TRP:CD1	2.32	0.65
1:C:255:PRO:O	1:C:259:GLU:HG3	1.97	0.65
1:E:151:ILE:HD13	1:E:189:ILE:HD11	1.79	0.65
1:G:124:TYR:CD1	1:G:125:PRO:HD3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:HG22	1:A:123:TYR:N	2.12	0.64
1:H:162:ASP:HB3	1:H:165:ASN:ND2	2.12	0.64
1:A:62:LEU:H	1:B:45:ASN:ND2	1.95	0.64
1:H:1:MET:HE3	1:H:48:GLU:HG3	1.80	0.64
1:A:184:ASP:HB3	3:A:1508:HOH:O	1.98	0.64
1:B:299:ILE:HD13	1:B:326:TYR:HB3	1.79	0.64
1:D:138:ILE:HG13	1:D:165:ASN:OD1	1.98	0.64
1:G:46:PRO:HG3	1:G:291:TRP:CD2	2.33	0.64
1:D:199:MET:HE3	1:D:257:ILE:HD13	1.80	0.63
1:A:103:PHE:CE2	1:A:129:ALA:HA	2.34	0.63
1:D:123:TYR:CZ	1:D:125:PRO:HG2	2.34	0.63
1:G:62:LEU:H	1:H:45:ASN:ND2	1.95	0.63
1:A:163:LYS:HD3	1:A:163:LYS:N	2.02	0.63
1:B:124:TYR:CG	1:B:125:PRO:HD3	2.34	0.63
1:A:151:ILE:CD1	1:A:189:ILE:HD11	2.28	0.63
1:B:163:LYS:HD3	1:B:163:LYS:N	2.03	0.63
1:A:17:LEU:HD22	2:A:1500:PPG:HNI2	1.65	0.62
1:A:123:TYR:CZ	1:A:125:PRO:HG2	2.34	0.62
1:F:46:PRO:HG3	1:F:291:TRP:CD2	2.33	0.62
1:G:151:ILE:CD1	1:G:189:ILE:HD11	2.28	0.62
1:C:99:VAL:HB	1:C:100:PRO:HD3	1.81	0.62
1:F:56:TYR:O	1:F:60:THR:HG22	1.99	0.62
1:D:50:ILE:O	1:D:54:LYS:HG3	2.00	0.62
1:E:122:VAL:HG22	1:E:123:TYR:H	1.64	0.62
1:E:99:VAL:HB	1:E:100:PRO:HD3	1.81	0.62
1:F:11:ARG:HG3	1:F:19:TRP:NE1	2.15	0.62
1:C:172:SER:O	1:C:204:GLU:HG2	2.00	0.62
1:F:342:MET:HE1	1:F:366:GLY:HA2	1.80	0.62
1:C:80:LYS:HD3	1:C:86:ASP:OD1	2.00	0.62
1:A:274:THR:HA	1:B:244:GLY:O	1.99	0.61
1:D:122:VAL:HG22	1:D:123:TYR:N	2.15	0.61
1:B:56:TYR:CE1	1:B:60:THR:HG21	2.35	0.61
1:B:206:HIS:HE1	2:B:2500:PPG:O3	1.82	0.61
1:G:17:LEU:HD22	2:G:7500:PPG:HNI2	1.66	0.61
1:A:300:ASP:O	1:A:303:GLN:HG2	1.99	0.61
1:E:219:PHE:O	1:E:222:ILE:HG12	2.01	0.61
1:H:56:TYR:CE1	1:H:60:THR:HG21	2.36	0.61
1:A:215:GLU:HB2	3:A:1556:HOH:O	2.01	0.61
1:E:107:ARG:HE	1:E:268:THR:HG21	1.65	0.61
1:F:206:HIS:HE1	2:F:6500:PPG:O3	1.83	0.61
1:C:47:PRO:O	1:C:51:GLU:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:375:PRO:HB2	1:G:378:VAL:HG23	1.82	0.61
1:B:122:VAL:HG22	1:B:123:TYR:N	2.17	0.60
1:G:183:LYS:O	1:G:187:GLN:HG2	2.02	0.60
1:H:41:MET:HG2	1:H:373:ALA:HB1	1.83	0.60
1:G:237:SER:HA	1:G:242:ILE:HG13	1.83	0.60
1:B:88:GLN:HB2	1:B:91:TRP:CD1	2.36	0.60
1:C:118:ILE:HG22	1:C:169:LEU:HB3	1.84	0.60
1:A:75:VAL:O	1:A:79:MET:HG2	2.01	0.60
1:C:162:ASP:HB3	1:C:165:ASN:ND2	2.17	0.60
1:H:1:MET:SD	1:H:47:PRO:HB2	2.41	0.60
1:B:11:ARG:HB2	1:B:19:TRP:CD1	2.37	0.60
1:H:47:PRO:O	1:H:51:GLU:HG2	2.02	0.60
1:H:18:LYS:HB2	1:H:38:VAL:HB	1.82	0.60
1:C:187:GLN:HE22	1:C:190:LYS:NZ	1.99	0.60
1:A:245:MET:HE3	1:A:280:ALA:HB2	1.82	0.59
1:C:112:PRO:HB3	1:C:134:GLU:HB3	1.84	0.59
1:D:124:TYR:CG	1:D:125:PRO:HD3	2.37	0.59
1:D:151:ILE:CD1	1:D:189:ILE:HD11	2.32	0.59
1:E:206:HIS:HE1	2:E:5500:PPG:O3	1.86	0.59
1:E:190:LYS:HG3	1:E:226:LEU:HD22	1.84	0.59
1:H:206:HIS:HE1	2:H:8500:PPG:O3	1.85	0.59
1:C:11:ARG:HB2	1:C:19:TRP:CD1	2.38	0.59
1:D:187:GLN:HA	1:D:187:GLN:HE21	1.66	0.59
1:H:384:GLU:HG3	1:H:388:LYS:NZ	2.18	0.59
1:C:46:PRO:HG3	1:C:291:TRP:CD2	2.38	0.59
1:A:307:LYS:O	1:A:311:GLU:HG3	2.03	0.59
1:B:11:ARG:HG3	1:B:19:TRP:NE1	2.18	0.59
1:A:124:TYR:CG	1:A:125:PRO:HD3	2.38	0.59
1:E:123:TYR:CZ	1:E:125:PRO:HG2	2.37	0.59
1:A:122:VAL:HG22	1:A:123:TYR:H	1.67	0.58
1:C:52:GLY:HA3	1:C:283:ILE:HD13	1.85	0.58
1:B:160:SER:OG	1:B:195:LYS:NZ	2.36	0.58
1:D:46:PRO:HG3	1:D:291:TRP:CD2	2.38	0.58
1:H:99:VAL:HB	1:H:100:PRO:HD3	1.84	0.58
1:A:118:ILE:HG22	1:A:169:LEU:HB3	1.85	0.58
1:H:52:GLY:HA3	1:H:283:ILE:HD13	1.86	0.58
1:C:206:HIS:HE1	2:C:3500:PPG:O3	1.86	0.58
1:H:195:LYS:HD2	1:H:195:LYS:O	2.03	0.58
1:C:138:ILE:HG13	1:C:165:ASN:OD1	2.02	0.58
1:G:220:GLN:HB3	1:G:230:THR:HG21	1.85	0.58
1:G:162:ASP:HB3	1:G:165:ASN:ND2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:SER:O	1:G:204:GLU:HG2	2.03	0.57
1:A:107:ARG:HE	1:A:268:THR:HG21	1.69	0.57
1:B:123:TYR:CZ	1:B:125:PRO:HG2	2.38	0.57
1:B:238:LYS:HZ1	2:B:2500:PPG:H5A1	1.67	0.57
1:B:151:ILE:HD13	1:B:189:ILE:HD11	1.86	0.57
1:C:238:LYS:HE2	2:C:3500:PPG:H4A2	1.86	0.57
1:D:163:LYS:H	1:D:163:LYS:CD	2.00	0.57
1:F:124:TYR:CD1	1:F:125:PRO:HD3	2.39	0.57
1:G:124:TYR:CG	1:G:125:PRO:HD3	2.39	0.57
1:A:388:LYS:HB3	3:A:1529:HOH:O	2.03	0.57
1:E:321:LEU:HD12	3:E:5620:HOH:O	2.03	0.57
1:F:111:LYS:HG2	1:F:114:ASP:OD1	2.04	0.57
1:A:195:LYS:HD2	1:A:195:LYS:C	2.29	0.57
1:F:69:GLU:O	1:F:73:LYS:HG3	2.04	0.57
1:G:50:ILE:O	1:G:54:LYS:HG3	2.04	0.57
1:A:187:GLN:HE22	1:A:190:LYS:NZ	2.03	0.57
1:E:39:ALA:HB2	2:E:5500:PPG:O2B	2.04	0.57
1:E:118:ILE:HG22	1:E:169:LEU:HB3	1.86	0.57
1:G:206:HIS:HE1	2:G:7500:PPG:O3	1.88	0.57
1:F:41:MET:HG2	1:F:373:ALA:CB	2.34	0.57
1:H:118:ILE:HG22	1:H:169:LEU:HB3	1.86	0.57
1:A:11:ARG:HB2	1:A:19:TRP:CD1	2.40	0.56
1:B:107:ARG:HD2	3:B:2510:HOH:O	2.04	0.56
1:A:91:TRP:CZ2	1:A:253:LYS:HG3	2.40	0.56
1:G:112:PRO:HB3	1:G:134:GLU:HB3	1.86	0.56
1:H:69:GLU:O	1:H:73:LYS:HG3	2.05	0.56
1:H:311:GLU:O	1:H:315:PRO:HG3	2.05	0.56
1:H:394:LYS:HD3	3:H:8521:HOH:O	2.03	0.56
1:H:111:LYS:HG2	1:H:114:ASP:OD1	2.04	0.56
1:A:167:ALA:HB2	1:A:199:MET:HB2	1.87	0.56
1:A:350:ALA:O	1:A:385:ARG:HD2	2.05	0.56
1:E:319:ALA:HB2	1:E:330:ILE:HG23	1.87	0.56
1:F:52:GLY:HA3	1:F:283:ILE:HD13	1.86	0.56
1:G:392:ASP:O	1:G:394:LYS:HE3	2.05	0.56
1:C:269:SER:CB	1:D:269:SER:HB3	2.34	0.56
1:B:99:VAL:HB	1:B:100:PRO:HD3	1.87	0.56
1:D:187:GLN:HA	1:D:187:GLN:NE2	2.21	0.56
1:E:69:GLU:O	1:E:73:LYS:HG3	2.06	0.56
1:E:98:VAL:HG21	1:E:205:ILE:HD12	1.88	0.56
1:A:205:ILE:HA	3:A:1526:HOH:O	2.05	0.55
1:C:122:VAL:HG22	1:C:123:TYR:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:TYR:CE1	2:B:2500:PPG:N4A	2.74	0.55
1:C:124:TYR:HB3	1:C:359:ILE:O	2.06	0.55
1:G:18:LYS:HD3	1:G:38:VAL:HB	1.89	0.55
1:A:123:TYR:CG	1:A:125:PRO:HD2	2.41	0.55
1:B:23:TYR:HE2	3:B:2660:HOH:O	1.90	0.55
1:B:107:ARG:NE	1:B:268:THR:HG21	2.21	0.55
1:C:98:VAL:HG13	1:C:233:PHE:HB3	1.87	0.55
1:G:69:GLU:O	1:G:73:LYS:HG3	2.06	0.55
1:B:145:LYS:HB2	3:B:2594:HOH:O	2.06	0.55
1:B:151:ILE:HD12	1:B:189:ILE:HD11	1.88	0.55
1:C:119:ILE:HG22	1:C:142:LEU:HG	1.88	0.55
1:G:238:LYS:NZ	2:G:7500:PPG:H4A1	2.22	0.55
1:H:46:PRO:HG3	1:H:291:TRP:CD2	2.41	0.55
1:H:174:HIS:HD2	1:H:177:VAL:HG22	1.70	0.55
1:F:80:LYS:HD3	1:F:86:ASP:OD1	2.07	0.55
1:E:107:ARG:NE	1:E:268:THR:HG21	2.22	0.54
1:A:50:ILE:O	1:A:54:LYS:HG3	2.08	0.54
1:F:99:VAL:HB	1:F:100:PRO:HD3	1.88	0.54
1:F:118:ILE:HG22	1:F:169:LEU:HB3	1.90	0.54
1:G:200:LEU:HB3	1:G:230:THR:OG1	2.07	0.54
1:F:272:PRO:HG3	3:F:6538:HOH:O	2.07	0.54
1:A:238:LYS:HZ1	2:A:1500:PPG:H4A1	1.73	0.54
1:B:192:ILE:O	1:B:195:LYS:HE3	2.08	0.54
1:E:122:VAL:HG22	1:E:123:TYR:N	2.23	0.54
1:F:195:LYS:HD2	1:F:195:LYS:O	2.08	0.54
1:A:155:LYS:O	1:A:159:LEU:HG	2.07	0.54
1:B:204:GLU:OE1	1:B:216:HIS:HE1	1.90	0.54
1:D:52:GLY:HA3	1:D:283:ILE:HD13	1.90	0.54
1:G:56:TYR:O	1:G:60:THR:HG22	2.08	0.54
1:G:99:VAL:HB	1:G:100:PRO:HD3	1.89	0.54
1:C:9:ILE:HD11	1:C:42:GLU:HA	1.90	0.54
1:E:299:ILE:HD13	1:E:326:TYR:HB3	1.90	0.53
1:H:124:TYR:CG	1:H:125:PRO:HD3	2.43	0.53
1:B:337:MET:HE1	1:B:345:PHE:HB2	1.90	0.53
1:C:275:THR:HG22	1:D:244:GLY:O	2.09	0.53
1:E:46:PRO:HG3	1:E:291:TRP:CD2	2.42	0.53
1:E:50:ILE:O	1:E:54:LYS:HG3	2.09	0.53
1:G:11:ARG:HB2	1:G:19:TRP:CD1	2.43	0.53
1:B:18:LYS:HB2	1:B:38:VAL:HB	1.91	0.53
1:D:275:THR:HG23	1:D:276:LEU:N	2.23	0.53
1:F:11:ARG:HG3	1:F:19:TRP:CE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:345:PHE:O	1:H:349:LYS:HB2	2.09	0.53
1:H:350:ALA:O	1:H:385:ARG:HD2	2.09	0.53
1:H:380:GLN:HG3	3:H:8519:HOH:O	2.08	0.53
1:E:51:GLU:HG3	3:E:5526:HOH:O	2.08	0.53
1:G:98:VAL:HG21	1:G:205:ILE:HD12	1.91	0.53
1:G:107:ARG:HB2	1:G:133:GLN:OE1	2.08	0.53
1:G:301:LYS:O	1:G:305:ILE:HG13	2.09	0.53
1:A:2:ILE:HG23	3:A:1592:HOH:O	2.09	0.53
1:A:97:GLY:C	1:A:100:PRO:HD2	2.33	0.53
1:C:392:ASP:C	1:C:394:LYS:H	2.15	0.53
1:E:317:ILE:HG23	1:E:331:ASP:O	2.08	0.53
1:H:65:THR:OG1	1:H:275:THR:HB	2.09	0.53
1:A:279:LYS:O	1:A:283:ILE:HG13	2.08	0.53
1:A:311:GLU:O	1:A:315:PRO:HG3	2.09	0.53
1:E:195:LYS:C	1:E:195:LYS:HD2	2.34	0.53
1:C:195:LYS:HD2	1:C:195:LYS:C	2.33	0.53
1:E:11:ARG:HB2	1:E:19:TRP:CD1	2.43	0.53
1:E:124:TYR:CG	1:E:125:PRO:HD3	2.44	0.53
1:G:138:ILE:HG22	1:G:159:LEU:HD13	1.90	0.53
1:G:350:ALA:O	1:G:385:ARG:HD2	2.09	0.53
1:H:195:LYS:HD2	1:H:195:LYS:C	2.33	0.53
1:C:356:GLU:O	1:C:359:ILE:HG12	2.09	0.53
1:G:354:PHE:HE1	1:G:370:ILE:HD12	1.73	0.53
1:H:123:TYR:CZ	1:H:125:PRO:HG2	2.44	0.53
1:B:236:PRO:HG2	1:B:242:ILE:HD11	1.91	0.52
1:C:297:LYS:HG2	3:C:3613:HOH:O	2.08	0.52
1:C:392:ASP:C	1:C:394:LYS:N	2.62	0.52
1:G:88:GLN:HB2	1:G:91:TRP:CD1	2.44	0.52
1:H:263:LYS:HG3	1:H:264:SER:N	2.24	0.52
1:A:45:ASN:ND2	1:B:62:LEU:H	1.94	0.52
1:D:47:PRO:O	1:D:51:GLU:HG2	2.09	0.52
1:F:157:GLU:O	1:F:160:SER:OG	2.25	0.52
1:F:160:SER:OG	1:F:195:LYS:NZ	2.43	0.52
1:F:55:LYS:O	1:F:59:GLU:HG3	2.10	0.52
1:H:80:LYS:HD3	1:H:86:ASP:OD1	2.09	0.52
1:H:124:TYR:CD1	1:H:125:PRO:HD3	2.45	0.52
1:D:116:VAL:HB	1:D:130:ILE:HD13	1.91	0.52
1:E:97:GLY:C	1:E:100:PRO:HD2	2.34	0.52
1:G:55:LYS:O	1:G:59:GLU:HG3	2.08	0.52
1:A:200:LEU:HD21	1:A:219:PHE:CD1	2.45	0.52
1:C:119:ILE:HD12	1:C:170:PHE:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:PHE:HA	3:H:8531:HOH:O	2.09	0.52
1:H:192:ILE:O	1:H:195:LYS:HE3	2.10	0.52
1:A:160:SER:OG	1:A:195:LYS:NZ	2.42	0.52
1:B:348:HIS:HD2	3:B:2678:HOH:O	1.93	0.52
1:C:123:TYR:CG	1:C:125:PRO:HD2	2.45	0.52
1:C:394:LYS:HB2	1:C:394:LYS:NZ	2.19	0.52
1:D:352:ILE:O	1:D:352:ILE:HG23	2.08	0.52
1:G:107:ARG:HE	1:G:268:THR:HG21	1.74	0.52
1:G:123:TYR:CG	1:G:125:PRO:HD2	2.44	0.52
1:H:384:GLU:HG2	3:H:8601:HOH:O	2.10	0.52
1:E:160:SER:OG	1:E:195:LYS:NZ	2.43	0.52
1:B:317:ILE:HD13	1:B:332:PHE:CE2	2.45	0.51
1:A:238:LYS:NZ	2:A:1500:PPG:H4A1	2.25	0.51
1:C:88:GLN:HB2	1:C:91:TRP:NE1	2.26	0.51
1:F:119:ILE:HG22	1:F:142:LEU:HG	1.93	0.51
1:E:151:ILE:CD1	1:E:189:ILE:HD11	2.39	0.51
1:H:98:VAL:O	1:H:102:VAL:HG23	2.10	0.51
1:A:1:MET:SD	1:A:47:PRO:HB2	2.50	0.51
1:F:392:ASP:C	1:F:394:LYS:N	2.63	0.51
1:D:350:ALA:O	1:D:385:ARG:HD2	2.11	0.51
1:A:46:PRO:HG3	1:A:291:TRP:CD2	2.45	0.51
1:D:317:ILE:HD13	1:D:332:PHE:CE2	2.45	0.51
1:E:332:PHE:O	1:E:335:LEU:HB2	2.10	0.51
1:E:189:ILE:O	1:E:193:VAL:HG23	2.11	0.51
1:G:117:ILE:HA	1:G:138:ILE:HB	1.92	0.51
1:H:123:TYR:CG	1:H:125:PRO:HD2	2.46	0.51
1:A:98:VAL:HG13	1:A:233:PHE:HB3	1.92	0.51
1:F:263:LYS:HG3	1:F:264:SER:N	2.26	0.51
1:H:56:TYR:O	1:H:60:THR:HG22	2.11	0.51
1:A:18:LYS:HE3	1:A:42:GLU:OE2	2.10	0.50
1:C:172:SER:HA	1:C:173:PRO:C	2.35	0.50
1:H:151:ILE:CD1	1:H:189:ILE:HD11	2.26	0.50
1:H:174:HIS:CD2	1:H:177:VAL:HG22	2.46	0.50
1:B:88:GLN:O	1:B:91:TRP:HB2	2.10	0.50
1:G:123:TYR:CD2	1:G:125:PRO:HD2	2.46	0.50
1:A:88:GLN:HB2	1:A:91:TRP:CD1	2.45	0.50
1:C:124:TYR:CD1	1:C:125:PRO:HD3	2.46	0.50
1:D:49:LEU:HA	1:D:283:ILE:HG21	1.94	0.50
1:G:44:LYS:HG3	3:G:7507:HOH:O	2.11	0.50
1:A:18:LYS:HB2	1:A:38:VAL:HB	1.94	0.50
1:A:163:LYS:CD	1:A:163:LYS:N	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:LYS:O	1:F:14:LEU:HG	2.10	0.50
1:H:122:VAL:HG22	1:H:123:TYR:H	1.73	0.50
1:H:228:ASP:O	1:H:254:ASN:HB2	2.11	0.50
1:E:245:MET:HE3	1:E:280:ALA:HB2	1.94	0.50
1:G:328:GLN:HB3	1:G:370:ILE:CG2	2.41	0.50
1:H:352:ILE:HG23	1:H:352:ILE:O	2.11	0.50
1:E:11:ARG:NH1	1:E:42:GLU:OE2	2.45	0.50
1:E:244:GLY:HA3	1:F:275:THR:HG22	1.93	0.50
1:E:317:ILE:HD11	1:E:335:LEU:HD13	1.94	0.50
1:B:124:TYR:CD1	1:B:125:PRO:HD3	2.47	0.50
1:A:148:TYR:OH	1:A:182:LYS:NZ	2.45	0.50
1:C:56:TYR:CD1	1:C:279:LYS:HG2	2.47	0.50
1:C:301:LYS:O	1:C:305:ILE:HG13	2.12	0.49
1:E:345:PHE:CE1	1:E:393:LEU:HD22	2.47	0.49
1:E:392:ASP:C	1:E:394:LYS:N	2.70	0.49
1:F:155:LYS:O	1:F:159:LEU:HG	2.12	0.49
1:B:123:TYR:CG	1:B:125:PRO:HD2	2.46	0.49
1:C:75:VAL:O	1:C:79:MET:HG2	2.11	0.49
1:C:98:VAL:CG2	1:C:205:ILE:HD12	2.41	0.49
1:C:301:LYS:HD3	1:C:305:ILE:HD11	1.94	0.49
1:H:303:GLN:HB3	1:H:372:LEU:HD13	1.94	0.49
1:A:215:GLU:HG3	3:A:1645:HOH:O	2.12	0.49
1:C:288:CYS:HA	3:C:3585:HOH:O	2.11	0.49
1:D:353:PHE:CD1	1:D:353:PHE:N	2.79	0.49
1:G:279:LYS:O	1:G:283:ILE:HG13	2.12	0.49
1:A:207:PHE:C	1:A:207:PHE:CD2	2.88	0.49
1:D:1:MET:CE	1:D:48:GLU:HG3	2.36	0.49
1:F:351:GLN:O	1:F:385:ARG:NH1	2.45	0.49
1:B:237:SER:HA	1:B:242:ILE:HG13	1.94	0.49
1:H:80:LYS:HE2	1:H:86:ASP:OD1	2.13	0.49
1:C:45:ASN:ND2	1:D:62:LEU:H	2.03	0.49
1:D:123:TYR:CD1	1:D:125:PRO:HD2	2.47	0.49
1:E:392:ASP:C	1:E:394:LYS:H	2.20	0.49
1:F:122:VAL:HG22	1:F:123:TYR:N	2.28	0.49
1:G:332:PHE:HD2	1:G:335:LEU:HD22	1.78	0.49
1:H:55:LYS:O	1:H:59:GLU:HG3	2.13	0.49
1:B:256:ASP:O	1:B:260:ARG:HG3	2.13	0.49
1:B:46:PRO:HG3	1:B:291:TRP:CD2	2.48	0.49
1:B:124:TYR:HB3	1:B:359:ILE:O	2.13	0.49
1:G:200:LEU:HD12	1:G:201:TRP:N	2.28	0.49
1:A:17:LEU:HD21	1:B:271:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:LYS:HD2	1:F:195:LYS:C	2.37	0.48
1:H:220:GLN:HB3	1:H:230:THR:HG21	1.95	0.48
1:H:309:PHE:CZ	1:H:387:ASN:HB2	2.47	0.48
1:H:22:MET:SD	1:H:35:PRO:HD3	2.53	0.48
1:E:303:GLN:HB3	1:E:372:LEU:HD13	1.95	0.48
1:C:41:MET:HB2	1:C:241:ASN:CG	2.39	0.48
1:G:128:MET:O	1:G:132:ASN:HB2	2.13	0.48
1:F:123:TYR:CD2	1:F:125:PRO:HD2	2.49	0.48
1:G:345:PHE:O	1:G:349:LYS:HB2	2.14	0.48
1:G:375:PRO:HD2	1:G:378:VAL:HG21	1.96	0.48
1:G:122:VAL:HG22	1:G:123:TYR:N	2.28	0.48
1:G:172:SER:O	1:G:204:GLU:HA	2.13	0.48
1:D:78:TRP:O	1:D:82:ARG:HB2	2.13	0.48
1:F:303:GLN:HB3	1:F:372:LEU:HD13	1.95	0.48
1:H:128:MET:O	1:H:132:ASN:HB2	2.13	0.48
1:C:111:LYS:HG2	1:C:114:ASP:OD1	2.14	0.48
1:D:49:LEU:O	1:D:53:LEU:HG	2.14	0.48
1:F:187:GLN:HE22	1:F:190:LYS:NZ	2.11	0.48
1:G:85:TRP:CE2	1:G:218:VAL:HG11	2.49	0.48
1:G:158:LYS:O	1:G:161:LYS:HB2	2.13	0.48
1:H:384:GLU:HG3	1:H:388:LYS:HZ2	1.79	0.48
1:H:386:LEU:O	1:H:390:LEU:HG	2.13	0.48
1:D:138:ILE:HG22	1:D:159:LEU:HD13	1.96	0.48
1:G:195:LYS:C	1:G:195:LYS:HD2	2.39	0.48
1:A:301:LYS:HG3	3:A:1621:HOH:O	2.13	0.47
1:D:172:SER:HA	1:D:173:PRO:C	2.39	0.47
1:E:300:ASP:O	1:E:303:GLN:HG2	2.14	0.47
1:A:41:MET:HB2	1:A:241:ASN:CG	2.39	0.47
1:B:41:MET:HB2	1:B:241:ASN:ND2	2.29	0.47
1:C:128:MET:O	1:C:132:ASN:HB2	2.14	0.47
1:C:244:GLY:O	1:D:274:THR:HA	2.13	0.47
1:D:160:SER:OG	1:D:195:LYS:NZ	2.47	0.47
1:F:392:ASP:C	1:F:394:LYS:H	2.22	0.47
1:H:328:GLN:HB3	1:H:370:ILE:CG2	2.44	0.47
1:C:119:ILE:HD12	1:C:170:PHE:CE1	2.50	0.47
1:C:350:ALA:O	1:C:385:ARG:HD2	2.14	0.47
1:E:97:GLY:O	1:E:100:PRO:HD2	2.14	0.47
1:E:109:PHE:CZ	1:E:257:ILE:HG23	2.49	0.47
1:E:328:GLN:HB3	1:E:370:ILE:CG2	2.44	0.47
1:G:157:GLU:O	1:G:161:LYS:HD3	2.14	0.47
1:A:151:ILE:HD12	1:A:189:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLN:HE22	1:B:190:LYS:NZ	2.12	0.47
1:C:1:MET:HE2	3:C:3553:HOH:O	2.14	0.47
1:A:37:SER:HB2	1:A:355:ASP:OD1	2.13	0.47
1:D:11:ARG:HG3	1:D:19:TRP:NE1	2.29	0.47
1:D:174:HIS:HD2	1:D:177:VAL:HG22	1.78	0.47
1:D:225:GLN:CD	1:D:225:GLN:H	2.21	0.47
1:H:138:ILE:HG13	1:H:165:ASN:OD1	2.14	0.47
1:E:98:VAL:CG2	1:E:205:ILE:HD12	2.45	0.47
1:F:299:ILE:HD13	1:F:326:TYR:HB3	1.97	0.47
1:B:163:LYS:HE2	3:B:2574:HOH:O	2.15	0.47
1:D:69:GLU:O	1:D:73:LYS:HG3	2.14	0.47
1:D:123:TYR:CG	1:D:125:PRO:HD2	2.49	0.47
1:D:206:HIS:HE1	2:D:4500:PPG:O3	1.97	0.47
1:D:228:ASP:O	1:D:254:ASN:HB2	2.14	0.47
1:G:11:ARG:CA	1:G:14:LEU:HD12	2.38	0.47
1:G:17:LEU:HD22	2:G:7500:PPG:NI	2.28	0.47
1:H:260:ARG:O	1:H:263:LYS:HG2	2.14	0.47
1:C:123:TYR:CZ	1:C:125:PRO:HG2	2.50	0.47
1:E:187:GLN:NE2	1:E:190:LYS:NZ	2.60	0.47
1:F:274:THR:HG23	1:F:274:THR:O	2.15	0.47
1:F:307:LYS:HD2	1:F:321:LEU:HG	1.96	0.47
1:A:351:GLN:O	1:A:385:ARG:NH1	2.48	0.47
1:D:327:LEU:HD13	1:D:369:ARG:NH1	2.29	0.47
1:E:172:SER:HA	1:E:173:PRO:C	2.40	0.47
1:E:263:LYS:HG3	1:E:264:SER:N	2.29	0.47
1:F:247:MET:HB3	3:F:6625:HOH:O	2.14	0.47
1:F:342:MET:HE1	1:F:366:GLY:CA	2.45	0.47
1:A:216:HIS:HD2	3:A:1550:HOH:O	1.98	0.47
1:B:191:ASP:HB2	3:B:2607:HOH:O	2.15	0.47
1:C:187:GLN:HE22	1:C:190:LYS:HZ1	1.63	0.47
1:F:225:GLN:O	1:F:228:ASP:HB2	2.15	0.47
1:A:22:MET:SD	1:A:35:PRO:HD3	2.55	0.46
1:D:19:TRP:O	1:D:23:TYR:HD1	1.98	0.46
1:E:260:ARG:HA	1:E:263:LYS:HG2	1.97	0.46
1:H:225:GLN:O	1:H:228:ASP:HB2	2.15	0.46
1:A:233:PHE:HD2	1:A:250:ILE:HD12	1.80	0.46
1:A:356:GLU:O	1:A:359:ILE:HG12	2.15	0.46
1:B:47:PRO:O	1:B:51:GLU:HG2	2.15	0.46
1:B:62:LEU:HD23	1:B:275:THR:HG21	1.98	0.46
1:B:80:LYS:HD3	1:B:86:ASP:OD1	2.15	0.46
1:B:387:ASN:OD1	1:B:391:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:HIS:HE1	1:G:208:ASP:OD1	1.98	0.46
1:C:11:ARG:HA	1:C:14:LEU:HD12	1.96	0.46
1:C:160:SER:OG	1:C:195:LYS:NZ	2.47	0.46
1:C:352:ILE:HG23	1:C:352:ILE:O	2.16	0.46
1:H:266:ASP:HA	1:H:270:GLY:HA2	1.97	0.46
1:D:120:THR:HB	1:D:121:PRO:HA	1.97	0.46
1:E:138:ILE:CG2	1:E:159:LEU:HD22	2.46	0.46
1:E:339:HIS:HB2	1:E:358:TYR:HD2	1.80	0.46
1:E:356:GLU:O	1:E:359:ILE:HG12	2.15	0.46
1:D:219:PHE:O	1:D:222:ILE:HG12	2.16	0.46
1:H:189:ILE:O	1:H:193:VAL:HG23	2.16	0.46
1:H:219:PHE:O	1:H:222:ILE:HG12	2.15	0.46
1:A:123:TYR:CD2	1:A:125:PRO:HD2	2.51	0.46
1:C:11:ARG:HG3	1:C:19:TRP:NE1	2.30	0.46
1:G:212:PRO:HB2	3:G:7532:HOH:O	2.16	0.46
1:H:75:VAL:O	1:H:79:MET:HG2	2.16	0.46
1:D:80:LYS:HD3	1:D:86:ASP:OD1	2.16	0.46
1:D:122:VAL:HG22	1:D:123:TYR:H	1.80	0.46
1:F:163:LYS:N	1:F:163:LYS:CD	2.64	0.46
1:C:113:GLY:HA2	1:C:136:LYS:NZ	2.30	0.46
1:D:17:LEU:HD23	2:D:4500:PPG:HNI2	1.81	0.46
1:E:123:TYR:CE1	2:E:5500:PPG:N4A	2.84	0.46
1:H:328:GLN:HB2	1:H:372:LEU:HD11	1.98	0.46
1:A:85:TRP:CD2	1:A:218:VAL:HG11	2.51	0.45
1:A:122:VAL:CG2	1:A:123:TYR:N	2.79	0.45
1:A:238:LYS:HZ1	2:A:1500:PPG:H5A1	1.81	0.45
1:C:172:SER:O	1:C:204:GLU:HA	2.17	0.45
1:D:142:LEU:HA	3:D:4571:HOH:O	2.16	0.45
1:F:84:GLN:HB3	3:F:6669:HOH:O	2.15	0.45
1:F:124:TYR:CG	1:F:125:PRO:HD3	2.51	0.45
1:G:17:LEU:HD11	1:H:271:MET:HE1	1.98	0.45
1:E:83:HIS:HB3	3:E:5566:HOH:O	2.16	0.45
1:G:56:TYR:CE1	1:G:60:THR:HG21	2.51	0.45
1:G:172:SER:HA	1:G:173:PRO:C	2.41	0.45
1:H:122:VAL:CG2	1:H:123:TYR:N	2.77	0.45
1:H:295:CYS:O	1:H:299:ILE:HG13	2.17	0.45
1:C:207:PHE:C	1:C:207:PHE:CD2	2.92	0.45
1:E:279:LYS:O	1:E:283:ILE:HG13	2.17	0.45
1:G:65:THR:O	1:G:273:PHE:HA	2.16	0.45
1:G:263:LYS:HG3	1:G:264:SER:N	2.32	0.45
1:F:195:LYS:HE3	1:F:195:LYS:HB3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:SER:HB2	1:F:243:ALA:HA	1.98	0.45
1:G:260:ARG:HA	1:G:263:LYS:HG2	1.97	0.45
1:A:107:ARG:CZ	1:A:268:THR:HG21	2.46	0.45
1:A:122:VAL:CG2	1:A:123:TYR:H	2.30	0.45
1:A:244:GLY:O	1:B:275:THR:HG22	2.17	0.45
1:F:233:PHE:HD2	1:F:250:ILE:HD12	1.82	0.45
1:G:12:LYS:O	1:G:14:LEU:HG	2.17	0.45
1:D:275:THR:HG23	1:D:276:LEU:H	1.80	0.45
1:A:272:PRO:HG3	3:A:1528:HOH:O	2.16	0.45
1:D:41:MET:HB2	1:D:241:ASN:ND2	2.32	0.45
1:D:195:LYS:HG3	1:G:88:GLN:HG3	1.99	0.45
1:E:117:ILE:HA	1:E:138:ILE:HB	1.98	0.45
1:E:266:ASP:HA	1:E:270:GLY:HA2	1.98	0.45
1:G:352:ILE:HD13	1:G:354:PHE:CZ	2.52	0.45
1:B:107:ARG:HE	1:B:268:THR:HG21	1.82	0.45
1:C:225:GLN:N	1:C:225:GLN:CD	2.75	0.45
1:D:116:VAL:HB	1:D:130:ILE:CD1	2.46	0.45
1:D:386:LEU:O	1:D:390:LEU:HG	2.17	0.45
1:F:38:VAL:HG13	2:F:6500:PPG:HBI	1.98	0.45
1:A:328:GLN:HB2	1:A:372:LEU:HD11	1.99	0.45
1:B:52:GLY:HA3	1:B:283:ILE:HD13	1.98	0.45
1:A:85:TRP:CE2	1:A:218:VAL:HG11	2.52	0.44
1:A:342:MET:HE3	1:A:368:GLU:OE1	2.17	0.44
1:B:122:VAL:HG22	1:B:123:TYR:H	1.81	0.44
1:D:37:SER:OG	1:D:38:VAL:N	2.50	0.44
1:E:71:TYR:O	1:E:75:VAL:HG23	2.17	0.44
1:G:46:PRO:HG3	1:G:291:TRP:CE3	2.52	0.44
1:D:205:ILE:HA	3:D:4566:HOH:O	2.17	0.44
1:E:123:TYR:CG	1:E:125:PRO:HD2	2.51	0.44
1:E:303:GLN:HG3	1:E:304:ARG:N	2.32	0.44
1:G:85:TRP:CD2	1:G:218:VAL:HG11	2.52	0.44
1:H:310:PHE:O	1:H:314:HIS:C	2.61	0.44
1:A:271:MET:HE1	1:B:17:LEU:HD11	1.98	0.44
1:C:176:PRO:HB3	1:C:369:ARG:HD3	1.99	0.44
1:C:225:GLN:CD	1:C:225:GLN:H	2.25	0.44
1:G:160:SER:OG	1:G:195:LYS:NZ	2.49	0.44
1:G:233:PHE:HD2	1:G:250:ILE:HD12	1.82	0.44
1:H:19:TRP:O	1:H:23:TYR:HD1	2.00	0.44
1:H:41:MET:HG2	1:H:373:ALA:CB	2.46	0.44
1:C:123:TYR:CD1	1:C:125:PRO:HD2	2.52	0.44
1:E:317:ILE:HD13	1:E:332:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:HIS:HB2	1:E:358:TYR:CD2	2.53	0.44
1:H:342:MET:O	1:H:346:MET:HG2	2.18	0.44
1:H:362:ASP:HB2	3:H:8553:HOH:O	2.15	0.44
1:D:260:ARG:O	1:D:263:LYS:HG2	2.18	0.44
1:E:3:TYR:CD2	1:E:291:TRP:HD1	2.36	0.44
1:H:131:LYS:HE3	1:H:131:LYS:HB2	1.82	0.44
1:A:263:LYS:NZ	1:F:341:ALA:HB2	2.32	0.44
1:C:133:GLN:O	1:C:134:GLU:HB2	2.18	0.44
1:C:300:ASP:O	1:C:303:GLN:HG2	2.18	0.44
1:D:21:LEU:O	1:D:21:LEU:HD12	2.17	0.44
1:G:19:TRP:O	1:G:23:TYR:HD1	2.00	0.44
1:G:98:VAL:CG2	1:G:205:ILE:HD12	2.48	0.44
1:A:11:ARG:HB2	1:A:19:TRP:CG	2.52	0.44
1:A:284:CYS:HA	1:A:288:CYS:SG	2.58	0.44
1:B:124:TYR:HA	1:B:127:PHE:HD1	1.82	0.44
1:B:162:ASP:HB3	1:B:165:ASN:HD22	1.80	0.44
1:C:317:ILE:HD13	1:C:332:PHE:CE2	2.53	0.44
1:D:83:HIS:O	1:D:84:GLN:C	2.61	0.44
1:F:216:HIS:HD2	3:F:6515:HOH:O	2.00	0.44
1:G:179:ARG:NE	1:G:323:GLU:OE1	2.43	0.44
1:E:1:MET:HE1	3:E:5526:HOH:O	2.17	0.44
1:A:116:VAL:HB	1:A:130:ILE:HD13	2.00	0.43
1:E:328:GLN:HB3	1:E:370:ILE:HG22	1.99	0.43
1:H:303:GLN:HG3	1:H:304:ARG:N	2.33	0.43
1:B:55:LYS:O	1:B:59:GLU:HG3	2.17	0.43
1:E:84:GLN:CD	1:E:84:GLN:N	2.76	0.43
1:E:112:PRO:HA	1:E:134:GLU:O	2.18	0.43
1:H:353:PHE:N	1:H:353:PHE:CD1	2.86	0.43
1:B:316:GLU:OE2	1:B:316:GLU:N	2.43	0.43
1:E:166:LYS:O	1:E:167:ALA:HB2	2.17	0.43
1:E:228:ASP:O	1:E:254:ASN:HB2	2.17	0.43
1:H:12:LYS:O	1:H:14:LEU:HG	2.18	0.43
1:A:184:ASP:O	1:A:188:LYS:HG3	2.18	0.43
1:C:342:MET:HE1	1:C:366:GLY:HA2	2.00	0.43
1:D:151:ILE:HD13	1:D:189:ILE:HD11	1.98	0.43
1:D:225:GLN:CD	1:D:225:GLN:N	2.75	0.43
1:F:68:THR:O	1:F:71:TYR:HB3	2.18	0.43
1:H:70:GLU:HB3	3:H:8552:HOH:O	2.17	0.43
1:A:17:LEU:HD21	1:B:271:MET:CE	2.48	0.43
1:A:299:ILE:HD13	1:A:326:TYR:HB3	2.01	0.43
1:B:356:GLU:O	1:B:359:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLU:O	1:D:161:LYS:HD3	2.19	0.43
1:D:207:PHE:C	1:D:207:PHE:CD2	2.94	0.43
1:E:254:ASN:HA	1:E:255:PRO:HD3	1.89	0.43
1:E:324:GLY:C	1:E:325:THR:HG23	2.44	0.43
1:G:352:ILE:HA	3:G:7598:HOH:O	2.17	0.43
1:A:374:ALA:HB2	3:A:1524:HOH:O	2.19	0.43
1:E:18:LYS:HD3	1:E:38:VAL:HB	2.00	0.43
1:H:172:SER:HA	1:H:173:PRO:C	2.43	0.43
1:D:98:VAL:HG13	1:D:233:PHE:HB3	2.00	0.43
1:D:162:ASP:O	1:D:164:ASN:N	2.52	0.43
1:F:311:GLU:O	1:F:315:PRO:HG3	2.17	0.43
1:G:120:THR:HA	1:G:121:PRO:C	2.44	0.43
1:G:145:LYS:HE3	1:G:145:LYS:HB3	1.90	0.43
1:A:302:ASN:O	1:A:306:VAL:HG23	2.19	0.43
1:B:303:GLN:HG3	1:B:321:LEU:HD22	2.01	0.43
1:E:352:ILE:HG23	1:E:352:ILE:O	2.18	0.43
1:F:352:ILE:HA	3:F:6580:HOH:O	2.18	0.43
1:A:328:GLN:HB3	1:A:370:ILE:CG2	2.49	0.43
1:A:352:ILE:O	1:A:352:ILE:CG2	2.67	0.43
1:C:120:THR:HB	1:C:121:PRO:HA	2.01	0.43
1:E:131:LYS:C	1:E:133:GLN:N	2.76	0.43
1:E:260:ARG:O	1:E:263:LYS:HG2	2.19	0.43
1:A:192:ILE:O	1:A:195:LYS:HE3	2.18	0.43
1:A:300:ASP:OD1	1:A:303:GLN:NE2	2.49	0.43
1:C:119:ILE:CG2	1:C:142:LEU:HG	2.49	0.43
1:D:392:ASP:C	1:D:394:LYS:N	2.76	0.43
1:E:241:ASN:ND2	1:F:61:VAL:HG13	2.34	0.43
1:G:41:MET:HG2	1:G:373:ALA:HB1	2.00	0.43
1:B:282:GLU:HG2	3:B:2603:HOH:O	2.18	0.42
1:B:353:PHE:CD1	1:B:353:PHE:N	2.87	0.42
1:F:80:LYS:HD2	1:F:80:LYS:HA	1.91	0.42
1:F:356:GLU:O	1:F:359:ILE:HG12	2.19	0.42
2:H:8500:PPG:HEI2	3:H:8556:HOH:O	2.19	0.42
1:C:203:ASP:OD1	2:C:3500:PPG:N1	2.52	0.42
1:E:12:LYS:HG2	1:E:13:ASN:ND2	2.34	0.42
1:G:107:ARG:NE	1:G:268:THR:HG21	2.34	0.42
1:G:216:HIS:CD2	3:G:7516:HOH:O	2.72	0.42
1:G:362:ASP:HA	1:G:365:ILE:HG13	2.01	0.42
1:B:12:LYS:HG2	1:B:13:ASN:ND2	2.34	0.42
1:B:266:ASP:HA	1:B:270:GLY:HA2	2.02	0.42
1:E:237:SER:HA	1:E:242:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LYS:O	1:E:311:GLU:HG3	2.19	0.42
1:F:332:PHE:O	1:F:335:LEU:HB2	2.20	0.42
1:G:303:GLN:HB3	1:G:372:LEU:HD13	2.01	0.42
1:A:11:ARG:HA	1:A:14:LEU:HD12	2.01	0.42
1:A:98:VAL:HG21	1:A:205:ILE:HD12	2.01	0.42
1:E:104:ASN:HB2	3:E:5536:HOH:O	2.18	0.42
1:E:274:THR:HA	1:F:244:GLY:O	2.19	0.42
1:E:313:ASN:C	1:E:315:PRO:HD3	2.44	0.42
1:E:327:LEU:HB3	1:E:369:ARG:HD2	2.02	0.42
1:F:386:LEU:O	1:F:390:LEU:HG	2.19	0.42
1:G:352:ILE:HG23	1:G:352:ILE:O	2.19	0.42
1:H:309:PHE:HZ	1:H:387:ASN:HB2	1.83	0.42
1:B:62:LEU:CD2	1:B:275:THR:HG21	2.49	0.42
1:B:69:GLU:O	1:B:73:LYS:HG3	2.20	0.42
1:E:303:GLN:CD	1:E:321:LEU:HD22	2.45	0.42
1:F:123:TYR:CZ	1:F:125:PRO:HG2	2.55	0.42
1:G:49:LEU:O	1:G:53:LEU:HG	2.19	0.42
1:G:332:PHE:O	1:G:335:LEU:HB2	2.19	0.42
1:H:124:TYR:HB3	1:H:359:ILE:O	2.20	0.42
1:D:252:ILE:O	1:D:258:ARG:NH1	2.44	0.42
1:D:303:GLN:HG3	1:D:321:LEU:HD22	2.02	0.42
1:E:119:ILE:CG2	1:E:142:LEU:HG	2.47	0.42
1:F:122:VAL:O	1:F:123:TYR:C	2.63	0.42
1:A:172:SER:O	1:A:204:GLU:HA	2.20	0.42
1:A:206:HIS:HE1	2:A:1500:PPG:O3	2.02	0.42
1:B:238:LYS:HD2	1:B:238:LYS:HA	1.88	0.42
1:C:18:LYS:HB2	1:C:38:VAL:HB	2.01	0.42
1:D:17:LEU:CD2	2:D:4500:PPG:HNI2	2.32	0.42
1:D:203:ASP:OD1	2:D:4500:PPG:N1	2.53	0.42
1:D:347:ILE:HG23	1:D:353:PHE:CE2	2.54	0.42
1:H:122:VAL:CG2	1:H:123:TYR:H	2.33	0.42
1:H:263:LYS:CG	1:H:264:SER:N	2.82	0.42
1:H:307:LYS:HB2	1:H:319:ALA:O	2.19	0.42
1:H:307:LYS:O	1:H:311:GLU:HG3	2.19	0.42
1:A:69:GLU:O	1:A:73:LYS:HG3	2.20	0.42
1:A:354:PHE:CD2	1:A:368:GLU:HB3	2.55	0.42
1:B:345:PHE:O	1:B:349:LYS:HB2	2.19	0.42
1:D:122:VAL:CG2	1:D:123:TYR:N	2.81	0.42
1:G:307:LYS:HD2	1:G:321:LEU:HG	2.02	0.42
1:G:328:GLN:HB3	1:G:370:ILE:HG22	2.02	0.42
1:H:207:PHE:CD2	1:H:207:PHE:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:THR:HB	3:B:2584:HOH:O	2.19	0.41
1:B:220:GLN:HG3	3:B:2526:HOH:O	2.20	0.41
1:C:41:MET:HB2	1:C:241:ASN:ND2	2.35	0.41
1:D:18:LYS:CD	1:D:38:VAL:HB	2.42	0.41
1:E:123:TYR:CD2	1:E:125:PRO:HD2	2.55	0.41
1:E:242:ILE:C	1:E:244:GLY:H	2.28	0.41
1:G:120:THR:HB	1:G:121:PRO:HA	2.02	0.41
1:A:207:PHE:HE2	1:A:208:ASP:OD2	2.03	0.41
1:D:342:MET:O	1:D:346:MET:HG2	2.20	0.41
1:F:157:GLU:O	1:F:161:LYS:HD3	2.20	0.41
1:G:269:SER:HB3	1:H:269:SER:HB3	2.02	0.41
1:H:111:LYS:HA	1:H:135:ARG:NH2	2.35	0.41
1:H:123:TYR:CD1	1:H:125:PRO:HD2	2.56	0.41
1:A:123:TYR:CE1	2:A:1500:PPG:N4A	2.89	0.41
1:F:352:ILE:O	1:F:352:ILE:HG23	2.19	0.41
1:G:223:ASP:OD1	1:G:225:GLN:N	2.54	0.41
1:A:187:GLN:HE22	1:A:190:LYS:HZ1	1.66	0.41
1:B:11:ARG:HB2	1:B:19:TRP:CG	2.55	0.41
1:C:89:THR:HG23	3:C:3535:HOH:O	2.18	0.41
1:C:263:LYS:HG3	1:C:264:SER:N	2.35	0.41
2:C:3500:PPG:H4A1	2:C:3500:PPG:H5A1	1.84	0.41
1:D:122:VAL:O	1:D:123:TYR:C	2.64	0.41
1:D:263:LYS:CG	1:D:264:SER:N	2.83	0.41
1:E:45:ASN:ND2	1:F:62:LEU:HG	2.35	0.41
1:E:52:GLY:HA3	1:E:283:ILE:HD13	2.01	0.41
1:E:362:ASP:C	1:E:364:GLY:H	2.29	0.41
1:H:119:ILE:HD12	1:H:170:PHE:CE1	2.55	0.41
1:A:123:TYR:CD1	1:A:125:PRO:HD2	2.55	0.41
1:B:122:VAL:CG2	1:B:123:TYR:N	2.82	0.41
1:D:162:ASP:C	1:D:164:ASN:N	2.78	0.41
1:F:216:HIS:CD2	3:F:6515:HOH:O	2.72	0.41
1:H:123:TYR:CD2	1:H:125:PRO:HD2	2.55	0.41
1:C:65:THR:HG22	1:C:66:GLY:N	2.36	0.41
1:D:162:ASP:C	1:D:164:ASN:H	2.29	0.41
1:E:336:LYS:HA	1:E:336:LYS:HD3	1.81	0.41
1:G:11:ARG:HG3	1:G:19:TRP:NE1	2.35	0.41
1:G:109:PHE:CZ	1:G:257:ILE:HG23	2.55	0.41
1:H:49:LEU:HA	1:H:283:ILE:HG21	2.03	0.41
1:A:207:PHE:C	1:A:207:PHE:HD2	2.29	0.41
1:C:220:GLN:HB3	1:C:230:THR:HG21	2.02	0.41
1:F:17:LEU:HD23	2:F:6500:PPG:NI	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:THR:O	1:A:71:TYR:HB3	2.21	0.41
3:C:3631:HOH:O	1:D:96:ALA:HB3	2.20	0.41
1:D:112:PRO:HB3	1:D:134:GLU:HB3	2.03	0.41
1:G:119:ILE:HG22	1:G:142:LEU:HG	2.02	0.41
1:H:205:ILE:HA	3:H:8605:HOH:O	2.21	0.41
1:A:184:ASP:CG	3:A:1521:HOH:O	2.64	0.41
1:A:265:ARG:O	1:A:265:ARG:HG2	2.20	0.41
1:A:345:PHE:O	1:A:349:LYS:HB2	2.20	0.41
1:B:143:LEU:O	1:B:149:TYR:HA	2.21	0.41
1:B:157:GLU:O	1:B:161:LYS:HD3	2.21	0.41
1:C:18:LYS:HD3	1:C:38:VAL:HB	2.03	0.41
1:C:136:LYS:HD2	1:C:136:LYS:N	2.36	0.41
1:D:343:GLU:OE2	1:D:356:GLU:HG3	2.20	0.41
1:E:83:HIS:O	1:E:84:GLN:C	2.63	0.41
1:F:9:ILE:HG12	3:F:6522:HOH:O	2.20	0.41
1:F:133:GLN:O	1:F:134:GLU:HB2	2.21	0.41
1:F:201:TRP:HB3	1:F:233:PHE:HE1	1.86	0.41
1:H:46:PRO:HA	1:H:47:PRO:HD3	1.93	0.41
1:H:107:ARG:HE	1:H:268:THR:HG21	1.85	0.41
1:H:123:TYR:CE1	2:H:8500:PPG:N4A	2.89	0.41
1:G:15:GLY:O	1:H:65:THR:HA	2.21	0.41
1:G:309:PHE:CZ	1:G:387:ASN:HB2	2.55	0.41
1:H:172:SER:O	1:H:204:GLU:HA	2.21	0.41
1:A:345:PHE:CE1	1:A:393:LEU:HD22	2.56	0.40
1:E:124:TYR:CD1	1:E:125:PRO:HD3	2.56	0.40
1:E:242:ILE:C	1:E:244:GLY:N	2.77	0.40
1:F:123:TYR:CG	1:F:125:PRO:HD2	2.56	0.40
1:G:74:THR:OG1	1:G:286:LYS:HE3	2.21	0.40
1:G:198:LEU:O	1:G:229:LYS:NZ	2.51	0.40
1:G:394:LYS:NZ	3:G:7573:HOH:O	2.53	0.40
1:A:70:GLU:HA	1:A:70:GLU:OE2	2.22	0.40
1:A:268:THR:OG1	1:A:269:SER:N	2.53	0.40
1:B:155:LYS:O	1:B:159:LEU:HG	2.21	0.40
1:C:122:VAL:CG2	1:C:123:TYR:N	2.84	0.40
1:D:188:LYS:HB3	1:D:188:LYS:HE2	1.90	0.40
1:D:353:PHE:HA	3:D:4636:HOH:O	2.21	0.40
1:E:112:PRO:HB3	1:E:134:GLU:HB3	2.03	0.40
1:E:163:LYS:N	1:E:163:LYS:CD	2.69	0.40
1:G:65:THR:HG22	1:G:66:GLY:N	2.36	0.40
1:B:393:LEU:O	1:B:394:LYS:CB	2.69	0.40
1:D:41:MET:C	1:D:43:PHE:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:HB	1:D:245:MET:HG2	2.03	0.40
1:G:207:PHE:C	1:G:207:PHE:CD2	2.99	0.40
1:H:41:MET:C	1:H:43:PHE:H	2.29	0.40
1:A:327:LEU:HB3	1:A:369:ARG:HD2	2.02	0.40
1:B:138:ILE:HG13	1:B:165:ASN:OD1	2.21	0.40
1:B:324:GLY:C	1:B:325:THR:HG23	2.47	0.40
1:C:67:PRO:HD3	1:C:278:TYR:CE2	2.56	0.40
1:C:303:GLN:HG3	1:C:321:LEU:HD22	2.03	0.40
1:E:45:ASN:HB2	1:E:50:ILE:HD11	2.03	0.40
1:E:49:LEU:O	1:E:53:LEU:HG	2.21	0.40
1:E:75:VAL:O	1:E:79:MET:HG2	2.22	0.40
1:E:88:GLN:HB2	1:E:91:TRP:CD1	2.57	0.40
1:E:341:ALA:O	1:E:344:GLU:HB3	2.21	0.40
1:F:41:MET:HB2	1:F:241:ASN:CG	2.46	0.40
1:F:136:LYS:HD2	1:F:136:LYS:N	2.36	0.40
1:G:233:PHE:CD2	1:G:250:ILE:HD12	2.56	0.40
1:C:106:VAL:O	1:C:110:THR:OG1	2.34	0.40
1:C:163:LYS:HG2	3:C:3612:HOH:O	2.21	0.40
1:C:198:LEU:O	1:C:229:LYS:HD2	2.22	0.40
1:C:266:ASP:HA	1:C:270:GLY:HA2	2.02	0.40
1:D:307:LYS:O	1:D:311:GLU:HG3	2.22	0.40
1:G:11:ARG:HB2	1:G:19:TRP:CG	2.56	0.40
1:H:83:HIS:HE1	1:H:208:ASP:OD1	2.03	0.40
1:H:106:VAL:O	1:H:110:THR:OG1	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	392/399 (98%)	368 (94%)	21 (5%)	3 (1%)	16 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	392/399 (98%)	371 (95%)	21 (5%)	0	100	100
1	C	392/399 (98%)	372 (95%)	19 (5%)	1 (0%)	36	55
1	D	392/399 (98%)	375 (96%)	16 (4%)	1 (0%)	36	55
1	E	392/399 (98%)	374 (95%)	16 (4%)	2 (0%)	24	43
1	F	392/399 (98%)	377 (96%)	15 (4%)	0	100	100
1	G	392/399 (98%)	369 (94%)	22 (6%)	1 (0%)	36	55
1	H	392/399 (98%)	371 (95%)	21 (5%)	0	100	100
All	All	3136/3192 (98%)	2977 (95%)	151 (5%)	8 (0%)	36	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS
1	A	274	THR
1	E	62	LEU
1	G	141	GLU
1	C	123	TYR
1	E	274	THR
1	A	38	VAL
1	A	246	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/358 (99%)	346 (98%)	7 (2%)	48	75
1	B	353/358 (99%)	344 (98%)	9 (2%)	42	69
1	C	353/358 (99%)	345 (98%)	8 (2%)	44	72
1	D	353/358 (99%)	345 (98%)	8 (2%)	44	72
1	E	353/358 (99%)	343 (97%)	10 (3%)	38	66
1	F	353/358 (99%)	343 (97%)	10 (3%)	38	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	353/358 (99%)	340 (96%)	13 (4%)	30	57
1	H	353/358 (99%)	346 (98%)	7 (2%)	48	75
All	All	2824/2864 (99%)	2752 (98%)	72 (2%)	42	69

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	A	163	LYS
1	A	176	PRO
1	A	207	PHE
1	A	238	LYS
1	A	301	LYS
1	A	355	ASP
1	B	134	GLU
1	B	157	GLU
1	B	163	LYS
1	B	176	PRO
1	B	207	PHE
1	B	238	LYS
1	B	275	THR
1	B	301	LYS
1	B	355	ASP
1	C	134	GLU
1	C	163	LYS
1	C	176	PRO
1	C	207	PHE
1	C	275	THR
1	C	301	LYS
1	C	355	ASP
1	C	394	LYS
1	D	134	GLU
1	D	144	GLU
1	D	163	LYS
1	D	176	PRO
1	D	199	MET
1	D	207	PHE
1	D	301	LYS
1	D	355	ASP
1	E	1	MET
1	E	84	GLN

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Mol	Chain	Res	Type
1	E	134	GLU
1	E	163	LYS
1	E	176	PRO
1	E	199	MET
1	E	207	PHE
1	E	301	LYS
1	E	335	LEU
1	E	355	ASP
1	F	11	ARG
1	F	134	GLU
1	F	163	LYS
1	F	175	ASN
1	F	176	PRO
1	F	207	PHE
1	F	238	LYS
1	F	275	THR
1	F	301	LYS
1	F	355	ASP
1	G	134	GLU
1	G	163	LYS
1	G	175	ASN
1	G	176	PRO
1	G	199	MET
1	G	207	PHE
1	G	238	LYS
1	G	274	THR
1	G	301	LYS
1	G	329	TRP
1	G	335	LEU
1	G	355	ASP
1	G	394	LYS
1	H	134	GLU
1	H	163	LYS
1	H	207	PHE
1	H	301	LYS
1	H	335	LEU
1	H	355	ASP
1	H	394	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	45	ASN
1	A	94	ASN
1	A	154	GLN
1	A	187	GLN
1	A	206	HIS
1	A	216	HIS
1	A	220	GLN
1	A	225	GLN
1	A	348	HIS
1	B	13	ASN
1	B	25	GLN
1	B	45	ASN
1	B	154	GLN
1	B	187	GLN
1	B	206	HIS
1	B	216	HIS
1	B	313	ASN
1	C	25	GLN
1	C	45	ASN
1	C	94	ASN
1	C	154	GLN
1	C	187	GLN
1	C	206	HIS
1	C	216	HIS
1	D	25	GLN
1	D	45	ASN
1	D	83	HIS
1	D	154	GLN
1	D	187	GLN
1	D	206	HIS
1	D	216	HIS
1	D	225	GLN
1	D	339	HIS
1	E	25	GLN
1	E	45	ASN
1	E	154	GLN
1	E	187	GLN
1	E	206	HIS
1	E	216	HIS
1	E	249	ASN
1	E	313	ASN
1	F	45	ASN

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Mol	Chain	Res	Type
1	F	83	HIS
1	F	94	ASN
1	F	154	GLN
1	F	187	GLN
1	F	206	HIS
1	F	216	HIS
1	F	348	HIS
1	G	25	GLN
1	G	45	ASN
1	G	187	GLN
1	G	206	HIS
1	G	216	HIS
1	G	220	GLN
1	G	225	GLN
1	H	13	ASN
1	H	25	GLN
1	H	45	ASN
1	H	84	GLN
1	H	154	GLN
1	H	187	GLN
1	H	206	HIS
1	H	249	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PPG	H	8500	-	25,26,26	2.71	9 (36%)	29,35,35	2.88	12 (41%)
2	PPG	A	1500	-	25,26,26	2.88	8 (32%)	29,35,35	2.10	10 (34%)
2	PPG	D	4500	-	25,26,26	2.73	8 (32%)	29,35,35	2.51	13 (44%)
2	PPG	G	7500	-	25,26,26	2.58	7 (28%)	29,35,35	2.28	12 (41%)
2	PPG	C	3500	-	25,26,26	2.75	9 (36%)	29,35,35	2.81	13 (44%)
2	PPG	E	5500	-	25,26,26	2.95	9 (36%)	29,35,35	2.39	12 (41%)
2	PPG	B	2500	-	25,26,26	3.30	9 (36%)	29,35,35	2.71	13 (44%)
2	PPG	F	6500	-	25,26,26	3.09	6 (24%)	29,35,35	2.64	14 (48%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPG	H	8500	-	-	5/20/21/21	0/1/1/1
2	PPG	A	1500	-	-	4/20/21/21	0/1/1/1
2	PPG	D	4500	-	-	5/20/21/21	0/1/1/1
2	PPG	G	7500	-	-	5/20/21/21	0/1/1/1
2	PPG	C	3500	-	-	6/20/21/21	0/1/1/1
2	PPG	E	5500	-	-	8/20/21/21	0/1/1/1
2	PPG	B	2500	-	-	5/20/21/21	0/1/1/1
2	PPG	F	6500	-	-	4/20/21/21	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2500	PPG	C5-C4	10.61	1.55	1.40
2	F	6500	PPG	C5-C4	9.86	1.54	1.40
2	A	1500	PPG	C5-C4	8.35	1.52	1.40
2	D	4500	PPG	C5-C4	7.97	1.51	1.40
2	E	5500	PPG	C5-C4	7.76	1.51	1.40
2	D	4500	PPG	O2B-CBC	7.70	1.41	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7500	PPG	C5-C4	7.47	1.50	1.40
2	F	6500	PPG	O2B-CBC	7.44	1.40	1.22
2	C	3500	PPG	C3-C2	7.39	1.48	1.41
2	A	1500	PPG	O2B-CBC	7.21	1.40	1.22
2	H	8500	PPG	C5-C4	7.19	1.50	1.40
2	E	5500	PPG	O2B-CBC	7.18	1.40	1.22
2	B	2500	PPG	C3-C2	6.99	1.48	1.41
2	G	7500	PPG	O2B-CBC	6.57	1.38	1.22
2	B	2500	PPG	O2B-CBC	6.53	1.38	1.22
2	H	8500	PPG	O2B-CBC	6.34	1.38	1.22
2	A	1500	PPG	C3-C2	6.12	1.47	1.41
2	C	3500	PPG	C5-C4	6.03	1.48	1.40
2	C	3500	PPG	O2B-CBC	5.94	1.37	1.22
2	F	6500	PPG	CAI-CBC	5.22	1.53	1.48
2	E	5500	PPG	C3-C2	5.17	1.46	1.41
2	H	8500	PPG	C3-C2	4.96	1.46	1.41
2	D	4500	PPG	C3-C2	4.28	1.45	1.41
2	F	6500	PPG	C2-N1	4.22	1.41	1.33
2	G	7500	PPG	C2-N1	4.21	1.41	1.33
2	E	5500	PPG	C4A-N4A	-4.09	1.40	1.46
2	H	8500	PPG	CAI-CBC	3.93	1.52	1.48
2	C	3500	PPG	CAI-CBC	3.91	1.52	1.48
2	F	6500	PPG	C3-C2	3.85	1.45	1.41
2	B	2500	PPG	C2-N1	3.83	1.40	1.33
2	E	5500	PPG	CAI-CBC	3.72	1.51	1.48
2	E	5500	PPG	CBI-CGI	3.55	1.44	1.31
2	F	6500	PPG	CBI-CGI	3.52	1.44	1.31
2	B	2500	PPG	CBI-CGI	3.48	1.44	1.31
2	B	2500	PPG	CAI-CBC	3.37	1.51	1.48
2	E	5500	PPG	C2-N1	3.33	1.39	1.33
2	D	4500	PPG	C2-N1	3.25	1.39	1.33
2	A	1500	PPG	C2-N1	3.05	1.39	1.33
2	A	1500	PPG	CBI-CGI	2.97	1.42	1.31
2	G	7500	PPG	C4A-C4	2.93	1.58	1.52
2	D	4500	PPG	C4A-C4	2.92	1.58	1.52
2	H	8500	PPG	CBI-CGI	2.90	1.42	1.31
2	H	8500	PPG	C2-N1	2.87	1.39	1.33
2	C	3500	PPG	C3-C4	2.87	1.44	1.40
2	A	1500	PPG	C5A-C5	2.87	1.58	1.50
2	H	8500	PPG	C3-C4	2.83	1.44	1.40
2	B	2500	PPG	C5A-C5	2.82	1.58	1.50
2	C	3500	PPG	C4A-N4A	-2.76	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3500	PPG	CBI-CGI	2.76	1.41	1.31
2	G	7500	PPG	C3-C2	2.76	1.43	1.41
2	C	3500	PPG	C2-N1	2.75	1.38	1.33
2	D	4500	PPG	CAI-CBC	2.74	1.50	1.48
2	H	8500	PPG	P-OP3	-2.72	1.44	1.54
2	E	5500	PPG	C3-C4	2.71	1.44	1.40
2	G	7500	PPG	CBI-CGI	2.67	1.41	1.31
2	G	7500	PPG	CAI-CBC	-2.62	1.45	1.48
2	H	8500	PPG	C2A-C2	2.41	1.54	1.50
2	A	1500	PPG	CAI-CBC	2.36	1.50	1.48
2	D	4500	PPG	CBI-CGI	2.29	1.40	1.31
2	A	1500	PPG	OET-CEI	2.28	1.50	1.43
2	C	3500	PPG	P-OP3	-2.17	1.46	1.54
2	B	2500	PPG	CBI-CAI	2.11	1.49	1.43
2	D	4500	PPG	C5A-C5	2.08	1.56	1.50
2	E	5500	PPG	P-OP3	-2.07	1.47	1.54
2	B	2500	PPG	C6-C5	2.03	1.41	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8500	PPG	C2A-C2-C3	8.56	130.81	120.80
2	C	3500	PPG	C2A-C2-C3	8.33	130.55	120.80
2	B	2500	PPG	C2A-C2-C3	6.57	128.49	120.80
2	E	5500	PPG	C2A-C2-C3	6.56	128.47	120.80
2	D	4500	PPG	C2A-C2-C3	6.50	128.41	120.80
2	H	8500	PPG	O3B-CBC-CAI	5.86	122.80	113.40
2	F	6500	PPG	C2A-C2-C3	5.65	127.41	120.80
2	B	2500	PPG	O3B-CBC-CAI	5.57	122.34	113.40
2	A	1500	PPG	C2A-C2-C3	5.50	127.24	120.80
2	F	6500	PPG	O3B-CBC-CAI	5.46	122.16	113.40
2	F	6500	PPG	C4A-C4-C5	5.43	125.65	119.76
2	G	7500	PPG	C2A-C2-C3	5.32	127.02	120.80
2	G	7500	PPG	O3B-CBC-CAI	5.06	121.51	113.40
2	C	3500	PPG	CBC-CAI-N4A	-4.99	114.68	122.12
2	H	8500	PPG	C6-N1-C2	4.81	127.91	119.20
2	D	4500	PPG	C4A-C4-C5	4.67	124.82	119.76
2	H	8500	PPG	C3-C2-N1	-4.66	115.08	120.96
2	B	2500	PPG	OP2-P-OP4	-4.56	94.77	106.67
2	C	3500	PPG	O3B-CBC-CAI	4.37	120.42	113.40
2	H	8500	PPG	CBC-CAI-N4A	-4.15	115.92	122.12
2	C	3500	PPG	CEI-OET-CGI	-4.08	101.85	114.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4500	PPG	O3B-CBC-CAI	4.07	119.93	113.40
2	C	3500	PPG	C3-C2-N1	-4.07	115.83	120.96
2	B	2500	PPG	C4A-C4-C5	4.06	124.16	119.76
2	A	1500	PPG	C4A-C4-C5	4.03	124.13	119.76
2	E	5500	PPG	C4A-C4-C5	4.02	124.12	119.76
2	C	3500	PPG	C6-N1-C2	4.02	126.48	119.20
2	F	6500	PPG	C6-N1-C2	4.00	126.45	119.20
2	E	5500	PPG	C6-N1-C2	3.93	126.33	119.20
2	B	2500	PPG	C6-N1-C2	3.84	126.15	119.20
2	D	4500	PPG	C6-N1-C2	3.71	125.92	119.20
2	G	7500	PPG	C4A-C4-C5	3.69	123.76	119.76
2	A	1500	PPG	O3B-CBC-CAI	3.64	119.23	113.40
2	D	4500	PPG	C3-C2-N1	-3.62	116.40	120.96
2	G	7500	PPG	C3-C2-N1	-3.58	116.44	120.96
2	G	7500	PPG	C6-N1-C2	3.56	125.66	119.20
2	H	8500	PPG	CEI-OET-CGI	-3.52	103.61	114.81
2	F	6500	PPG	O3-C3-C4	3.52	128.39	118.18
2	F	6500	PPG	C5-C6-N1	-3.46	118.20	123.83
2	E	5500	PPG	C3-C2-N1	-3.46	116.60	120.96
2	C	3500	PPG	C6-C5-C4	3.39	120.62	118.06
2	F	6500	PPG	O3-C3-C2	-3.30	110.73	117.58
2	A	1500	PPG	C6-N1-C2	3.27	125.12	119.20
2	E	5500	PPG	C6-C5-C4	3.24	120.51	118.06
2	E	5500	PPG	O3B-CBC-CAI	3.21	118.55	113.40
2	B	2500	PPG	O3-C3-C4	3.21	127.48	118.18
2	H	8500	PPG	O3-C3-C4	3.21	127.48	118.18
2	D	4500	PPG	OP2-P-OP4	-3.18	98.37	106.67
2	F	6500	PPG	CEI-OET-CGI	-3.18	104.70	114.81
2	D	4500	PPG	CEI-OET-CGI	-3.15	104.80	114.81
2	G	7500	PPG	C5-C6-N1	-3.14	118.72	123.83
2	B	2500	PPG	C5-C6-N1	-3.11	118.78	123.83
2	C	3500	PPG	O3-C3-C4	3.07	127.10	118.18
2	B	2500	PPG	O3-C3-C2	-3.07	111.22	117.58
2	F	6500	PPG	C3-C2-N1	-3.02	117.15	120.96
2	B	2500	PPG	C3-C2-N1	-2.98	117.20	120.96
2	E	5500	PPG	O3-C3-C4	2.97	126.80	118.18
2	E	5500	PPG	CEI-OET-CGI	-2.97	105.37	114.81
2	D	4500	PPG	O3-C3-C4	2.97	126.79	118.18
2	F	6500	PPG	C6-C5-C4	2.95	120.29	118.06
2	A	1500	PPG	O3-C3-C4	2.93	126.67	118.18
2	A	1500	PPG	C3-C2-N1	-2.92	117.27	120.96
2	D	4500	PPG	O2B-CBC-CAI	-2.90	117.44	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	PPG	CEI-OET-CGI	-2.84	105.78	114.81
2	B	2500	PPG	C6-C5-C4	2.82	120.19	118.06
2	H	8500	PPG	C5-C6-N1	-2.77	119.33	123.83
2	B	2500	PPG	O2B-CBC-CAI	-2.75	117.67	122.02
2	B	2500	PPG	CEI-OET-CGI	-2.68	106.27	114.81
2	G	7500	PPG	CBC-CAI-N4A	-2.65	118.17	122.12
2	D	4500	PPG	O3-C3-C2	-2.63	112.12	117.58
2	E	5500	PPG	C3-C4-C5	-2.63	116.34	118.73
2	D	4500	PPG	C5-C6-N1	-2.62	119.57	123.83
2	G	7500	PPG	C6-C5-C4	2.61	120.04	118.06
2	H	8500	PPG	O3B-CBC-O2B	-2.60	117.71	123.90
2	E	5500	PPG	C5-C6-N1	-2.58	119.63	123.83
2	B	2500	PPG	C3-C4-C5	-2.58	116.39	118.73
2	G	7500	PPG	O3-C3-C4	2.54	125.54	118.18
2	E	5500	PPG	O3B-CBC-O2B	-2.47	118.02	123.90
2	A	1500	PPG	CBC-CAI-N4A	-2.46	118.45	122.12
2	C	3500	PPG	C5-C6-N1	-2.45	119.84	123.83
2	E	5500	PPG	O3-C3-C2	-2.42	112.57	117.58
2	C	3500	PPG	OP2-P-OP4	-2.41	100.38	106.67
2	C	3500	PPG	O2B-CBC-CAI	-2.39	118.25	122.02
2	A	1500	PPG	O3-C3-C2	-2.35	112.71	117.58
2	H	8500	PPG	O3-C3-C2	-2.33	112.76	117.58
2	F	6500	PPG	OP2-P-OP4	-2.30	100.67	106.67
2	G	7500	PPG	CEI-OET-CGI	-2.29	107.52	114.81
2	C	3500	PPG	O3-C3-C2	-2.22	112.98	117.58
2	H	8500	PPG	OP4-C5A-C5	2.21	113.50	109.36
2	D	4500	PPG	C6-C5-C4	2.21	119.73	118.06
2	A	1500	PPG	C5-C6-N1	-2.19	120.27	123.83
2	G	7500	PPG	OP2-P-OP4	-2.17	101.02	106.67
2	G	7500	PPG	O3B-CBC-O2B	-2.17	118.74	123.90
2	C	3500	PPG	C2A-C2-N1	-2.14	113.61	117.64
2	H	8500	PPG	OP2-P-OP4	-2.14	101.09	106.67
2	F	6500	PPG	CBC-CAI-N4A	-2.14	118.93	122.12
2	F	6500	PPG	O2B-CBC-CAI	-2.11	118.69	122.02
2	F	6500	PPG	O3B-CBC-O2B	-2.00	119.13	123.90
2	D	4500	PPG	OP4-C5A-C5	2.00	113.11	109.36

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1500	PPG	CBI-CAI-N4A-C4A

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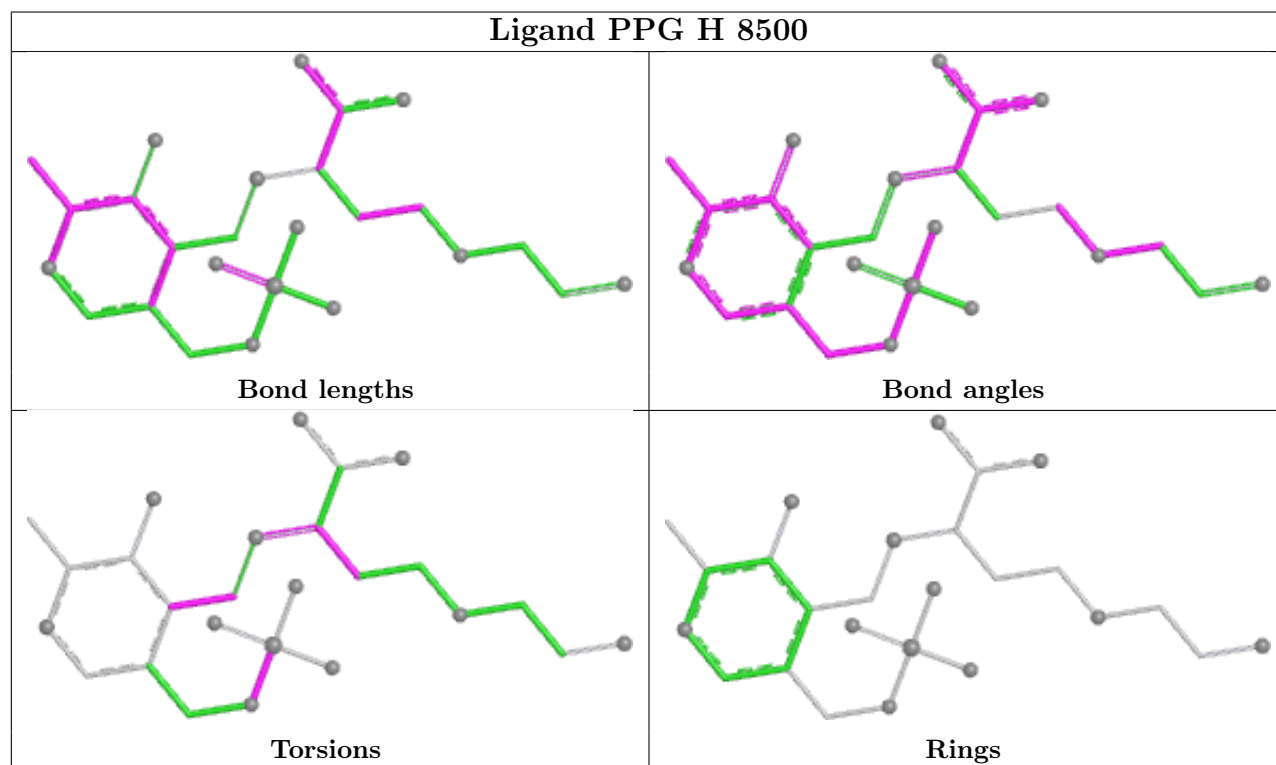
Mol	Chain	Res	Type	Atoms
2	A	1500	PPG	N4A-CAI-CBI-CGI
2	A	1500	PPG	CBC-CAI-CBI-CGI
2	A	1500	PPG	CAI-CBI-CGI-OET
2	B	2500	PPG	C5A-OP4-P-OP1
2	B	2500	PPG	CBI-CAI-N4A-C4A
2	B	2500	PPG	CAI-CBI-CGI-OET
2	C	3500	PPG	CBI-CAI-N4A-C4A
2	C	3500	PPG	N4A-CAI-CBI-CGI
2	C	3500	PPG	CBC-CAI-CBI-CGI
2	C	3500	PPG	CAI-CBI-CGI-OET
2	D	4500	PPG	CBI-CAI-N4A-C4A
2	D	4500	PPG	CAI-CBI-CGI-OET
2	E	5500	PPG	CBI-CAI-N4A-C4A
2	E	5500	PPG	N4A-CAI-CBC-O2B
2	E	5500	PPG	N4A-CAI-CBC-O3B
2	E	5500	PPG	CBI-CAI-CBC-O2B
2	E	5500	PPG	CBI-CAI-CBC-O3B
2	E	5500	PPG	N4A-CAI-CBI-CGI
2	E	5500	PPG	CBC-CAI-CBI-CGI
2	E	5500	PPG	CAI-CBI-CGI-OET
2	F	6500	PPG	CBI-CAI-N4A-C4A
2	F	6500	PPG	CAI-CBI-CGI-OET
2	G	7500	PPG	CBI-CAI-N4A-C4A
2	G	7500	PPG	CAI-CBI-CGI-OET
2	H	8500	PPG	CBI-CAI-N4A-C4A
2	H	8500	PPG	N4A-CAI-CBI-CGI
2	H	8500	PPG	CBC-CAI-CBI-CGI
2	B	2500	PPG	N4A-CAI-CBI-CGI
2	B	2500	PPG	CBC-CAI-CBI-CGI
2	F	6500	PPG	N4A-CAI-CBI-CGI
2	F	6500	PPG	CBC-CAI-CBI-CGI
2	C	3500	PPG	C5-C4-C4A-N4A
2	D	4500	PPG	C5A-OP4-P-OP1
2	H	8500	PPG	C5A-OP4-P-OP1
2	D	4500	PPG	N4A-CAI-CBI-CGI
2	D	4500	PPG	CBC-CAI-CBI-CGI
2	C	3500	PPG	C3-C4-C4A-N4A
2	G	7500	PPG	C6-C5-C5A-OP4
2	H	8500	PPG	C3-C4-C4A-N4A
2	G	7500	PPG	N4A-CAI-CBI-CGI
2	G	7500	PPG	CBC-CAI-CBI-CGI

There are no ring outliers.

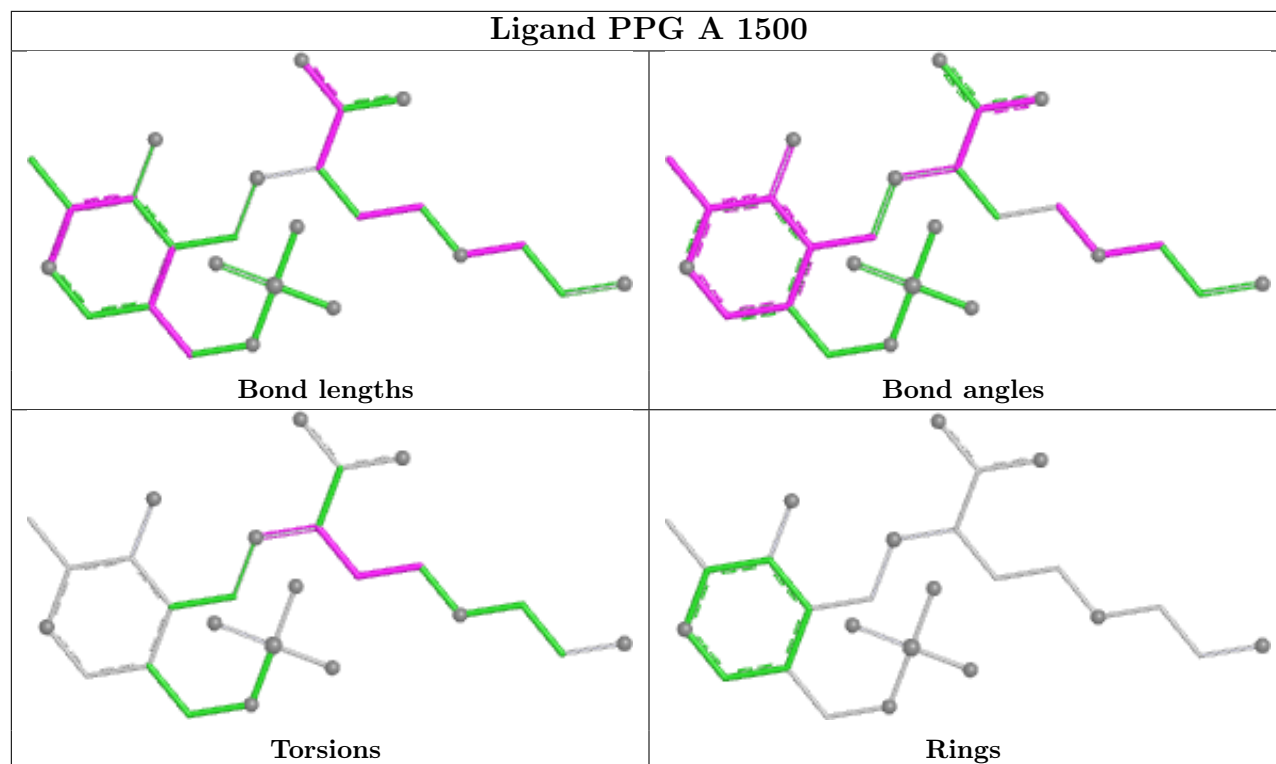
8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	8500	PPG	3	0
2	A	1500	PPG	7	0
2	D	4500	PPG	4	0
2	G	7500	PPG	4	0
2	C	3500	PPG	4	0
2	E	5500	PPG	3	0
2	B	2500	PPG	4	0
2	F	6500	PPG	3	0

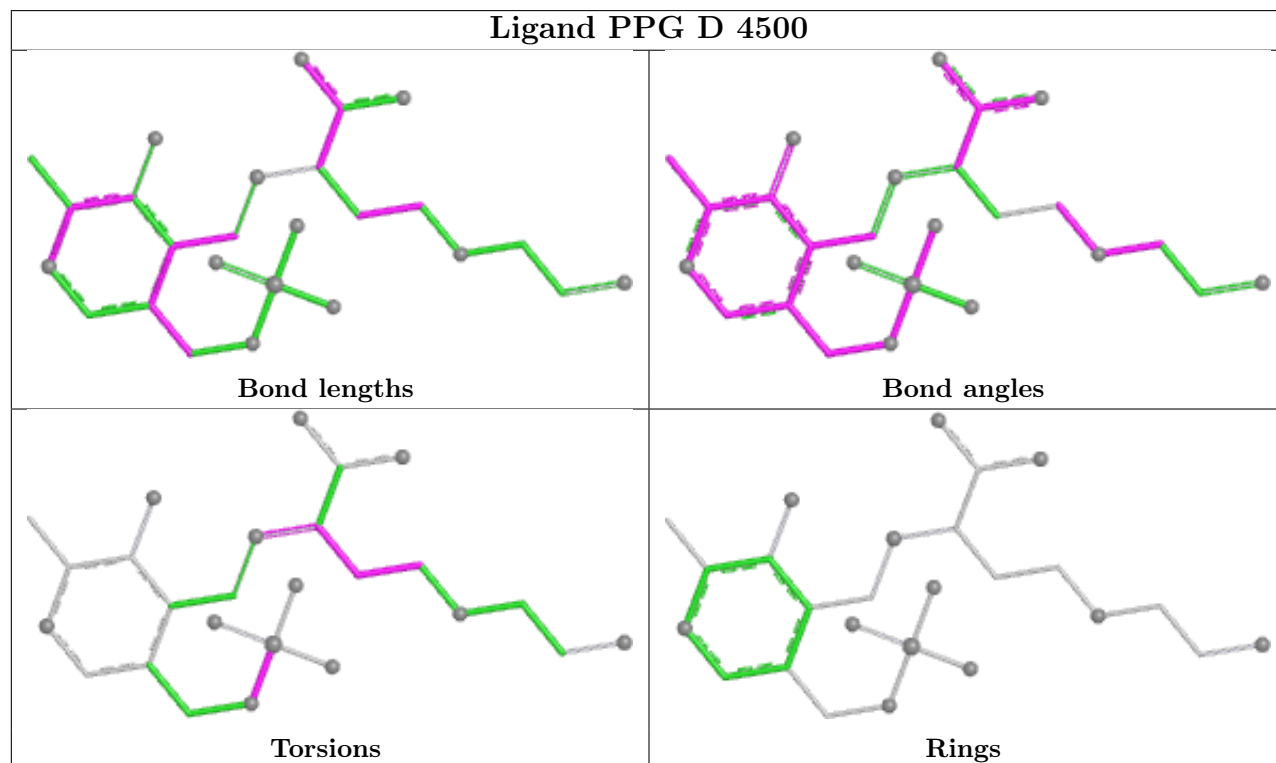
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



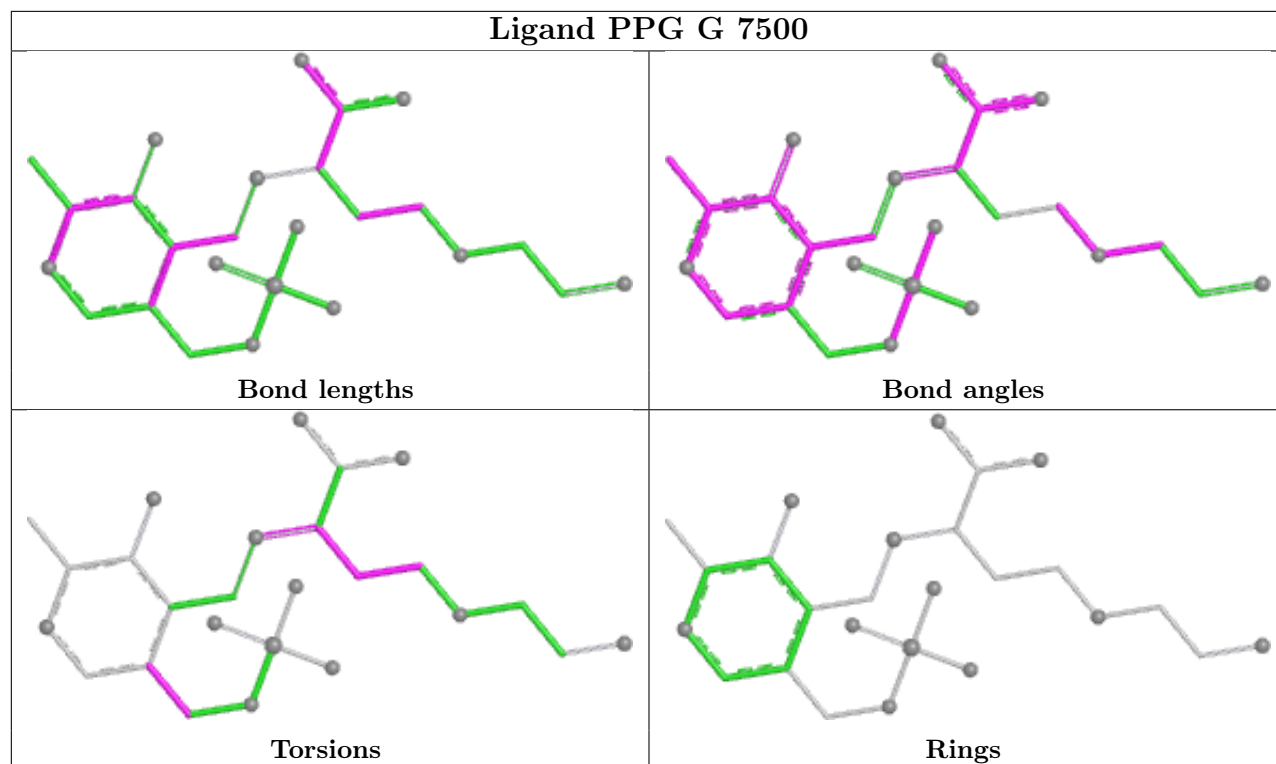
Ligand PPG A 1500



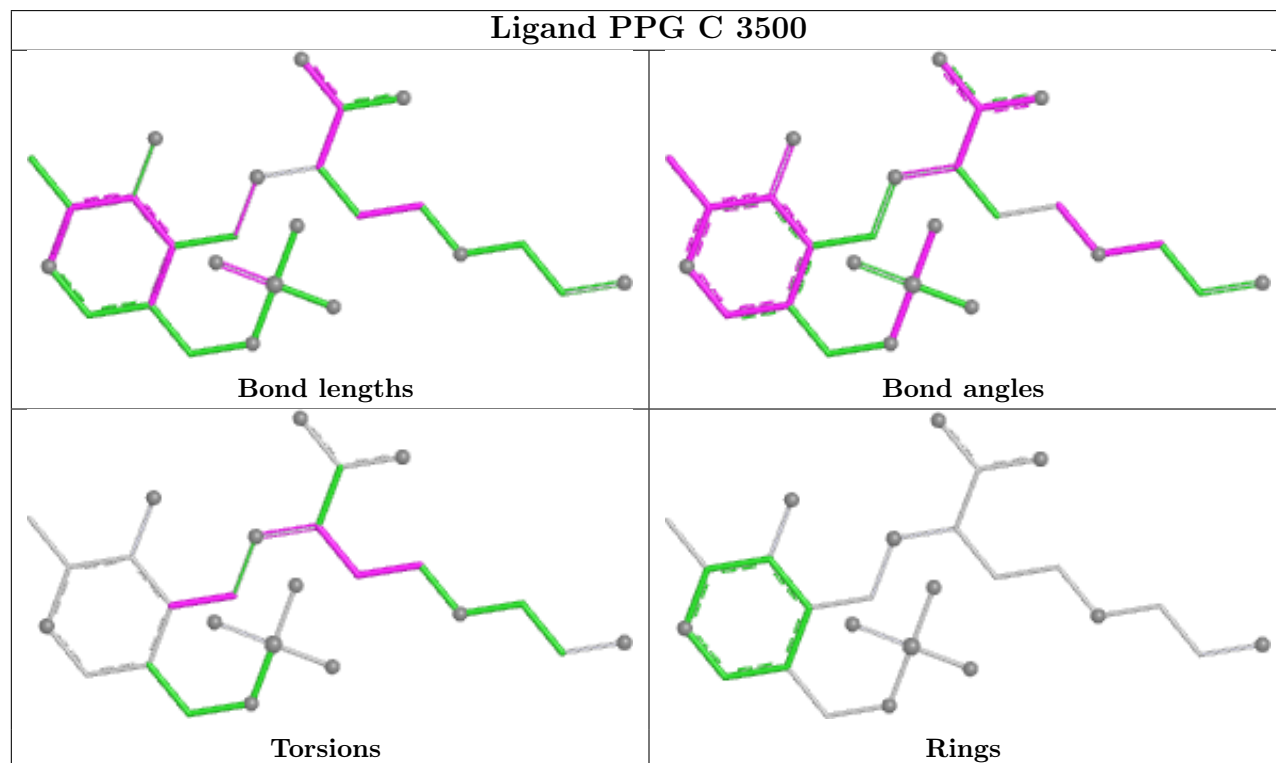
Ligand PPG D 4500



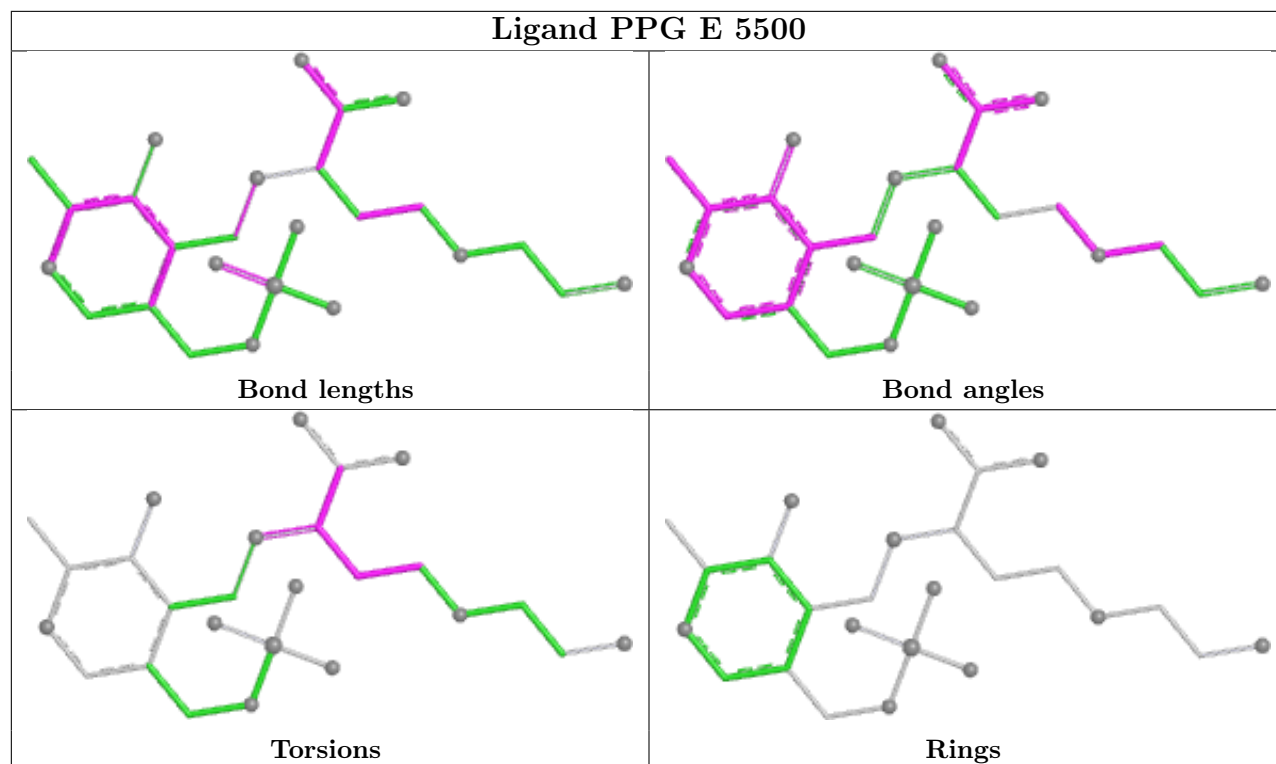
Ligand PPG G 7500



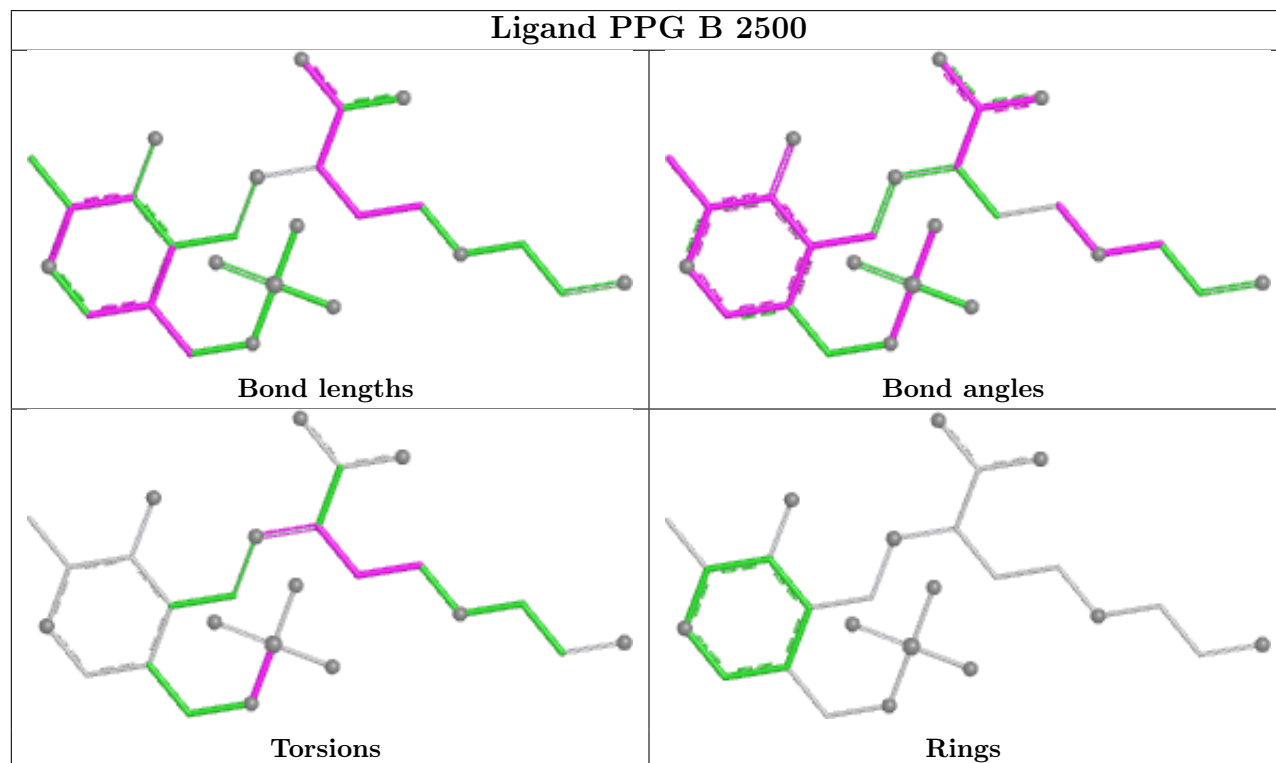
Ligand PPG C 3500

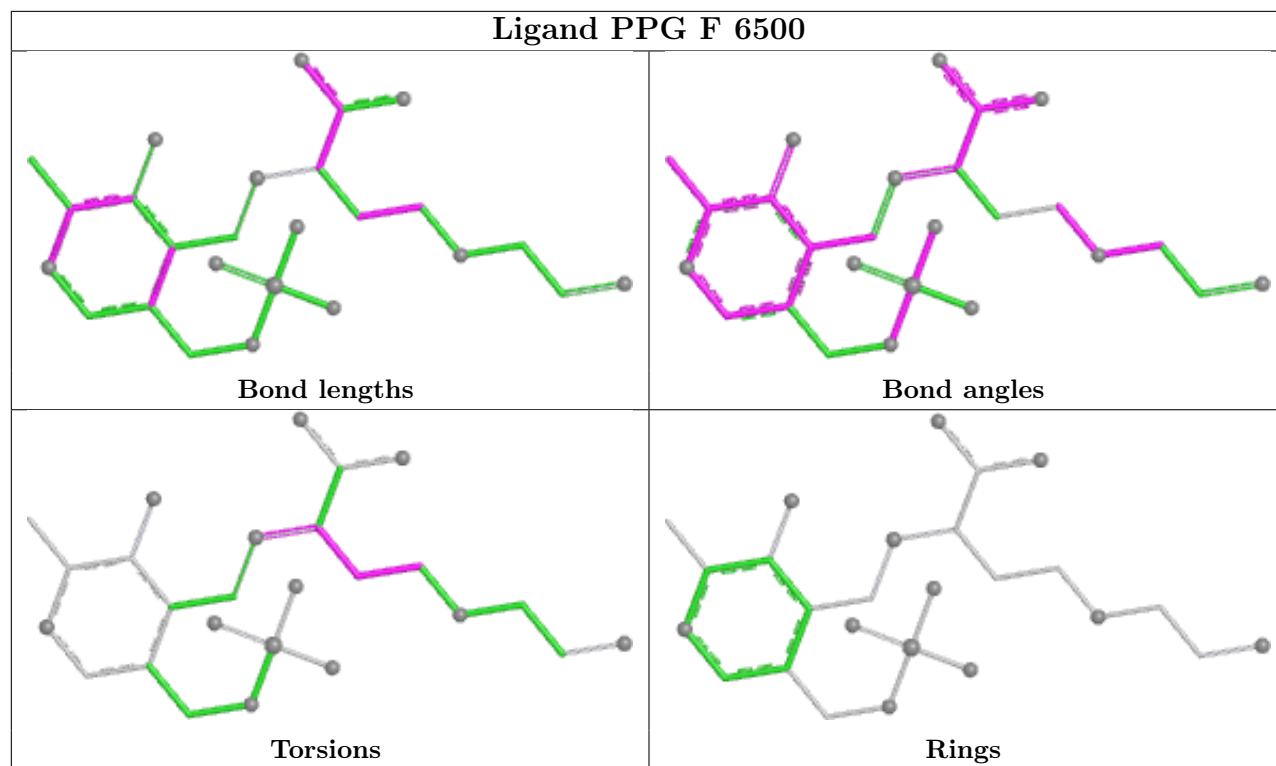


Ligand PPG E 5500



Ligand PPG B 2500





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	394/399 (98%)	-1.73	0 100 100	19, 30, 44, 71	0
1	B	394/399 (98%)	-1.77	0 100 100	12, 23, 36, 70	0
1	C	394/399 (98%)	-1.75	0 100 100	17, 28, 42, 78	0
1	D	394/399 (98%)	-1.71	0 100 100	19, 32, 48, 69	0
1	E	394/399 (98%)	-1.71	0 100 100	18, 32, 48, 64	0
1	F	394/399 (98%)	-1.77	0 100 100	12, 24, 38, 72	0
1	G	394/399 (98%)	-1.70	0 100 100	19, 33, 46, 57	0
1	H	394/399 (98%)	-1.72	0 100 100	16, 30, 47, 74	0
All	All	3152/3192 (98%)	-1.73	0 100 100	12, 29, 45, 78	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

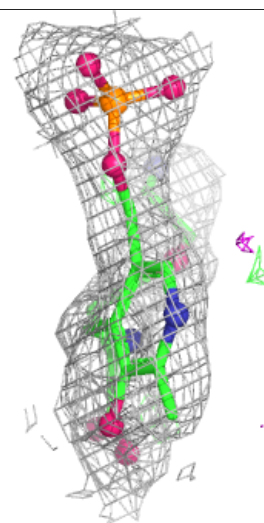
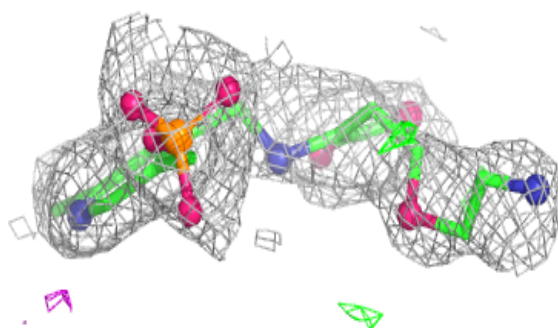
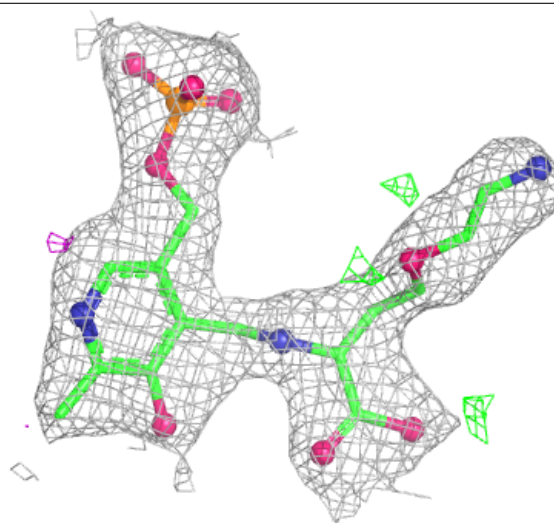
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PPG	A	1500	26/26	0.99	0.03	33,37,50,51	0
2	PPG	C	3500	26/26	0.99	0.03	32,37,54,57	0
2	PPG	D	4500	26/26	0.99	0.03	34,40,49,54	0
2	PPG	E	5500	26/26	0.99	0.03	28,39,52,53	0
2	PPG	G	7500	26/26	0.99	0.04	37,45,56,58	0
2	PPG	F	6500	26/26	1.00	0.02	17,26,44,45	0
2	PPG	B	2500	26/26	1.00	0.02	27,32,47,51	0
2	PPG	H	8500	26/26	1.00	0.03	30,35,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

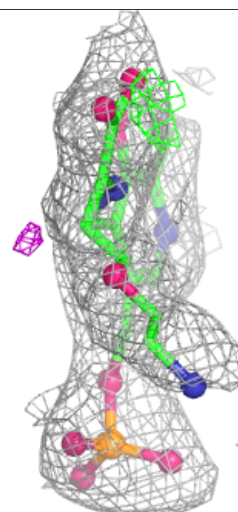
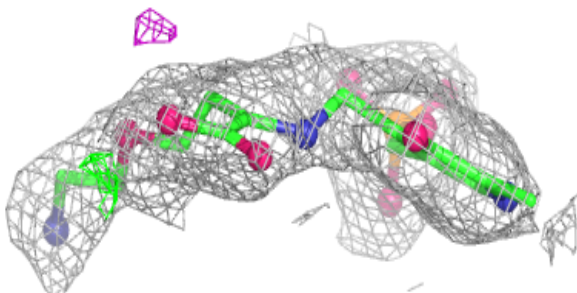
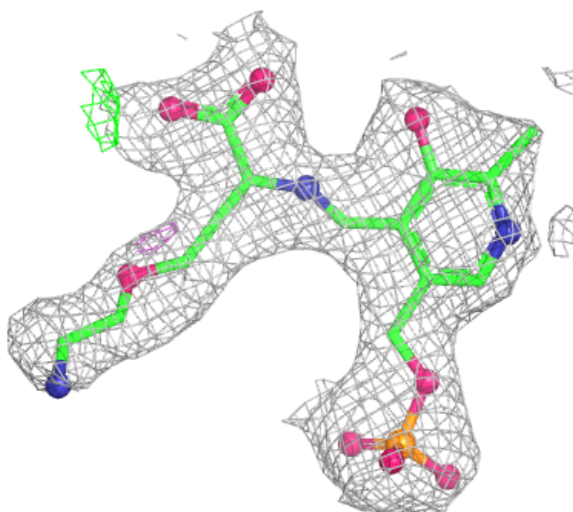
Electron density around PPG A 1500:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



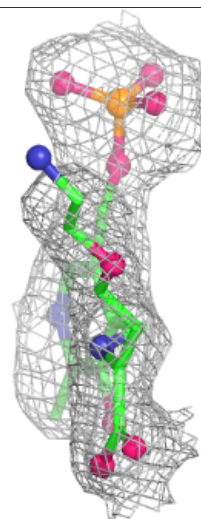
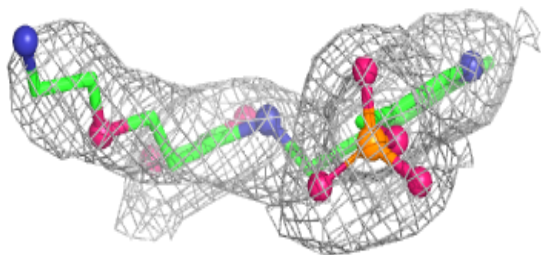
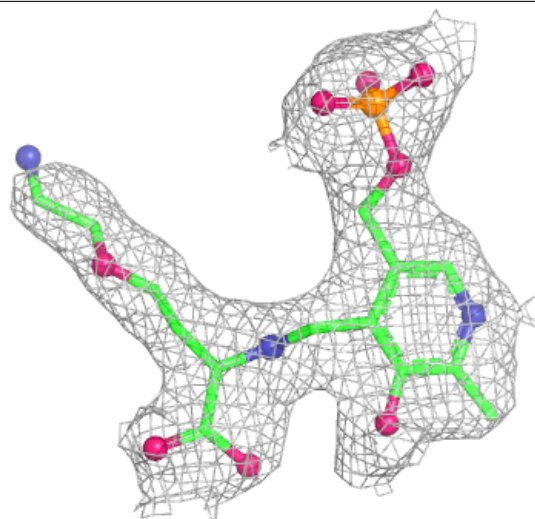
Electron density around PPG C 3500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



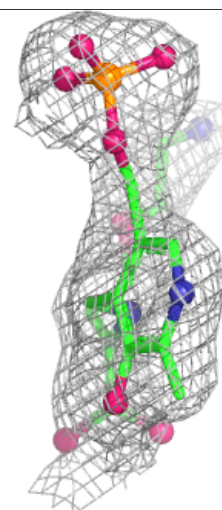
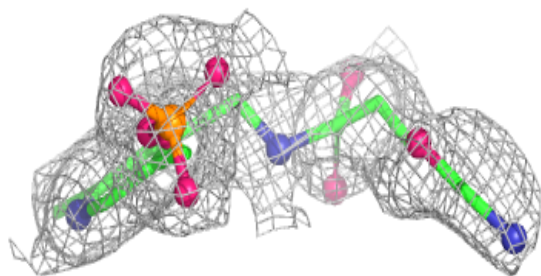
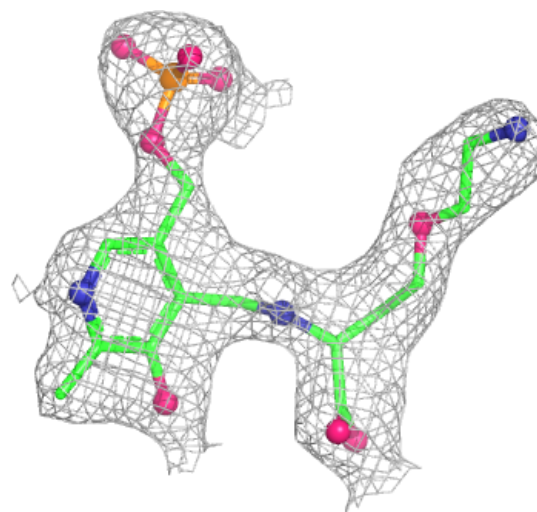
Electron density around PPG D 4500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



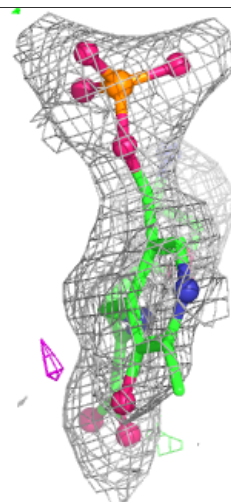
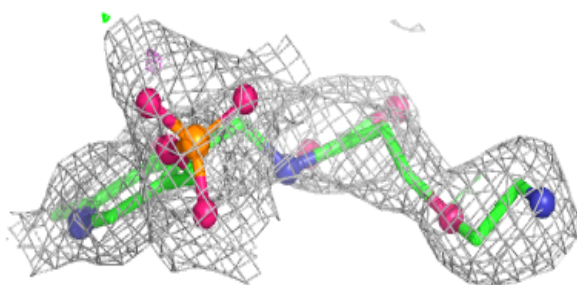
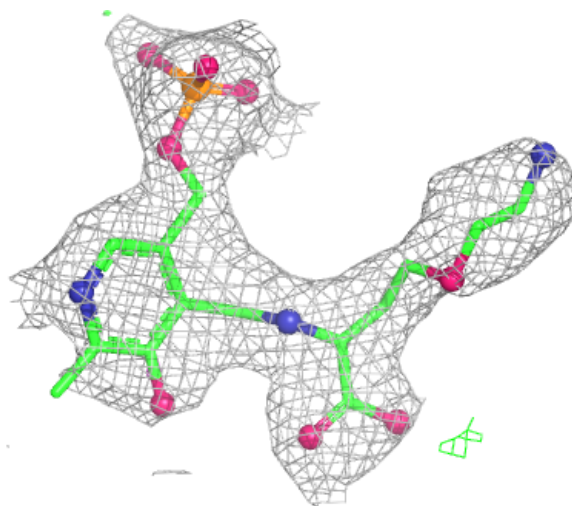
Electron density around PPG E 5500:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



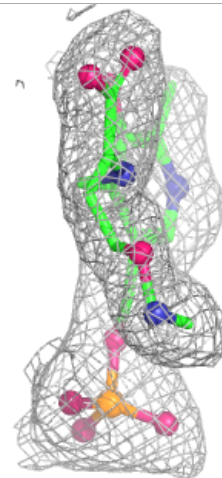
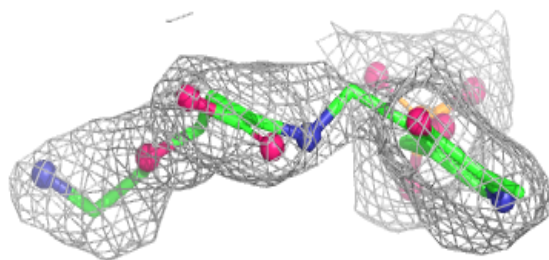
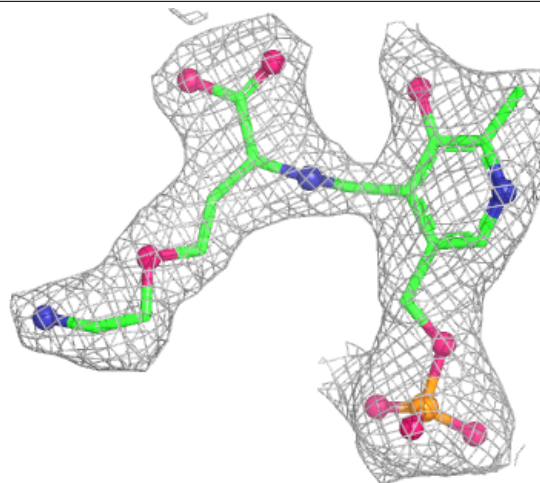
Electron density around PPG G 7500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



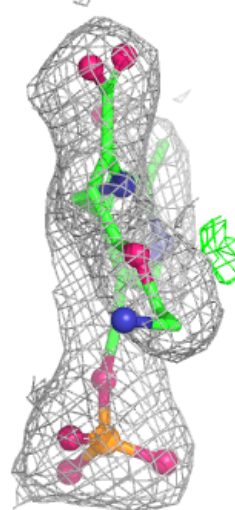
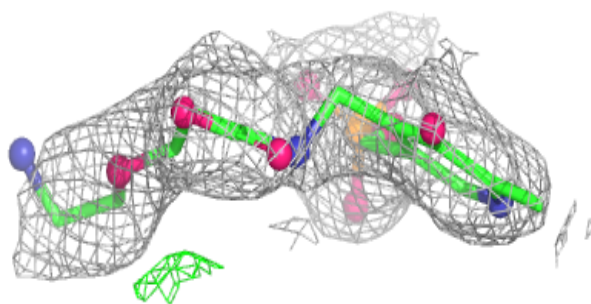
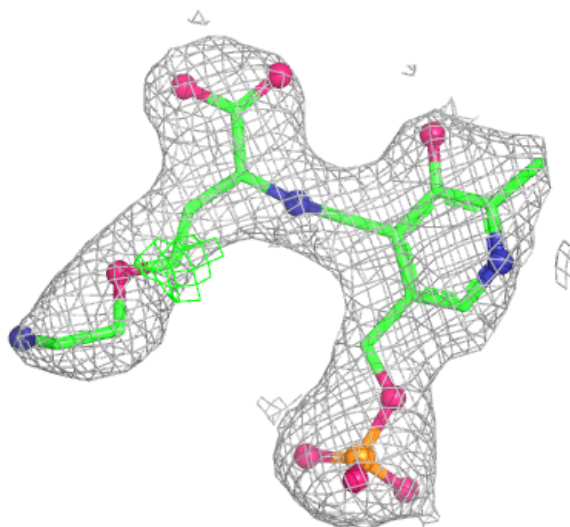
Electron density around PPG F 6500:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



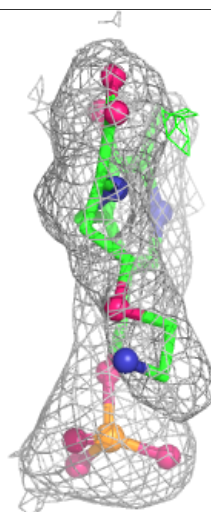
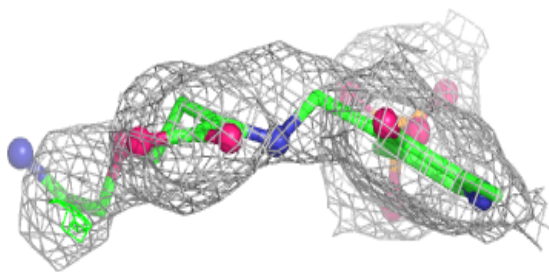
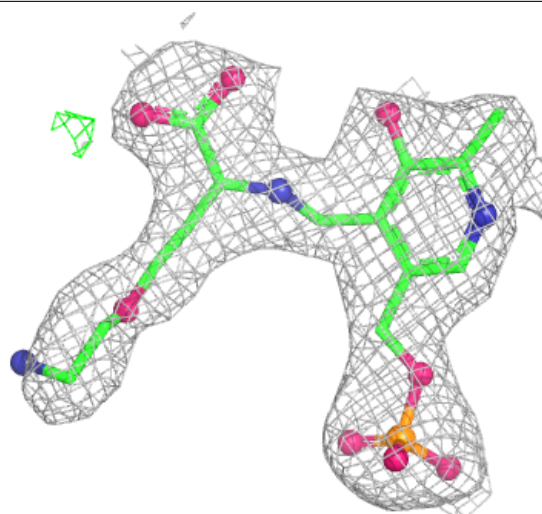
Electron density around PPG B 2500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PPG H 8500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.