



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:38 AM UTC

PDB ID : 3X43 / pdb_00003x43
Title : Crystal structure of O-ureido-L-serine synthase
Authors : Matoba, Y.; Uda, N.; Oda, K.; Sugiyama, M.
Deposited on : 2015-03-13
Resolution : 2.25 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:

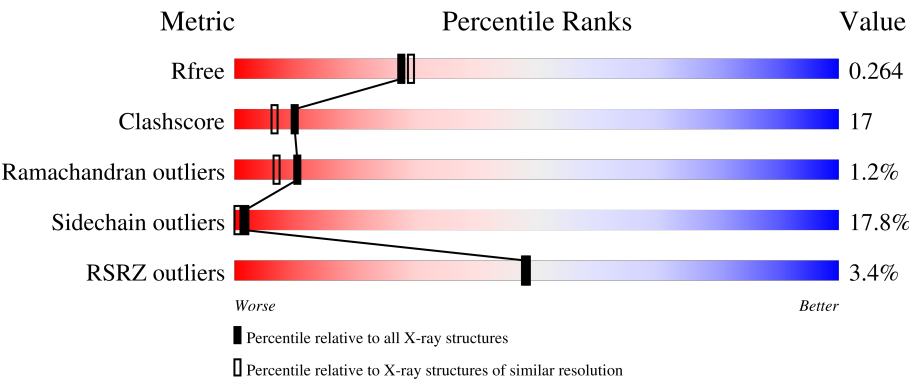
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	332	2% 59%28%7%5%
1	B	332	4% 58%28%11%.
1	C	332	2% 58%29%8%5%
1	D	332	3% 63%26%6%. 5%
1	E	332	5% 55%31%9%5%

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Mol	Chain	Length	Quality of chain
1	F	332	2% 61% 25% 9% 5%
1	G	332	2% 60% 26% 9% 5%
1	H	332	7% 58% 29% 9% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20024 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 O-ureido-L-serine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2381	1502	419	452	8			
1	B	319	Total	C	N	O	S	0	0	0
			2404	1516	422	458	8			
1	C	317	Total	C	N	O	S	0	0	0
			2389	1508	420	453	8			
1	D	316	Total	C	N	O	S	0	0	0
			2381	1502	419	452	8			
1	E	317	Total	C	N	O	S	0	0	0
			2389	1508	420	453	8			
1	F	316	Total	C	N	O	S	0	0	0
			2381	1502	419	452	8			
1	G	317	Total	C	N	O	S	0	0	0
			2389	1508	420	453	8			
1	H	316	Total	C	N	O	S	0	0	0
			2381	1502	419	452	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	LEU	-	expression tag	UNP D2Z027
A	326	GLU	-	expression tag	UNP D2Z027
A	327	HIS	-	expression tag	UNP D2Z027
A	328	HIS	-	expression tag	UNP D2Z027
A	329	HIS	-	expression tag	UNP D2Z027
A	330	HIS	-	expression tag	UNP D2Z027
A	331	HIS	-	expression tag	UNP D2Z027
A	332	HIS	-	expression tag	UNP D2Z027
B	325	LEU	-	expression tag	UNP D2Z027
B	326	GLU	-	expression tag	UNP D2Z027
B	327	HIS	-	expression tag	UNP D2Z027
B	328	HIS	-	expression tag	UNP D2Z027
B	329	HIS	-	expression tag	UNP D2Z027

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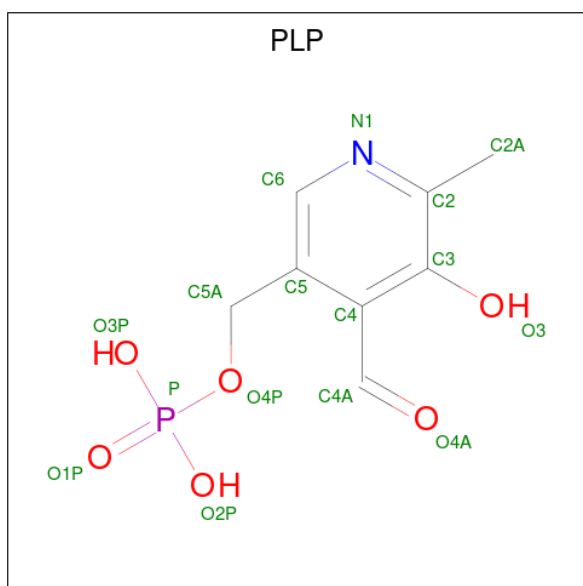
Chain	Residue	Modelled	Actual	Comment	Reference
B	330	HIS	-	expression tag	UNP D2Z027
B	331	HIS	-	expression tag	UNP D2Z027
B	332	HIS	-	expression tag	UNP D2Z027
C	325	LEU	-	expression tag	UNP D2Z027
C	326	GLU	-	expression tag	UNP D2Z027
C	327	HIS	-	expression tag	UNP D2Z027
C	328	HIS	-	expression tag	UNP D2Z027
C	329	HIS	-	expression tag	UNP D2Z027
C	330	HIS	-	expression tag	UNP D2Z027
C	331	HIS	-	expression tag	UNP D2Z027
C	332	HIS	-	expression tag	UNP D2Z027
D	325	LEU	-	expression tag	UNP D2Z027
D	326	GLU	-	expression tag	UNP D2Z027
D	327	HIS	-	expression tag	UNP D2Z027
D	328	HIS	-	expression tag	UNP D2Z027
D	329	HIS	-	expression tag	UNP D2Z027
D	330	HIS	-	expression tag	UNP D2Z027
D	331	HIS	-	expression tag	UNP D2Z027
D	332	HIS	-	expression tag	UNP D2Z027
E	325	LEU	-	expression tag	UNP D2Z027
E	326	GLU	-	expression tag	UNP D2Z027
E	327	HIS	-	expression tag	UNP D2Z027
E	328	HIS	-	expression tag	UNP D2Z027
E	329	HIS	-	expression tag	UNP D2Z027
E	330	HIS	-	expression tag	UNP D2Z027
E	331	HIS	-	expression tag	UNP D2Z027
E	332	HIS	-	expression tag	UNP D2Z027
F	325	LEU	-	expression tag	UNP D2Z027
F	326	GLU	-	expression tag	UNP D2Z027
F	327	HIS	-	expression tag	UNP D2Z027
F	328	HIS	-	expression tag	UNP D2Z027
F	329	HIS	-	expression tag	UNP D2Z027
F	330	HIS	-	expression tag	UNP D2Z027
F	331	HIS	-	expression tag	UNP D2Z027
F	332	HIS	-	expression tag	UNP D2Z027
G	325	LEU	-	expression tag	UNP D2Z027
G	326	GLU	-	expression tag	UNP D2Z027
G	327	HIS	-	expression tag	UNP D2Z027
G	328	HIS	-	expression tag	UNP D2Z027
G	329	HIS	-	expression tag	UNP D2Z027
G	330	HIS	-	expression tag	UNP D2Z027
G	331	HIS	-	expression tag	UNP D2Z027

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Chain	Residue	Modelled	Actual	Comment	Reference
G	332	HIS	-	expression tag	UNP D2Z027
H	325	LEU	-	expression tag	UNP D2Z027
H	326	GLU	-	expression tag	UNP D2Z027
H	327	HIS	-	expression tag	UNP D2Z027
H	328	HIS	-	expression tag	UNP D2Z027
H	329	HIS	-	expression tag	UNP D2Z027
H	330	HIS	-	expression tag	UNP D2Z027
H	331	HIS	-	expression tag	UNP D2Z027
H	332	HIS	-	expression tag	UNP D2Z027

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

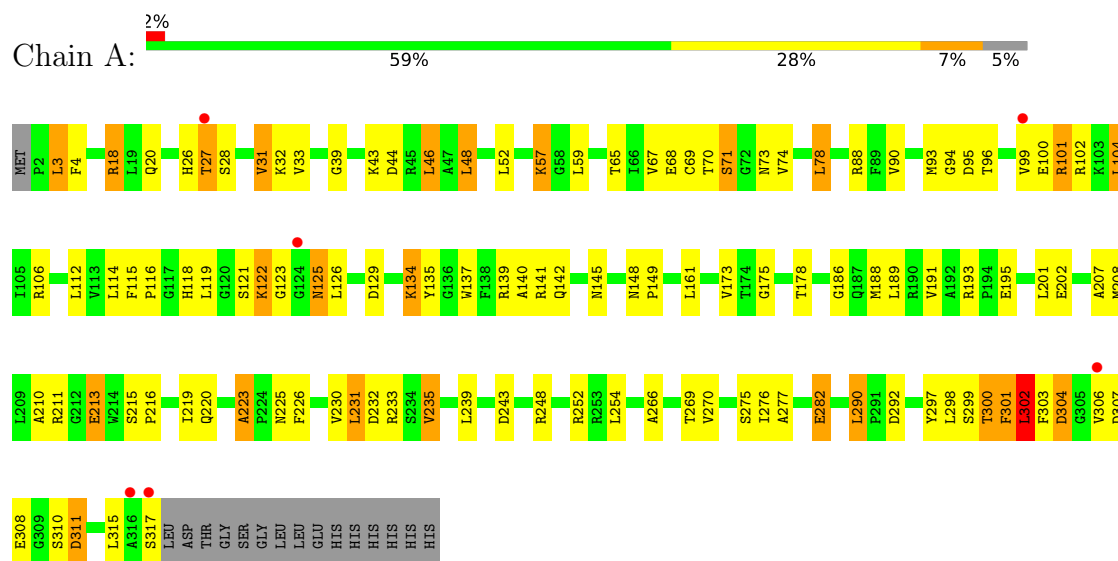
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	B	102	Total	O	0	0
			102	102		
3	C	96	Total	O	0	0
			96	96		
3	D	114	Total	O	0	0
			114	114		
3	E	106	Total	O	0	0
			106	106		
3	F	98	Total	O	0	0
			98	98		
3	G	97	Total	O	0	0
			97	97		
3	H	85	Total	O	0	0
			85	85		

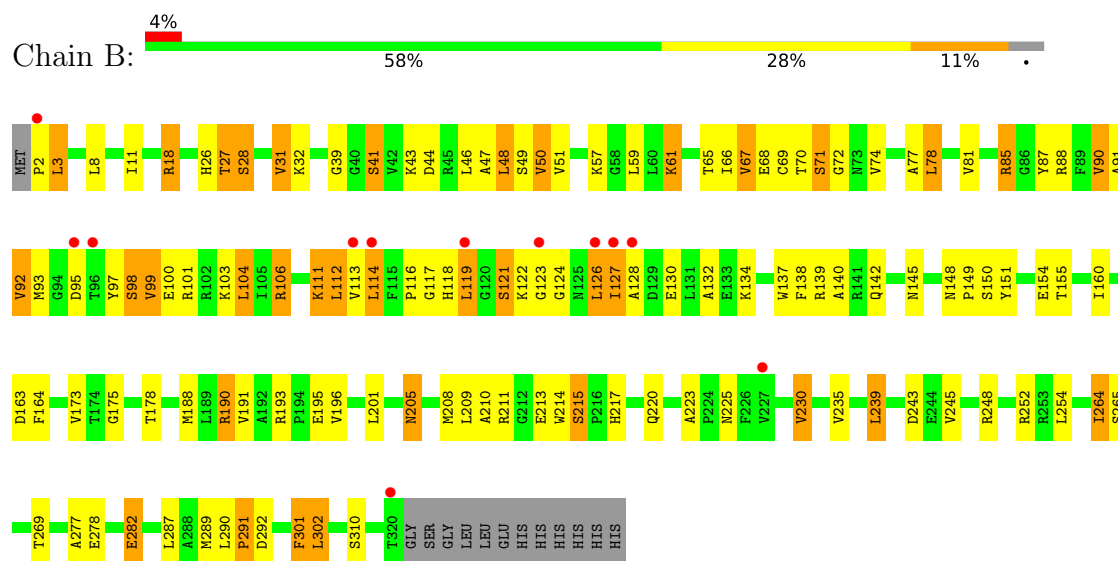
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

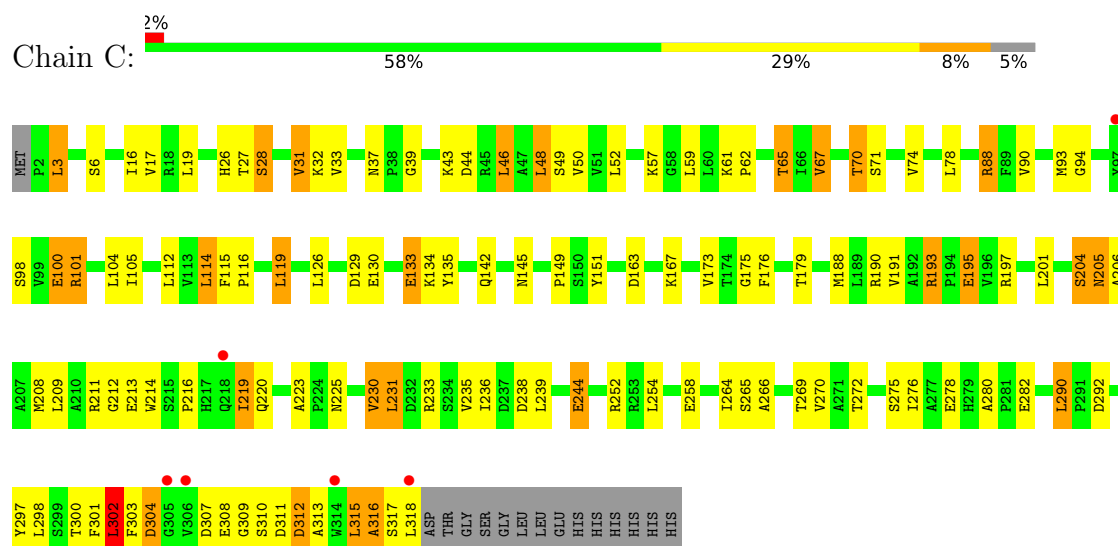
• Molecule 1: O-ureido-L-serine synthase



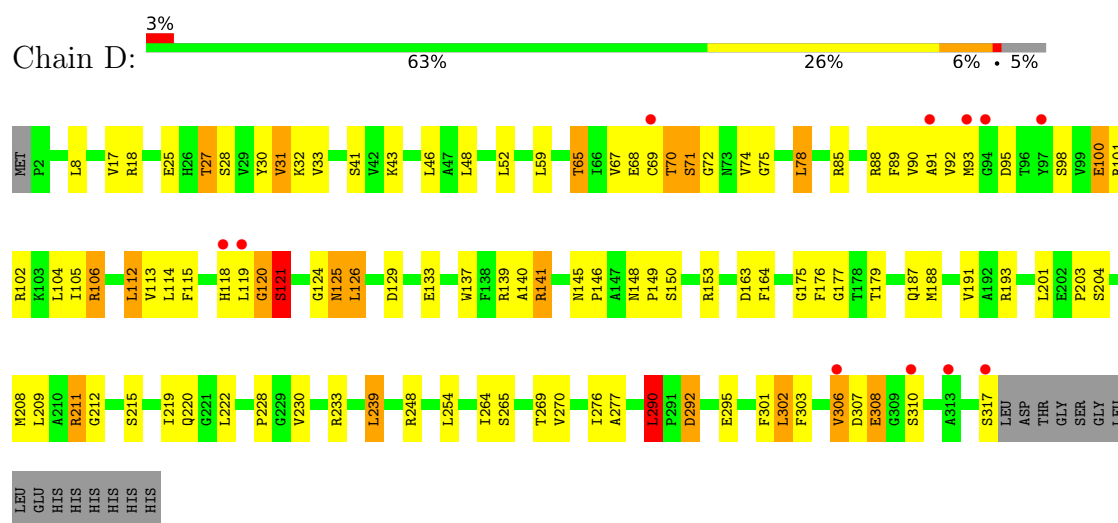
• Molecule 1: O-ureido-L-serine synthase



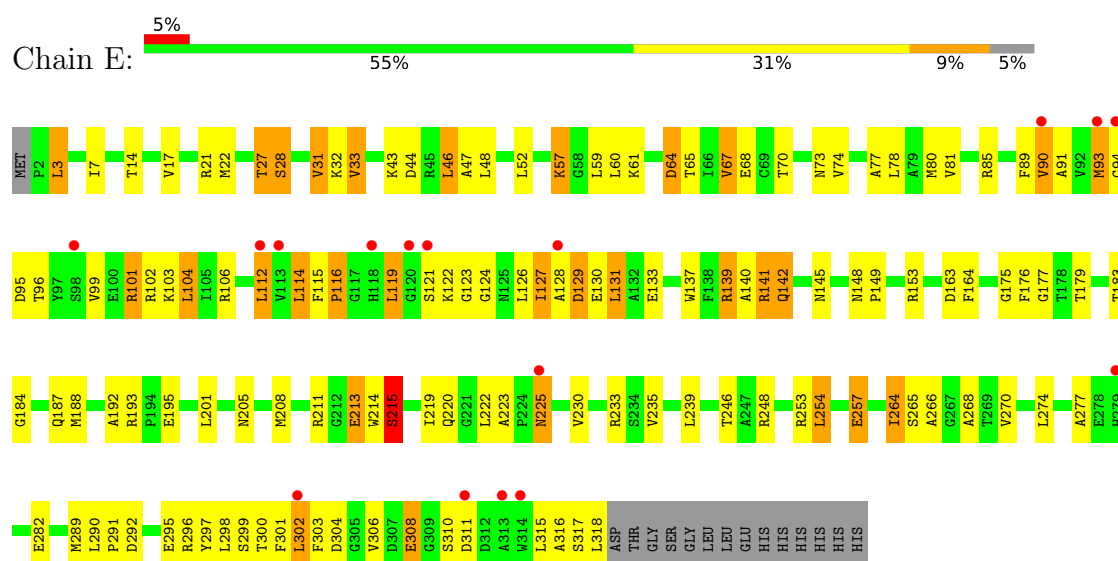
• Molecule 1: O-ureido-L-serine synthase



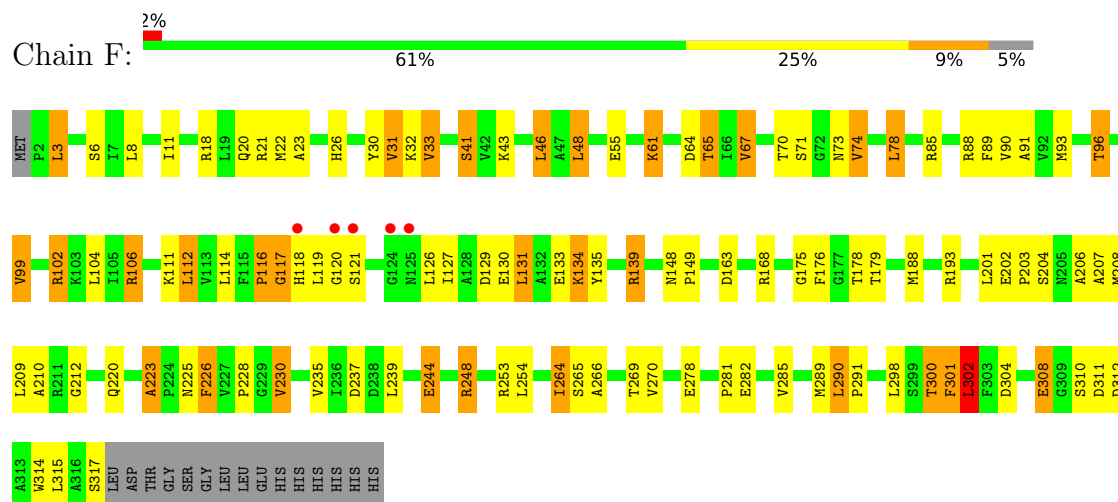
• Molecule 1: O-ureido-L-serine synthase



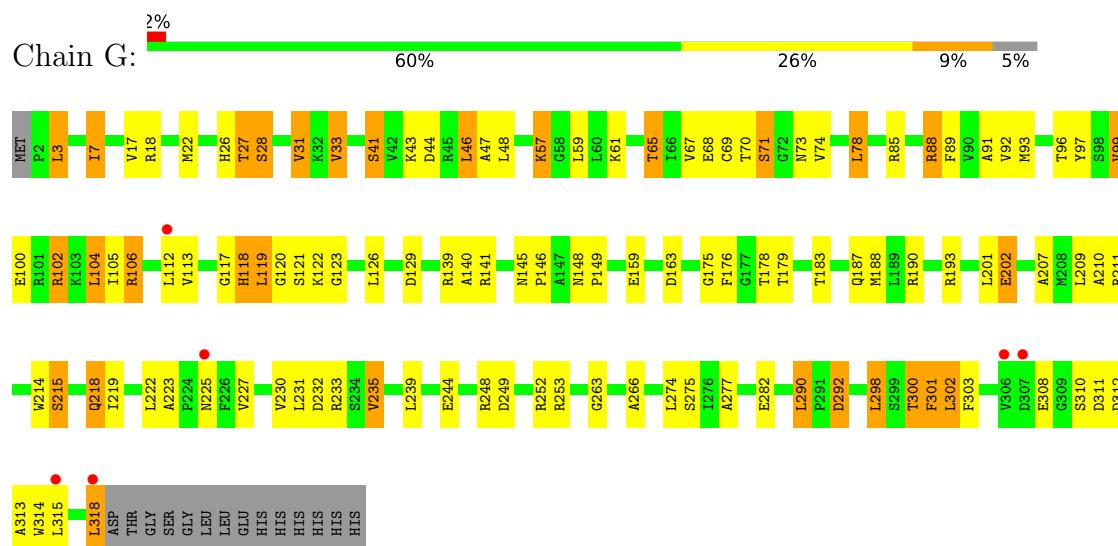
• Molecule 1: O-ureido-L-serine synthase



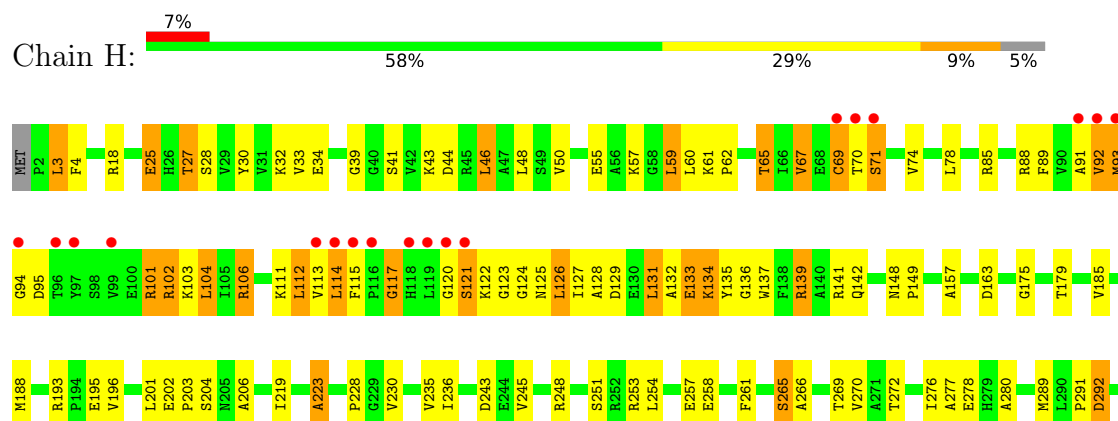
• Molecule 1: O-ureido-L-serine synthase



• Molecule 1: O-ureido-L-serine synthase



• Molecule 1: O-ureido-L-serine synthase



E295	E296	Y297	L298	S299	T300	F301	L302	F303	D304	G305	V306	D307	E308	G309	S310	D311	D312	A313	W314	L315	A316	S317	LEU	ASP	THR	GLY	SER	GLY	GLY	LEU	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.48Å 154.13Å 118.52Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	29.83 – 2.25 29.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.83-2.25) 99.9 (29.83-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.24Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.264 0.209 , 0.264	Depositor DCC
R_{free} test set	6181 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20024	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3181e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PLP

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	0.43	0/2427	0.94	11/3295 (0.3%)
1	B	0.41	0/2450	0.90	7/3327 (0.2%)
1	C	0.42	0/2435	0.92	6/3306 (0.2%)
1	D	0.46	0/2427	0.93	6/3295 (0.2%)
1	E	0.40	0/2435	0.90	5/3306 (0.2%)
1	F	0.47	0/2427	0.94	11/3295 (0.3%)
1	G	0.40	0/2435	0.92	7/3306 (0.2%)
1	H	0.42	0/2427	0.91	7/3295 (0.2%)
All	All	0.42	0/19463	0.92	60/26425 (0.2%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	175	GLY	N-CA-C	-8.08	99.81	112.58
1	F	175	GLY	N-CA-C	-7.67	102.06	112.57
1	G	33	VAL	N-CA-C	7.15	116.92	106.55
1	H	175	GLY	N-CA-C	-7.09	102.86	112.57
1	E	292	ASP	N-CA-C	6.92	117.73	108.38
1	D	71	SER	N-CA-C	-6.86	104.22	114.64
1	D	292	ASP	N-CA-C	6.82	118.15	108.74
1	B	291	PRO	N-CA-C	6.75	122.76	113.65
1	G	73	ASN	N-CA-C	6.66	119.38	111.33
1	A	101	ARG	N-CA-C	-6.63	105.00	113.23
1	C	292	ASP	N-CA-C	6.42	117.05	108.38
1	D	175	GLY	N-CA-C	-6.36	103.86	112.57
1	G	290	LEU	CA-C-N	6.29	125.79	119.24
1	G	290	LEU	C-N-CA	6.29	125.79	119.24
1	F	290	LEU	CA-C-N	6.23	125.72	119.24
1	F	290	LEU	C-N-CA	6.23	125.72	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	175	GLY	N-CA-C	-6.21	102.77	112.58
1	B	175	GLY	N-CA-C	-6.19	102.80	112.58
1	C	290	LEU	CA-C-N	6.19	127.58	119.84
1	C	290	LEU	C-N-CA	6.19	127.58	119.84
1	C	175	GLY	N-CA-C	-6.12	104.19	112.57
1	H	302	LEU	N-CA-C	-6.11	104.17	111.69
1	A	302	LEU	N-CA-C	-6.08	104.77	111.82
1	B	3	LEU	N-CA-C	-6.04	101.34	110.28
1	F	33	VAL	N-CA-C	5.92	115.14	106.55
1	B	173	VAL	N-CA-C	5.84	116.35	108.17
1	A	223	ALA	N-CA-C	5.80	122.64	109.81
1	F	237	ASP	N-CA-C	-5.80	106.25	113.55
1	A	175	GLY	N-CA-C	-5.74	103.80	112.41
1	B	178	THR	N-CA-C	-5.73	106.29	113.28
1	E	246	THR	N-CA-C	-5.67	105.18	111.36
1	G	44	ASP	N-CA-C	-5.67	105.19	111.71
1	A	73	ASN	N-CA-C	5.60	117.06	111.07
1	A	292	ASP	N-CA-C	5.60	116.47	108.74
1	B	264	ILE	N-CA-C	5.55	115.75	110.53
1	C	173	VAL	N-CA-C	5.54	115.92	108.17
1	G	292	ASP	N-CA-C	5.53	116.38	108.74
1	C	302	LEU	N-CA-C	-5.53	105.80	112.54
1	H	33	VAL	N-CA-C	5.51	114.54	106.55
1	F	178	THR	N-CA-C	-5.46	106.46	113.23
1	E	73	ASN	N-CA-C	5.42	117.89	111.33
1	B	71	SER	N-CA-C	-5.40	106.19	112.89
1	D	290	LEU	CA-C-N	5.40	124.85	119.24
1	D	290	LEU	C-N-CA	5.40	124.85	119.24
1	E	177	GLY	N-CA-C	-5.32	100.56	113.18
1	A	71	SER	N-CA-C	-5.32	106.84	113.38
1	A	173	VAL	N-CA-C	5.30	115.59	108.17
1	H	204	SER	N-CA-C	5.30	117.47	111.11
1	F	223	ALA	N-CA-C	5.28	121.48	109.81
1	A	231	LEU	N-CA-C	5.27	117.09	110.24
1	F	302	LEU	N-CA-C	-5.26	106.82	113.18
1	H	236	ILE	N-CA-C	5.25	115.83	108.89
1	A	178	THR	N-CA-C	-5.25	106.72	113.23
1	H	292	ASP	N-CA-C	5.25	115.98	108.74
1	F	73	ASN	N-CA-C	5.20	116.94	111.28
1	H	223	ALA	N-CA-C	5.14	121.17	109.81
1	A	191	VAL	N-CA-C	5.12	115.34	110.42
1	F	264	ILE	N-CA-C	5.11	115.88	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	23	ALA	N-CA-C	5.10	117.32	110.29
1	D	177	GLY	N-CA-C	-5.02	101.28	113.18

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	2381	0	2374	79	0
1	B	2404	0	2396	101	0
1	C	2389	0	2385	92	0
1	D	2381	0	2374	91	0
1	E	2389	0	2385	106	0
1	F	2381	0	2374	74	0
1	G	2389	0	2385	86	0
1	H	2381	0	2374	84	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
2	E	15	0	6	0	0
2	F	15	0	6	0	0
2	G	15	0	6	0	0
2	H	15	0	6	0	0
3	A	111	0	0	2	0
3	B	102	0	0	1	0
3	C	96	0	0	6	0
3	D	114	0	0	2	0
3	E	106	0	0	0	0
3	F	98	0	0	1	0
3	G	97	0	0	1	0
3	H	85	0	0	1	0
All	All	20024	0	19095	665	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 17.

All (665) 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:A:57:LYS:HB3	1:A:59:LEU:HD13	1.30	1.07
1:B:114:LEU:H	1:C:310:SER:HB2	1.21	1.06
1:D:68:GLU:HA	1:D:139:ARG:HH21	1.17	1.04
1:B:67:VAL:HG12	1:B:90:VAL:HB	1.44	0.95
1:F:26:HIS:HB2	1:F:282:GLU:HG2	1.48	0.94
1:A:300:THR:HG22	1:A:302:LEU:H	1.32	0.92
1:E:214:TRP:O	1:E:215:SER:HB3	1.69	0.91
1:D:67:VAL:HG12	1:D:90:VAL:HB	1.53	0.90
1:B:31:VAL:HG22	1:B:290:LEU:HD13	1.53	0.90
1:E:67:VAL:HG13	1:E:90:VAL:HB	1.52	0.90
1:A:67:VAL:HG12	1:A:90:VAL:HB	1.51	0.89
1:C:116:PRO:HB2	1:C:119:LEU:HD23	1.56	0.88
1:H:93:MET:HE3	1:H:112:LEU:HB3	1.56	0.87
1:H:69:CYS:HB2	1:H:125:ASN:HD21	1.39	0.86
1:B:57:LYS:HB3	1:B:59:LEU:HD13	1.58	0.86
1:E:116:PRO:HB2	1:E:119:LEU:HD23	1.58	0.85
1:C:129:ASP:O	1:C:133:GLU:HG2	1.76	0.85
1:A:27:THR:HG21	1:A:277:ALA:HB1	1.58	0.85
1:H:300:THR:HG22	1:H:301:PHE:H	1.41	0.84
1:B:210:ALA:HB2	1:B:239:LEU:HD13	1.60	0.83
1:D:208:MET:HE3	1:D:212:GLY:HA2	1.58	0.83
1:G:248:ARG:HG2	1:G:302:LEU:HD23	1.57	0.83
1:D:70:THR:HG21	1:D:75:GLY:H	1.42	0.82
1:G:300:THR:HG22	1:G:302:LEU:H	1.46	0.81
1:H:65:THR:HB	1:H:88:ARG:HB3	1.62	0.80
1:C:31:VAL:HG13	1:C:290:LEU:HD22	1.64	0.78
1:D:93:MET:HE1	1:D:102:ARG:HA	1.66	0.78
1:B:124:GLY:HA2	1:B:127:ILE:HG22	1.66	0.77
1:D:95:ASP:HA	1:D:114:LEU:HD22	1.64	0.77
1:F:3:LEU:HD13	1:G:163:ASP:HB3	1.67	0.76
1:A:70:THR:O	1:A:93:MET:HG3	1.87	0.74
1:G:57:LYS:HB3	1:G:59:LEU:HD13	1.68	0.74
1:H:70:THR:OG1	1:H:93:MET:HB3	1.86	0.74
1:E:300:THR:HG22	1:E:301:PHE:H	1.52	0.74
1:A:3:LEU:HD13	1:D:163:ASP:HB3	1.67	0.74
1:A:67:VAL:HG11	1:A:137:TRP:CE3	2.22	0.74
1:H:43:LYS:HE2	1:H:74:VAL:HG23	1.70	0.74
1:B:3:LEU:HD13	1:C:163:ASP:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:LEU:HD23	1:G:123:GLY:HA3	1.70	0.73
1:C:190:ARG:HD2	3:C:506:HOH:O	1.87	0.73
1:B:116:PRO:HG2	1:B:119:LEU:HD12	1.70	0.73
1:C:65:THR:HB	1:C:88:ARG:HB3	1.68	0.73
1:G:31:VAL:HG13	1:G:290:LEU:HD22	1.70	0.73
1:B:114:LEU:N	1:C:310:SER:HB2	2.01	0.73
1:E:31:VAL:HG13	1:E:290:LEU:HD22	1.71	0.72
1:E:163:ASP:HB3	1:H:3:LEU:HD13	1.71	0.72
1:C:74:VAL:HG21	1:C:142:GLN:OE1	1.89	0.72
1:F:207:ALA:HB1	1:F:210:ALA:HB3	1.72	0.72
1:D:68:GLU:HA	1:D:139:ARG:NH2	2.00	0.72
1:E:31:VAL:CG1	1:E:290:LEU:HD22	2.20	0.72
1:G:300:THR:CG2	1:G:302:LEU:H	2.02	0.72
1:H:70:THR:HG21	1:H:91:ALA:HB1	1.72	0.71
1:F:31:VAL:HG13	1:F:290:LEU:HD22	1.72	0.71
1:D:69:CYS:HB3	1:D:125:ASN:HD22	1.55	0.71
1:D:31:VAL:HG22	1:D:290:LEU:HD13	1.73	0.71
1:C:254:LEU:HD11	1:C:270:VAL:HG21	1.73	0.70
1:F:65:THR:HB	1:F:88:ARG:HD2	1.71	0.70
1:C:116:PRO:O	1:C:119:LEU:HB2	1.91	0.70
1:A:67:VAL:HG11	1:A:137:TRP:HE3	1.57	0.70
1:F:135:TYR:OH	1:G:318:LEU:HG	1.92	0.70
1:G:231:LEU:HD12	1:G:232:ASP:N	2.07	0.70
1:A:68:GLU:OE2	1:A:140:ALA:HB3	1.90	0.70
1:E:68:GLU:OE2	1:E:140:ALA:HB3	1.92	0.70
1:B:99:VAL:O	1:B:103:LYS:HG3	1.91	0.70
1:A:26:HIS:HB2	1:A:282:GLU:HG2	1.71	0.70
1:C:188:MET:HE3	1:D:188:MET:HE3	1.74	0.69
1:G:231:LEU:HD12	1:G:232:ASP:H	1.56	0.69
1:A:31:VAL:HG22	1:A:290:LEU:HD13	1.74	0.69
1:H:300:THR:HG22	1:H:301:PHE:N	2.07	0.69
1:A:311:ASP:CG	1:D:106:ARG:HH22	2.01	0.69
1:F:70:THR:O	1:F:93:MET:HG2	1.92	0.69
1:A:31:VAL:HG13	1:A:290:LEU:HD22	1.76	0.68
1:C:31:VAL:CG1	1:C:290:LEU:HD22	2.24	0.68
1:A:149:PRO:HG3	1:A:230:VAL:HG13	1.75	0.67
1:E:298:LEU:HA	1:E:303:PHE:CD1	2.28	0.67
1:B:67:VAL:CG1	1:B:90:VAL:HB	2.24	0.67
1:F:129:ASP:O	1:F:133:GLU:HG2	1.93	0.67
1:D:70:THR:HG21	1:D:75:GLY:N	2.09	0.67
1:C:43:LYS:HE2	1:C:74:VAL:CG2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:HIS:HB2	1:B:282:GLU:HG2	1.77	0.66
1:E:77:ALA:O	1:E:81:VAL:HG23	1.95	0.66
1:B:106:ARG:NH2	1:B:112:LEU:H	1.94	0.66
1:C:31:VAL:HG22	1:C:290:LEU:HD13	1.77	0.66
1:C:43:LYS:HE2	1:C:74:VAL:HG23	1.78	0.66
1:A:122:LYS:HB2	1:A:225:ASN:HD21	1.58	0.66
1:D:254:LEU:HD11	1:D:270:VAL:HG21	1.75	0.66
1:H:92:VAL:HG21	1:H:128:ALA:HB2	1.75	0.66
1:E:310:SER:HB2	1:H:114:LEU:HG	1.77	0.66
1:G:311:ASP:O	1:G:313:ALA:N	2.28	0.65
1:B:43:LYS:HE2	1:B:74:VAL:CG2	2.25	0.65
1:G:300:THR:HG23	1:G:301:PHE:N	2.09	0.65
1:D:65:THR:HB	1:D:88:ARG:HB3	1.78	0.65
1:E:43:LYS:HE2	1:E:74:VAL:HG22	1.78	0.65
1:G:31:VAL:CG1	1:G:290:LEU:HD22	2.26	0.65
1:H:123:GLY:O	1:H:126:LEU:HB2	1.96	0.65
1:D:113:VAL:O	1:D:113:VAL:HG23	1.97	0.64
1:G:218:GLN:HG3	1:G:244:GLU:OE1	1.98	0.64
1:B:114:LEU:HG	1:C:310:SER:CB	2.27	0.64
1:E:214:TRP:CG	1:E:215:SER:H	2.13	0.64
1:H:70:THR:CG2	1:H:91:ALA:HB1	2.27	0.64
1:H:149:PRO:HG3	1:H:230:VAL:HG13	1.79	0.64
1:B:31:VAL:HG22	1:B:290:LEU:CD1	2.24	0.64
1:B:43:LYS:HE2	1:B:74:VAL:HG22	1.80	0.64
1:D:67:VAL:HG11	1:D:137:TRP:CE3	2.32	0.64
1:F:301:PHE:HA	1:F:304:ASP:HB2	1.78	0.64
1:H:106:ARG:NH1	1:H:112:LEU:HD11	2.13	0.64
1:A:201:LEU:HD21	1:A:269:THR:HG22	1.80	0.64
1:A:57:LYS:HB3	1:A:59:LEU:CD1	2.19	0.64
1:A:231:LEU:HD12	1:A:232:ASP:H	1.63	0.63
1:C:67:VAL:HG13	1:C:90:VAL:HB	1.79	0.63
1:B:248:ARG:HG2	1:B:302:LEU:HD23	1.80	0.63
1:F:134:LYS:HE3	1:G:318:LEU:HD21	1.78	0.63
1:E:43:LYS:HE2	1:E:74:VAL:CG2	2.28	0.63
1:D:69:CYS:HB3	1:D:125:ASN:ND2	2.12	0.63
1:H:69:CYS:HB2	1:H:125:ASN:ND2	2.11	0.63
1:E:163:ASP:HB3	1:H:3:LEU:CD1	2.29	0.63
1:E:208:MET:HE2	1:E:225:ASN:C	2.24	0.62
1:A:207:ALA:HB1	1:A:210:ALA:HB3	1.81	0.62
1:B:264:ILE:HD11	1:B:302:LEU:HB2	1.81	0.62
1:B:98:SER:HB2	1:B:100:GLU:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:OG1	1:A:88:ARG:HD2	1.99	0.62
1:E:306:VAL:HG13	1:H:106:ARG:HG2	1.80	0.62
1:F:265:SER:O	1:F:269:THR:HG23	1.99	0.62
1:G:183:THR:O	1:G:187:GLN:HG3	2.00	0.62
1:H:27:THR:HG21	1:H:277:ALA:HB1	1.82	0.62
1:H:67:VAL:HG22	1:H:137:TRP:HB3	1.82	0.62
1:A:67:VAL:HG23	1:A:139:ARG:HD2	1.81	0.61
1:D:264:ILE:HD11	1:D:302:LEU:HB2	1.82	0.61
1:H:148:ASN:HB3	1:H:149:PRO:CD	2.29	0.61
1:B:39:GLY:N	1:B:44:ASP:OD1	2.32	0.61
1:D:233:ARG:HG3	3:D:517:HOH:O	2.00	0.61
1:C:276:ILE:O	1:C:280:ALA:HB2	1.99	0.61
1:G:43:LYS:HE2	1:G:74:VAL:HG22	1.80	0.61
1:G:219:ILE:HG21	1:G:222:LEU:HD12	1.81	0.61
1:H:298:LEU:HD12	1:H:303:PHE:HE2	1.66	0.61
1:D:31:VAL:CG2	1:D:290:LEU:HD13	2.30	0.61
1:H:65:THR:HG21	1:H:88:ARG:HH11	1.66	0.61
1:B:114:LEU:HG	1:C:310:SER:HB2	1.82	0.61
1:B:70:THR:CG2	1:B:91:ALA:HB1	2.31	0.61
1:C:266:ALA:HB1	1:C:290:LEU:HG	1.82	0.61
1:C:298:LEU:HA	1:C:303:PHE:CD1	2.35	0.61
1:D:302:LEU:HD22	1:D:302:LEU:O	1.99	0.61
1:E:266:ALA:O	1:E:270:VAL:HG23	2.01	0.60
1:F:61:LYS:HD2	1:F:64:ASP:OD1	2.00	0.60
1:F:31:VAL:HG22	1:F:290:LEU:HD13	1.82	0.60
1:C:300:THR:HG22	1:C:301:PHE:N	2.17	0.60
1:G:141:ARG:HG3	1:G:141:ARG:HH11	1.67	0.60
1:H:57:LYS:O	1:H:59:LEU:HD13	2.02	0.59
1:E:93:MET:O	1:E:114:LEU:HD12	2.01	0.59
1:G:129:ASP:CG	1:G:139:ARG:HH11	2.10	0.59
1:F:41:SER:HB3	3:F:539:HOH:O	2.02	0.59
1:G:190:ARG:HD2	3:G:517:HOH:O	2.02	0.59
1:G:214:TRP:CD1	1:G:225:ASN:HA	2.36	0.59
1:H:289:MET:O	1:H:291:PRO:HD3	2.01	0.59
1:H:298:LEU:HD12	1:H:303:PHE:CE2	2.37	0.59
1:D:148:ASN:HB3	1:D:149:PRO:CD	2.32	0.59
1:E:219:ILE:HG21	1:E:222:LEU:HD12	1.82	0.59
1:G:99:VAL:HA	1:G:102:ARG:HD3	1.83	0.59
1:C:134:LYS:HE2	1:C:135:TYR:CZ	2.38	0.58
1:F:46:LEU:HD12	1:F:46:LEU:C	2.28	0.58
1:F:99:VAL:HA	1:F:102:ARG:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:C	1:B:46:LEU:HD12	2.29	0.58
1:G:46:LEU:HD12	1:G:47:ALA:N	2.19	0.58
1:E:148:ASN:HB3	1:E:149:PRO:CD	2.34	0.58
1:F:18:ARG:NH1	1:F:20:GLN:HE22	2.01	0.58
1:A:116:PRO:HB2	1:A:119:LEU:HD13	1.84	0.58
1:E:164:PHE:O	1:E:193:ARG:NH2	2.36	0.58
1:B:69:CYS:HA	1:B:92:VAL:HG23	1.84	0.58
1:C:278:GLU:HG2	3:C:595:HOH:O	2.03	0.58
1:E:119:LEU:O	1:E:123:GLY:HA3	2.04	0.58
1:F:43:LYS:HE2	1:F:74:VAL:HG23	1.86	0.58
1:F:74:VAL:HG13	1:F:78:LEU:HD22	1.85	0.58
1:A:31:VAL:HG22	1:A:290:LEU:CD1	2.34	0.57
1:B:66:ILE:HG23	1:B:138:PHE:HD2	1.68	0.57
1:B:114:LEU:HD21	1:C:309:GLY:HA2	1.86	0.57
1:F:18:ARG:HH12	1:F:20:GLN:HE22	1.52	0.57
1:H:148:ASN:HB3	1:H:149:PRO:HD3	1.86	0.57
1:E:188:MET:HE3	1:F:188:MET:HE3	1.86	0.57
1:A:116:PRO:HB2	1:A:119:LEU:CD1	2.33	0.57
1:B:50:VAL:HG22	1:B:145:ASN:ND2	2.20	0.57
1:D:27:THR:CG2	1:D:28:SER:N	2.68	0.57
1:D:67:VAL:HG11	1:D:137:TRP:HE3	1.69	0.57
1:H:128:ALA:HA	1:H:131:LEU:HD12	1.85	0.57
1:B:46:LEU:HD12	1:B:47:ALA:N	2.19	0.57
1:B:132:ALA:HA	1:B:137:TRP:HB2	1.86	0.57
1:C:57:LYS:HB3	1:C:59:LEU:HD13	1.86	0.57
1:H:102:ARG:HG3	1:H:102:ARG:HH21	1.68	0.57
1:D:126:LEU:HD22	1:D:129:ASP:OD2	2.05	0.56
1:H:43:LYS:HE2	1:H:74:VAL:CG2	2.35	0.56
1:B:148:ASN:HB3	1:B:149:PRO:CD	2.35	0.56
1:B:67:VAL:HA	1:B:90:VAL:O	2.06	0.56
1:D:70:THR:HG22	1:D:72:GLY:H	1.70	0.56
1:H:266:ALA:O	1:H:270:VAL:HG23	2.05	0.56
1:E:57:LYS:HB3	1:E:59:LEU:HD13	1.87	0.56
1:E:302:LEU:O	1:E:302:LEU:HD22	2.06	0.56
1:B:31:VAL:HG13	1:B:290:LEU:HD22	1.88	0.56
1:D:65:THR:HB	1:D:88:ARG:HD2	1.88	0.56
1:G:41:SER:HB2	1:G:292:ASP:HB3	1.86	0.56
1:H:101:ARG:HA	1:H:104:LEU:HD23	1.87	0.56
1:C:231:LEU:HD21	1:C:233:ARG:HG2	1.87	0.56
1:B:70:THR:HG22	1:B:91:ALA:HB1	1.88	0.55
1:D:8:LEU:HD12	1:D:85:ARG:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:PHE:HD2	1:E:306:VAL:HG21	1.71	0.55
1:F:208:MET:HE3	1:F:212:GLY:HA2	1.88	0.55
1:G:65:THR:HB	1:G:88:ARG:HB3	1.88	0.55
1:H:113:VAL:HG23	1:H:113:VAL:O	2.05	0.55
1:A:211:ARG:HB2	1:A:213:GLU:HG2	1.87	0.55
1:C:48:LEU:HD22	1:C:52:LEU:HG	1.88	0.55
1:C:61:LYS:HB3	1:C:62:PRO:HD2	1.89	0.55
1:A:122:LYS:HB2	1:A:225:ASN:ND2	2.21	0.55
1:D:101:ARG:O	1:D:105:ILE:HD12	2.06	0.55
1:D:126:LEU:HA	1:D:129:ASP:HB2	1.88	0.55
1:H:93:MET:O	1:H:114:LEU:HA	2.07	0.55
1:C:26:HIS:HB2	1:C:282:GLU:OE2	2.06	0.55
1:E:31:VAL:HG22	1:E:290:LEU:HD13	1.89	0.55
1:G:27:THR:CG2	1:G:28:SER:N	2.70	0.55
1:E:124:GLY:HA2	1:E:127:ILE:HG13	1.89	0.54
1:G:148:ASN:HB3	1:G:149:PRO:CD	2.36	0.54
1:G:201:LEU:C	1:G:201:LEU:HD12	2.32	0.54
1:B:93:MET:SD	1:B:112:LEU:HD11	2.47	0.54
1:C:46:LEU:O	1:C:50:VAL:HG23	2.07	0.54
1:E:93:MET:HE2	1:E:112:LEU:HD11	1.89	0.54
1:F:31:VAL:HG22	1:F:290:LEU:CD1	2.37	0.54
1:B:248:ARG:HB2	1:B:301:PHE:CZ	2.43	0.54
1:C:201:LEU:HD12	1:C:201:LEU:C	2.33	0.54
1:E:265:SER:O	1:E:268:ALA:HB3	2.08	0.54
1:G:300:THR:CG2	1:G:301:PHE:N	2.71	0.54
1:A:104:LEU:HD11	1:D:295:GLU:HG3	1.89	0.54
1:A:188:MET:HE3	1:B:188:MET:HE3	1.89	0.54
1:E:141:ARG:O	1:E:145:ASN:HB2	2.08	0.54
1:G:188:MET:HE3	1:H:188:MET:HE3	1.90	0.54
1:A:148:ASN:HB3	1:A:149:PRO:CD	2.38	0.54
1:A:65:THR:HB	1:A:137:TRP:CD1	2.42	0.54
1:E:211:ARG:O	1:E:213:GLU:HG2	2.08	0.54
1:D:306:VAL:O	1:D:307:ASP:HB2	2.07	0.54
1:H:253:ARG:O	1:H:257:GLU:HB2	2.08	0.54
1:A:297:TYR:O	1:A:300:THR:HB	2.07	0.54
1:D:102:ARG:HB3	1:D:112:LEU:HD21	1.90	0.54
1:A:302:LEU:HD13	1:A:303:PHE:CE1	2.43	0.53
1:E:27:THR:HG23	1:E:28:SER:N	2.23	0.53
1:G:43:LYS:HE2	1:G:74:VAL:CG2	2.38	0.53
1:G:263:GLY:O	1:G:266:ALA:HB3	2.08	0.53
1:C:37:ASN:HB3	1:C:44:ASP:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:LYS:O	1:E:290:LEU:HB2	2.08	0.53
1:B:68:GLU:HG3	1:B:69:CYS:N	2.23	0.53
1:A:310:SER:HB2	1:D:114:LEU:H	1.72	0.53
1:B:97:TYR:O	1:B:98:SER:C	2.51	0.53
1:G:31:VAL:HG22	1:G:290:LEU:CD1	2.38	0.53
1:A:43:LYS:HE2	1:A:74:VAL:CG2	2.39	0.53
1:C:297:TYR:CB	1:C:302:LEU:HD12	2.38	0.53
1:C:300:THR:C	1:C:302:LEU:H	2.16	0.53
1:E:148:ASN:HB3	1:E:149:PRO:HD3	1.91	0.53
1:F:116:PRO:HB2	1:F:118:HIS:CD2	2.44	0.53
1:B:114:LEU:H	1:C:310:SER:CB	2.09	0.53
1:B:39:GLY:HA3	1:B:44:ASP:OD2	2.09	0.53
1:F:31:VAL:CG1	1:F:290:LEU:HD22	2.38	0.53
1:F:67:VAL:HG23	1:F:139:ARG:HG2	1.90	0.53
1:G:96:THR:OG1	1:G:117:GLY:HA3	2.09	0.53
1:H:70:THR:OG1	1:H:71:SER:N	2.42	0.53
1:H:134:LYS:HE2	1:H:135:TYR:CZ	2.43	0.53
1:C:208:MET:O	1:C:212:GLY:HA2	2.08	0.53
1:C:264:ILE:HD12	1:C:297:TYR:CD1	2.44	0.53
1:F:93:MET:O	1:F:114:LEU:HA	2.09	0.53
1:E:70:THR:O	1:E:93:MET:HG2	2.09	0.53
1:F:264:ILE:HD13	1:F:301:PHE:HE2	1.74	0.52
1:H:276:ILE:O	1:H:280:ALA:HB2	2.09	0.52
1:E:59:LEU:HD12	1:E:59:LEU:N	2.24	0.52
1:E:68:GLU:CD	1:E:140:ALA:HB3	2.34	0.52
1:H:89:PHE:CE2	1:H:91:ALA:HB2	2.44	0.52
1:D:126:LEU:HA	1:D:129:ASP:OD2	2.09	0.52
1:C:19:LEU:HD22	1:C:258:GLU:HG3	1.90	0.52
1:F:163:ASP:HB3	1:G:3:LEU:HD13	1.90	0.52
1:B:193:ARG:HB3	1:B:196:VAL:HG23	1.92	0.52
1:D:92:VAL:HG22	1:D:113:VAL:CG2	2.40	0.52
1:A:119:LEU:HB3	1:A:123:GLY:HA3	1.92	0.52
1:E:99:VAL:HG22	1:E:103:LYS:HD2	1.92	0.52
1:C:201:LEU:HD12	1:C:201:LEU:O	2.09	0.52
1:E:129:ASP:O	1:E:133:GLU:HG3	2.10	0.52
1:E:201:LEU:HD12	1:E:201:LEU:C	2.35	0.52
1:F:308:GLU:CD	1:F:308:GLU:H	2.18	0.52
1:H:94:GLY:HA2	1:H:115:PHE:O	2.09	0.52
1:C:315:LEU:O	1:C:316:ALA:HB2	2.09	0.52
1:C:297:TYR:HB2	1:C:302:LEU:HD12	1.93	0.51
1:G:31:VAL:HG22	1:G:290:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TYR:HB2	1:A:302:LEU:HD12	1.91	0.51
1:F:96:THR:OG1	1:F:117:GLY:HA3	2.10	0.51
1:B:70:THR:HG23	1:B:70:THR:O	2.10	0.51
1:F:289:MET:O	1:F:291:PRO:HD3	2.10	0.51
1:D:153:ARG:HD3	1:D:187:GLN:OE1	2.11	0.51
1:H:254:LEU:O	1:H:258:GLU:HB2	2.11	0.51
1:F:127:ILE:HG22	1:F:131:LEU:HD11	1.91	0.51
1:B:163:ASP:HB3	1:C:3:LEU:HD13	1.91	0.51
1:D:106:ARG:NH1	1:D:112:LEU:HB2	2.25	0.51
1:F:114:LEU:HD12	1:G:310:SER:H	1.76	0.51
1:C:98:SER:OG	1:C:100:GLU:HG3	2.11	0.50
1:F:203:PRO:HB2	1:F:206:ALA:HB3	1.93	0.50
1:A:298:LEU:HA	1:A:303:PHE:CD1	2.46	0.50
1:D:102:ARG:HD2	1:D:112:LEU:HD21	1.94	0.50
1:F:176:PHE:CZ	1:F:209:LEU:HG	2.45	0.50
1:B:74:VAL:HG12	1:B:78:LEU:HD22	1.93	0.50
1:E:295:GLU:HG2	1:H:295:GLU:HG2	1.93	0.50
1:F:179:THR:HG23	1:F:228:PRO:HG2	1.93	0.50
1:H:179:THR:HG23	1:H:228:PRO:HG2	1.93	0.50
1:C:16:ILE:HG12	1:C:32:LYS:HG3	1.93	0.50
1:E:46:LEU:C	1:E:46:LEU:HD12	2.35	0.50
1:E:116:PRO:O	1:E:119:LEU:HB2	2.10	0.50
1:A:46:LEU:HD12	1:A:46:LEU:C	2.37	0.50
1:A:266:ALA:O	1:A:270:VAL:HG23	2.12	0.50
1:H:265:SER:O	1:H:269:THR:HG23	2.12	0.50
1:A:74:VAL:HG23	3:A:529:HOH:O	2.10	0.50
1:A:300:THR:CG2	1:A:301:PHE:N	2.74	0.50
1:A:306:VAL:HG12	1:D:106:ARG:HG2	1.93	0.50
1:B:113:VAL:HG23	1:B:113:VAL:O	2.11	0.50
1:B:211:ARG:HB3	1:B:213:GLU:HG2	1.94	0.50
1:C:191:VAL:HG21	1:D:191:VAL:HG21	1.94	0.50
1:D:95:ASP:HB3	1:D:114:LEU:HB3	1.92	0.50
1:D:208:MET:HE3	1:D:212:GLY:CA	2.36	0.50
1:E:27:THR:HG21	1:E:277:ALA:HB1	1.94	0.50
1:G:266:ALA:HB1	1:G:290:LEU:HG	1.94	0.50
1:H:65:THR:HG21	1:H:88:ARG:NH1	2.27	0.50
1:G:159:GLU:HG2	3:H:508:HOH:O	2.11	0.50
1:H:61:LYS:HB3	1:H:62:PRO:HD2	1.93	0.50
1:A:254:LEU:HD11	1:A:270:VAL:HG21	1.94	0.50
1:D:201:LEU:HD21	1:D:269:THR:HA	1.92	0.50
1:E:128:ALA:HB3	1:E:139:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:PHE:HA	1:E:304:ASP:CG	2.37	0.50
1:F:18:ARG:NH1	1:F:20:GLN:NE2	2.59	0.50
1:F:65:THR:HB	1:F:88:ARG:HB3	1.94	0.49
1:E:31:VAL:HG11	1:E:290:LEU:HD22	1.94	0.49
1:A:231:LEU:HD12	1:A:232:ASP:N	2.27	0.49
1:B:243:ASP:OD1	1:B:245:VAL:HB	2.12	0.49
1:G:46:LEU:HD12	1:G:46:LEU:C	2.36	0.49
1:E:300:THR:HG22	1:E:301:PHE:N	2.24	0.49
1:F:114:LEU:HD12	1:G:310:SER:N	2.27	0.49
1:F:281:PRO:O	1:F:282:GLU:C	2.55	0.49
1:G:106:ARG:NH1	1:G:112:LEU:HD12	2.27	0.49
1:H:300:THR:CG2	1:H:301:PHE:H	2.19	0.49
1:B:85:ARG:NH1	1:B:85:ARG:HG2	2.28	0.49
1:E:115:PHE:CE1	1:E:119:LEU:HB3	2.47	0.49
1:E:214:TRP:CG	1:E:215:SER:N	2.81	0.49
1:B:77:ALA:O	1:B:81:VAL:HG23	2.13	0.49
1:D:93:MET:CE	1:D:112:LEU:HD11	2.43	0.49
1:A:39:GLY:N	1:A:44:ASP:OD1	2.35	0.49
1:A:102:ARG:HG2	1:A:112:LEU:HD21	1.93	0.49
1:E:115:PHE:HE1	1:E:119:LEU:HB3	1.77	0.49
1:C:46:LEU:HD12	1:C:46:LEU:C	2.38	0.49
1:B:85:ARG:HH11	1:B:85:ARG:CG	2.26	0.48
1:D:118:HIS:C	1:D:120:GLY:H	2.21	0.48
1:F:55:GLU:CD	1:F:85:ARG:HH21	2.20	0.48
1:E:127:ILE:O	1:E:131:LEU:HD12	2.12	0.48
1:G:68:GLU:OE2	1:G:140:ALA:HB3	2.12	0.48
1:A:94:GLY:HA2	1:A:115:PHE:O	2.13	0.48
1:B:164:PHE:O	1:B:193:ARG:NH2	2.46	0.48
1:D:176:PHE:CD1	1:D:179:THR:HG22	2.48	0.48
1:E:17:VAL:HG12	1:H:4:PHE:HB2	1.95	0.48
1:H:39:GLY:N	1:H:44:ASP:OD1	2.35	0.48
1:B:302:LEU:O	1:B:302:LEU:HD22	2.13	0.48
1:G:233:ARG:C	1:G:235:VAL:H	2.21	0.48
1:C:94:GLY:HA2	1:C:115:PHE:O	2.13	0.48
1:G:59:LEU:N	1:G:59:LEU:HD12	2.29	0.48
1:B:8:LEU:HD13	1:B:48:LEU:HD23	1.94	0.48
1:C:31:VAL:HG22	1:C:290:LEU:CD1	2.41	0.48
1:C:272:THR:O	1:C:276:ILE:HG13	2.14	0.48
1:C:317:SER:O	1:C:318:LEU:HB2	2.13	0.48
1:G:148:ASN:HB3	1:G:149:PRO:HD3	1.94	0.48
1:C:211:ARG:HH21	1:C:213:GLU:CD	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLU:HG2	1:D:101:ARG:N	2.29	0.48
1:H:203:PRO:HB3	1:H:219:ILE:HD12	1.95	0.48
1:B:2:PRO:HG2	3:C:510:HOH:O	2.12	0.48
1:C:70:THR:O	1:C:93:MET:HB3	2.14	0.48
1:C:101:ARG:HA	1:C:101:ARG:HD3	1.49	0.48
1:B:148:ASN:HB3	1:B:149:PRO:HD3	1.96	0.48
1:H:127:ILE:HG22	1:H:131:LEU:HD11	1.95	0.48
1:C:57:LYS:CB	1:C:59:LEU:HD13	2.44	0.47
1:D:27:THR:HG23	1:D:28:SER:N	2.30	0.47
1:E:67:VAL:HA	1:E:90:VAL:O	2.14	0.47
1:F:248:ARG:HB3	1:F:301:PHE:CZ	2.49	0.47
1:G:118:HIS:C	1:G:120:GLY:H	2.22	0.47
1:G:225:ASN:C	1:G:225:ASN:OD1	2.56	0.47
1:H:18:ARG:HB2	1:H:30:TYR:CE2	2.49	0.47
1:H:128:ALA:HB3	1:H:139:ARG:NH2	2.29	0.47
1:E:126:LEU:O	1:E:130:GLU:HG3	2.15	0.47
1:E:214:TRP:O	1:E:215:SER:CB	2.52	0.47
1:E:248:ARG:HG2	1:E:302:LEU:HD23	1.95	0.47
1:G:207:ALA:HB1	1:G:210:ALA:HB3	1.96	0.47
1:B:27:THR:HG21	1:B:277:ALA:HB1	1.96	0.47
1:B:149:PRO:HG3	1:B:230:VAL:HG22	1.96	0.47
1:C:193:ARG:NH1	3:C:547:HOH:O	2.46	0.47
1:D:92:VAL:HG22	1:D:113:VAL:HG21	1.95	0.47
1:E:289:MET:O	1:E:291:PRO:HD3	2.14	0.47
1:F:18:ARG:HB2	1:F:30:TYR:CE2	2.49	0.47
1:H:115:PHE:CD2	1:H:117:GLY:HA3	2.49	0.47
1:H:201:LEU:HD22	1:H:272:THR:OG1	2.14	0.47
1:A:248:ARG:CZ	1:A:252:ARG:NH1	2.77	0.47
1:E:106:ARG:NH1	1:H:307:ASP:HB3	2.29	0.47
1:E:124:GLY:HA2	1:E:127:ILE:CG1	2.44	0.47
1:A:300:THR:HG22	1:A:302:LEU:N	2.14	0.47
1:D:211:ARG:HG2	1:D:211:ARG:HH11	1.80	0.47
1:A:93:MET:O	1:A:114:LEU:HA	2.15	0.47
1:A:211:ARG:HB2	1:A:213:GLU:CG	2.45	0.47
1:B:31:VAL:CG2	1:B:290:LEU:CD1	2.92	0.47
1:C:197:ARG:NH2	1:C:238:ASP:OD1	2.48	0.47
1:H:254:LEU:HD11	1:H:270:VAL:HG21	1.97	0.47
1:B:106:ARG:NH1	1:B:112:LEU:HB3	2.29	0.47
1:C:201:LEU:HD21	1:C:269:THR:HA	1.96	0.47
1:E:310:SER:OG	1:H:113:VAL:HA	2.15	0.47
1:H:115:PHE:CE2	1:H:124:GLY:HA3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:PRO:HG2	1:B:119:LEU:CD1	2.41	0.47
1:D:18:ARG:HB2	1:D:30:TYR:CE2	2.50	0.47
1:F:225:ASN:O	1:F:226:PHE:HB3	2.15	0.47
1:C:67:VAL:CG1	1:C:90:VAL:HB	2.45	0.47
1:F:149:PRO:HG3	1:F:230:VAL:HG22	1.96	0.47
1:D:43:LYS:HE2	1:D:74:VAL:CG2	2.45	0.47
1:B:18:ARG:NH2	3:B:588:HOH:O	2.47	0.46
1:E:99:VAL:HG13	1:E:103:LYS:HD2	1.97	0.46
1:C:317:SER:N	3:C:550:HOH:O	2.47	0.46
1:B:265:SER:O	1:B:269:THR:HG23	2.15	0.46
1:C:149:PRO:HG3	1:C:230:VAL:HG22	1.96	0.46
1:F:65:THR:HG21	1:F:88:ARG:HH11	1.79	0.46
1:G:176:PHE:HZ	1:G:202:GLU:OE1	1.99	0.46
1:D:219:ILE:HG21	1:D:222:LEU:HD12	1.97	0.46
1:A:18:ARG:NH1	1:A:20:GLN:OE1	2.49	0.46
1:A:300:THR:HG23	1:A:301:PHE:N	2.31	0.46
1:D:70:THR:O	1:D:93:MET:HB3	2.15	0.46
1:B:68:GLU:HG3	1:B:69:CYS:H	1.81	0.46
1:F:315:LEU:HD11	1:G:113:VAL:HG22	1.97	0.46
1:E:22:MET:HE2	1:E:274:LEU:HD11	1.98	0.46
1:E:192:ALA:HB2	1:F:188:MET:CE	2.46	0.46
1:F:8:LEU:HD12	1:F:85:ARG:HD3	1.98	0.46
1:E:102:ARG:HD2	1:H:308:GLU:O	2.16	0.46
1:G:218:GLN:HG3	1:G:244:GLU:CD	2.41	0.46
1:H:115:PHE:O	1:H:115:PHE:CG	2.68	0.46
1:B:208:MET:SD	1:B:214:TRP:HB2	2.56	0.46
1:E:139:ARG:HD2	1:E:141:ARG:NH2	2.31	0.46
1:E:316:ALA:C	1:E:318:LEU:H	2.24	0.46
1:G:248:ARG:HD2	1:G:248:ARG:C	2.40	0.46
1:A:74:VAL:HG21	1:A:142:GLN:OE1	2.16	0.46
1:F:168:ARG:O	1:F:285:VAL:HG11	2.16	0.46
1:D:93:MET:HE2	1:D:112:LEU:HD11	1.98	0.45
1:G:27:THR:HG21	1:G:277:ALA:HB1	1.97	0.45
1:F:163:ASP:O	1:G:3:LEU:HD22	2.15	0.45
1:G:7:ILE:O	1:G:7:ILE:HG13	2.15	0.45
1:H:129:ASP:O	1:H:132:ALA:HB3	2.17	0.45
1:H:203:PRO:HG2	1:H:206:ALA:HB3	1.98	0.45
1:B:67:VAL:HG11	1:B:137:TRP:CE3	2.51	0.45
1:D:101:ARG:HA	1:D:101:ARG:HD3	1.72	0.45
1:D:120:GLY:O	1:D:121:SER:C	2.59	0.45
1:E:254:LEU:HD11	1:E:270:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:LEU:HD21	1:G:104:LEU:HD13	1.97	0.45
1:H:300:THR:CG2	1:H:301:PHE:N	2.77	0.45
1:F:3:LEU:CD1	1:G:163:ASP:HB3	2.42	0.45
1:B:32:LYS:O	1:B:290:LEU:HB2	2.16	0.45
1:D:65:THR:HG21	1:D:88:ARG:HH11	1.81	0.45
1:E:7:ILE:O	1:E:7:ILE:HG13	2.16	0.45
1:F:244:GLU:H	1:F:244:GLU:HG2	1.50	0.45
1:B:49:SER:HB2	1:B:151:TYR:CD1	2.51	0.45
1:C:205:ASN:OD1	1:C:205:ASN:N	2.38	0.45
1:C:209:LEU:HD22	1:C:233:ARG:CZ	2.46	0.45
1:F:22:MET:HE3	1:F:253:ARG:HB3	1.99	0.45
1:A:43:LYS:HE2	1:A:74:VAL:HG23	1.99	0.45
1:B:92:VAL:HG11	1:B:127:ILE:HG23	1.97	0.45
1:C:219:ILE:CD1	1:C:244:GLU:HB3	2.46	0.45
1:C:219:ILE:HG23	1:C:264:ILE:HG22	1.98	0.45
1:D:203:PRO:HB3	1:D:219:ILE:HD12	1.98	0.45
1:H:248:ARG:HG3	1:H:301:PHE:CE1	2.52	0.45
1:A:129:ASP:OD1	1:A:139:ARG:NH1	2.50	0.45
1:B:90:VAL:HG13	1:B:111:LYS:O	2.16	0.45
1:G:69:CYS:HA	1:G:92:VAL:O	2.16	0.45
1:G:70:THR:O	1:G:93:MET:HB3	2.16	0.45
1:D:31:VAL:CG2	1:D:290:LEU:CD1	2.94	0.45
1:F:102:ARG:CB	1:F:112:LEU:HD21	2.47	0.45
1:C:252:ARG:HH21	1:C:302:LEU:C	2.25	0.45
1:B:201:LEU:C	1:B:201:LEU:HD12	2.42	0.44
1:A:148:ASN:HB3	1:A:149:PRO:HD3	1.99	0.44
1:D:145:ASN:HA	1:D:146:PRO:HD2	1.87	0.44
1:D:303:PHE:O	1:D:306:VAL:HG22	2.18	0.44
1:F:302:LEU:HD22	1:F:302:LEU:O	2.18	0.44
1:A:208:MET:HE2	1:A:226:PHE:HA	1.99	0.44
1:E:27:THR:CG2	1:E:28:SER:N	2.78	0.44
1:E:298:LEU:HD23	1:E:303:PHE:CE1	2.53	0.44
1:G:71:SER:HB3	1:G:97:TYR:CZ	2.52	0.44
1:A:95:ASP:HA	1:A:102:ARG:HH11	1.82	0.44
1:B:217:HIS:CD2	1:B:217:HIS:H	2.33	0.44
1:E:65:THR:HB	1:E:137:TRP:CD1	2.52	0.44
1:D:41:SER:HB2	1:D:292:ASP:HB3	1.98	0.44
1:F:55:GLU:OE1	1:F:85:ARG:NH2	2.45	0.44
1:F:301:PHE:HA	1:F:304:ASP:CB	2.46	0.44
1:G:219:ILE:CG2	1:G:222:LEU:HD12	2.46	0.44
1:G:233:ARG:C	1:G:235:VAL:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:VAL:HA	1:C:310:SER:HB2	2.00	0.44
1:B:151:TYR:CE2	1:B:155:THR:HG21	2.53	0.44
1:B:205:ASN:OD1	1:B:205:ASN:N	2.33	0.44
1:E:3:LEU:HD22	1:H:163:ASP:O	2.18	0.44
1:E:153:ARG:HG2	1:E:184:GLY:O	2.17	0.44
1:G:89:PHE:CE2	1:G:91:ALA:HB2	2.52	0.44
1:C:65:THR:HA	1:C:88:ARG:O	2.18	0.44
1:G:298:LEU:HD22	1:G:303:PHE:CZ	2.52	0.44
1:H:46:LEU:HD12	1:H:46:LEU:C	2.43	0.44
1:B:68:GLU:CD	1:B:140:ALA:HB3	2.43	0.44
1:D:120:GLY:O	1:D:121:SER:O	2.35	0.44
1:F:102:ARG:H	1:F:102:ARG:HG2	1.58	0.44
1:H:261:PHE:HZ	1:H:303:PHE:HZ	1.66	0.44
1:C:176:PHE:CD1	1:C:179:THR:HG22	2.53	0.44
1:C:300:THR:CG2	1:C:301:PHE:N	2.80	0.44
1:G:178:THR:C	1:G:179:THR:HG23	2.42	0.44
1:B:230:VAL:O	1:B:230:VAL:HG13	2.18	0.43
1:E:264:ILE:HG12	1:E:297:TYR:CE1	2.54	0.43
1:B:92:VAL:HG11	1:B:127:ILE:CG2	2.49	0.43
1:H:120:GLY:O	1:H:121:SER:C	2.61	0.43
1:D:140:ALA:O	1:D:141:ARG:HB2	2.18	0.43
1:E:114:LEU:HD12	1:E:114:LEU:HA	1.88	0.43
1:F:266:ALA:O	1:F:270:VAL:HG23	2.17	0.43
1:D:78:LEU:HB3	1:D:89:PHE:CE1	2.53	0.43
1:D:164:PHE:O	1:D:193:ARG:NH2	2.51	0.43
1:G:214:TRP:CD2	1:G:215:SER:N	2.86	0.43
1:E:104:LEU:HD13	1:E:104:LEU:HA	1.87	0.43
1:F:201:LEU:HD21	1:F:269:THR:HA	2.01	0.43
1:G:141:ARG:HH11	1:G:141:ARG:CG	2.31	0.43
1:C:27:THR:HG22	1:C:28:SER:N	2.34	0.43
1:E:303:PHE:CD2	1:E:306:VAL:HG21	2.52	0.43
1:F:89:PHE:CE2	1:F:91:ALA:HB2	2.54	0.43
1:H:32:LYS:HE3	1:H:34:GLU:OE1	2.19	0.43
1:H:65:THR:HB	1:H:88:ARG:HD2	2.01	0.43
1:A:193:ARG:HD2	3:A:523:HOH:O	2.17	0.43
1:C:204:SER:C	1:C:206:ALA:H	2.26	0.43
1:C:225:ASN:OD1	1:C:225:ASN:C	2.61	0.43
1:D:91:ALA:O	1:D:113:VAL:HG22	2.19	0.43
1:E:48:LEU:HD11	1:E:52:LEU:HD11	2.01	0.43
1:F:32:LYS:O	1:F:290:LEU:HB2	2.19	0.43
1:A:67:VAL:CG1	1:A:137:TRP:CE3	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ASP:HA	1:C:315:LEU:HB2	2.01	0.43
1:D:27:THR:HG21	1:D:277:ALA:HB1	2.00	0.43
1:D:32:LYS:O	1:D:290:LEU:HB2	2.19	0.43
1:E:253:ARG:O	1:E:257:GLU:HB2	2.19	0.43
1:A:48:LEU:HD22	1:A:52:LEU:HG	2.01	0.43
1:D:85:ARG:HA	1:D:85:ARG:HD2	1.92	0.43
1:D:308:GLU:H	1:D:308:GLU:HG2	1.44	0.43
1:F:300:THR:C	1:F:302:LEU:H	2.27	0.43
1:G:118:HIS:C	1:G:120:GLY:N	2.76	0.43
1:C:70:THR:OG1	1:C:71:SER:N	2.51	0.43
1:C:206:ALA:C	1:C:208:MET:H	2.27	0.43
1:A:186:GLY:HA3	1:A:235:VAL:HG11	2.01	0.42
1:B:27:THR:HG23	1:B:28:SER:N	2.33	0.42
1:C:100:GLU:HG3	1:C:100:GLU:H	1.59	0.42
1:G:78:LEU:HD12	1:G:78:LEU:HA	1.89	0.42
1:A:215:SER:O	1:A:216:PRO:C	2.62	0.42
1:B:8:LEU:HD22	1:B:11:ILE:HD11	2.01	0.42
1:E:183:THR:O	1:E:187:GLN:HG3	2.19	0.42
1:G:249:ASP:O	1:G:253:ARG:HG3	2.19	0.42
1:H:127:ILE:O	1:H:131:LEU:HD12	2.19	0.42
1:C:195:GLU:HG3	3:C:543:HOH:O	2.18	0.42
1:E:106:ARG:NH2	1:H:311:ASP:OD2	2.52	0.42
1:H:102:ARG:HG3	1:H:102:ARG:NH2	2.34	0.42
1:A:118:HIS:CD2	1:A:119:LEU:HD12	2.54	0.42
1:B:117:GLY:C	1:B:119:LEU:H	2.27	0.42
1:C:49:SER:OG	1:C:151:TYR:HB2	2.19	0.42
1:C:93:MET:O	1:C:114:LEU:HA	2.17	0.42
1:C:300:THR:C	1:C:302:LEU:N	2.77	0.42
1:F:148:ASN:HB3	1:F:149:PRO:CD	2.49	0.42
1:G:74:VAL:HG12	1:G:78:LEU:HD22	2.01	0.42
1:A:4:PHE:HB2	1:D:17:VAL:HG12	2.01	0.42
1:B:190:ARG:HG3	1:B:191:VAL:N	2.31	0.42
1:E:68:GLU:OE1	1:E:142:GLN:NE2	2.47	0.42
1:E:115:PHE:O	1:E:116:PRO:C	2.61	0.42
1:G:209:LEU:HB2	1:G:239:LEU:HD11	2.01	0.42
1:H:39:GLY:HA3	1:H:44:ASP:OD2	2.19	0.42
1:B:95:ASP:HB3	1:B:117:GLY:H	1.85	0.42
1:D:25:GLU:C	1:D:27:THR:H	2.27	0.42
1:D:115:PHE:CZ	1:D:124:GLY:HA3	2.54	0.42
1:B:65:THR:HB	1:B:137:TRP:CD1	2.55	0.42
1:B:310:SER:N	1:C:114:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LYS:CB	1:E:59:LEU:HD13	2.49	0.42
1:E:59:LEU:N	1:E:59:LEU:CD1	2.82	0.42
1:G:27:THR:HG23	1:G:28:SER:N	2.35	0.42
1:B:289:MET:O	1:B:291:PRO:HD3	2.20	0.42
1:C:298:LEU:HA	1:C:303:PHE:CE1	2.55	0.42
1:D:8:LEU:CD1	1:D:85:ARG:HD3	2.50	0.42
1:E:112:LEU:HD13	1:E:112:LEU:HA	1.90	0.42
1:A:69:CYS:HB3	1:A:125:ASN:HD22	1.84	0.42
1:B:126:LEU:C	1:B:128:ALA:H	2.27	0.42
1:C:167:LYS:O	1:C:193:ARG:NH2	2.53	0.42
1:D:209:LEU:CB	1:D:239:LEU:HD11	2.49	0.42
1:E:253:ARG:HG2	1:E:257:GLU:OE2	2.19	0.42
1:G:210:ALA:C	1:G:211:ARG:HD2	2.44	0.42
1:H:133:GLU:H	1:H:133:GLU:HG2	1.37	0.42
1:A:141:ARG:O	1:A:145:ASN:HB2	2.20	0.42
1:B:85:ARG:HG2	1:B:85:ARG:HH11	1.85	0.42
1:B:121:SER:C	1:B:123:GLY:N	2.78	0.42
1:D:179:THR:HG23	1:D:228:PRO:HG2	2.01	0.42
1:E:94:GLY:C	1:E:96:THR:N	2.77	0.42
1:G:233:ARG:O	1:G:235:VAL:N	2.52	0.42
1:E:153:ARG:NH1	1:E:187:GLN:OE1	2.53	0.41
1:F:202:GLU:CD	1:F:207:ALA:HA	2.45	0.41
1:E:176:PHE:CD1	1:E:179:THR:HG22	2.55	0.41
1:G:300:THR:HG22	1:G:302:LEU:HB2	2.02	0.41
1:B:41:SER:HB2	1:B:292:ASP:HB3	2.01	0.41
1:E:46:LEU:HD12	1:E:47:ALA:N	2.35	0.41
1:E:89:PHE:CE2	1:E:91:ALA:HB2	2.54	0.41
1:E:289:MET:HE3	1:E:289:MET:HB3	1.86	0.41
1:F:11:ILE:HD12	1:F:48:LEU:HG	2.02	0.41
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.93	0.41
1:B:27:THR:CG2	1:B:28:SER:N	2.83	0.41
1:C:206:ALA:HA	1:C:214:TRP:HA	2.02	0.41
1:C:297:TYR:HB3	1:C:302:LEU:HD12	2.02	0.41
1:E:176:PHE:HB2	1:E:179:THR:HA	2.03	0.41
1:G:113:VAL:O	1:G:113:VAL:HG12	2.20	0.41
1:H:55:GLU:OE1	1:H:85:ARG:NH2	2.54	0.41
1:H:132:ALA:O	1:H:136:GLY:N	2.52	0.41
1:A:297:TYR:CB	1:A:302:LEU:HD12	2.51	0.41
1:B:104:LEU:HD13	1:B:104:LEU:HA	1.90	0.41
1:D:48:LEU:HD11	1:D:52:LEU:HD11	2.02	0.41
1:D:65:THR:HG23	1:D:137:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:VAL:O	1:D:113:VAL:CG2	2.68	0.41
1:F:67:VAL:HG13	1:F:90:VAL:HB	2.03	0.41
1:F:106:ARG:NH2	1:G:311:ASP:OD2	2.53	0.41
1:A:306:VAL:CG1	1:D:106:ARG:HG2	2.50	0.41
1:B:8:LEU:HD11	1:B:81:VAL:HG13	2.02	0.41
1:D:204:SER:HB2	3:D:556:HOH:O	2.20	0.41
1:E:94:GLY:C	1:E:96:THR:H	2.28	0.41
1:B:3:LEU:HD12	1:B:3:LEU:HA	1.87	0.41
1:B:49:SER:HB2	1:B:151:TYR:CG	2.56	0.41
1:B:61:LYS:O	1:B:87:TYR:HE1	2.04	0.41
1:C:219:ILE:HG22	1:C:265:SER:HA	2.02	0.41
1:D:265:SER:O	1:D:269:THR:HG23	2.19	0.41
1:E:93:MET:O	1:E:114:LEU:HA	2.21	0.41
1:E:266:ALA:HB1	1:E:290:LEU:HG	2.02	0.41
1:E:101:ARG:H	1:E:101:ARG:HG2	1.61	0.41
1:F:102:ARG:HB3	1:F:112:LEU:HD21	2.03	0.41
1:G:145:ASN:HA	1:G:146:PRO:HD2	1.96	0.41
1:A:32:LYS:O	1:A:290:LEU:HB2	2.21	0.41
1:A:134:LYS:HG2	1:A:135:TYR:CE2	2.55	0.41
1:A:248:ARG:NE	1:A:252:ARG:NH1	2.68	0.41
1:A:298:LEU:CD1	1:D:100:GLU:HB2	2.51	0.41
1:B:160:ILE:HG12	1:B:287:LEU:HD21	2.02	0.41
1:C:39:GLY:HA3	1:C:44:ASP:OD2	2.21	0.41
1:C:50:VAL:HG13	1:C:145:ASN:ND2	2.35	0.41
1:D:69:CYS:CB	1:D:125:ASN:HD22	2.29	0.41
1:D:148:ASN:HB3	1:D:149:PRO:HD3	2.00	0.41
1:E:44:ASP:OD1	1:E:80:MET:HE1	2.21	0.41
1:G:118:HIS:CE1	1:G:119:LEU:HD12	2.56	0.41
1:H:60:LEU:HD23	1:H:60:LEU:HA	1.96	0.41
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.93	0.41
1:C:219:ILE:HD13	1:C:219:ILE:N	2.35	0.41
1:G:100:GLU:O	1:G:104:LEU:HD22	2.20	0.41
1:H:41:SER:HB2	1:H:292:ASP:HB3	2.03	0.41
1:A:300:THR:C	1:A:302:LEU:H	2.29	0.40
1:E:102:ARG:HE	1:E:102:ARG:HB2	1.76	0.40
1:A:69:CYS:HB3	1:A:125:ASN:ND2	2.37	0.40
1:B:50:VAL:HG12	1:B:51:VAL:N	2.36	0.40
1:B:205:ASN:HB2	1:B:215:SER:OG	2.21	0.40
1:G:22:MET:HE2	1:G:274:LEU:HD11	2.02	0.40
1:H:25:GLU:C	1:H:27:THR:H	2.27	0.40
1:H:157:ALA:HB2	1:H:185:VAL:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ARG:CG	1:B:302:LEU:HA	2.51	0.40
1:C:311:ASP:C	1:C:313:ALA:H	2.29	0.40
1:D:248:ARG:C	1:D:248:ARG:HD2	2.46	0.40
1:D:302:LEU:HD13	1:D:303:PHE:CE1	2.56	0.40
1:E:14:THR:HB	1:E:33:VAL:O	2.21	0.40
1:F:311:ASP:HB3	1:F:314:TRP:HB3	2.03	0.40
1:A:161:LEU:HD22	1:B:154:GLU:HG2	2.02	0.40
1:E:298:LEU:HA	1:E:303:PHE:CE1	2.56	0.40
1:F:111:LYS:HE3	1:G:314:TRP:CE2	2.56	0.40
1:G:26:HIS:HB2	1:G:282:GLU:HG2	2.03	0.40
1:H:193:ARG:HB3	1:H:196:VAL:HG23	2.03	0.40
1:E:308:GLU:H	1:E:308:GLU:HG2	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	314/332 (95%)	294 (94%)	17 (5%)	3 (1%)	12	10
1	B	317/332 (96%)	293 (92%)	19 (6%)	5 (2%)	7	4
1	C	315/332 (95%)	285 (90%)	26 (8%)	4 (1%)	9	6
1	D	314/332 (95%)	292 (93%)	20 (6%)	2 (1%)	21	21
1	E	315/332 (95%)	288 (91%)	23 (7%)	4 (1%)	9	6
1	F	314/332 (95%)	294 (94%)	15 (5%)	5 (2%)	7	4
1	G	315/332 (95%)	288 (91%)	24 (8%)	3 (1%)	12	10
1	H	314/332 (95%)	286 (91%)	24 (8%)	4 (1%)	9	6
All	All	2518/2656 (95%)	2320 (92%)	168 (7%)	30 (1%)	10	7

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	ALA
1	D	121	SER
1	E	215	SER
1	G	312	ASP
1	H	117	GLY
1	H	121	SER
1	D	120	GLY
1	E	64	ASP
1	F	120	GLY
1	A	304	ASP
1	B	98	SER
1	B	225	ASN
1	B	118	HIS
1	C	223	ALA
1	C	304	ASP
1	E	116	PRO
1	H	223	ALA
1	H	307	ASP
1	A	307	ASP
1	B	223	ALA
1	C	216	PRO
1	A	223	ALA
1	E	223	ALA
1	F	223	ALA
1	F	226	PHE
1	G	118	HIS
1	F	116	PRO
1	F	117	GLY
1	G	223	ALA
1	B	72	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	247/261 (95%)	203 (82%)	44 (18%)	2	0
1	B	250/261 (96%)	203 (81%)	47 (19%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	248/261 (95%)	206 (83%)	42 (17%)	2	0
1	D	247/261 (95%)	213 (86%)	34 (14%)	3	2
1	E	248/261 (95%)	197 (79%)	51 (21%)	1	0
1	F	247/261 (95%)	203 (82%)	44 (18%)	2	0
1	G	248/261 (95%)	204 (82%)	44 (18%)	2	0
1	H	247/261 (95%)	200 (81%)	47 (19%)	1	0
All	All	1982/2088 (95%)	1629 (82%)	353 (18%)	2	0

All (353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	18	ARG
1	A	27	THR
1	A	28	SER
1	A	31	VAL
1	A	33	VAL
1	A	46	LEU
1	A	48	LEU
1	A	57	LYS
1	A	71	SER
1	A	78	LEU
1	A	96	THR
1	A	99	VAL
1	A	100	GLU
1	A	101	ARG
1	A	104	LEU
1	A	106	ARG
1	A	121	SER
1	A	122	LYS
1	A	125	ASN
1	A	126	LEU
1	A	134	LYS
1	A	195	GLU
1	A	202	GLU
1	A	213	GLU
1	A	219	ILE
1	A	220	GLN
1	A	233	ARG
1	A	235	VAL

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Mol	Chain	Res	Type
1	A	239	LEU
1	A	243	ASP
1	A	275	SER
1	A	276	ILE
1	A	282	GLU
1	A	290	LEU
1	A	299	SER
1	A	300	THR
1	A	301	PHE
1	A	302	LEU
1	A	304	ASP
1	A	308	GLU
1	A	311	ASP
1	A	315	LEU
1	A	317	SER
1	B	18	ARG
1	B	27	THR
1	B	28	SER
1	B	31	VAL
1	B	41	SER
1	B	48	LEU
1	B	50	VAL
1	B	61	LYS
1	B	67	VAL
1	B	71	SER
1	B	78	LEU
1	B	85	ARG
1	B	88	ARG
1	B	90	VAL
1	B	92	VAL
1	B	99	VAL
1	B	101	ARG
1	B	104	LEU
1	B	106	ARG
1	B	111	LYS
1	B	112	LEU
1	B	114	LEU
1	B	119	LEU
1	B	121	SER
1	B	122	LYS
1	B	126	LEU
1	B	127	ILE

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Mol	Chain	Res	Type
1	B	130	GLU
1	B	134	LYS
1	B	139	ARG
1	B	142	GLN
1	B	150	SER
1	B	190	ARG
1	B	195	GLU
1	B	205	ASN
1	B	209	LEU
1	B	215	SER
1	B	220	GLN
1	B	230	VAL
1	B	235	VAL
1	B	239	LEU
1	B	252	ARG
1	B	254	LEU
1	B	278	GLU
1	B	282	GLU
1	B	301	PHE
1	B	302	LEU
1	C	3	LEU
1	C	6	SER
1	C	17	VAL
1	C	28	SER
1	C	31	VAL
1	C	33	VAL
1	C	46	LEU
1	C	48	LEU
1	C	65	THR
1	C	67	VAL
1	C	70	THR
1	C	78	LEU
1	C	88	ARG
1	C	100	GLU
1	C	101	ARG
1	C	104	LEU
1	C	105	ILE
1	C	112	LEU
1	C	114	LEU
1	C	119	LEU
1	C	126	LEU
1	C	130	GLU

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Mol	Chain	Res	Type
1	C	133	GLU
1	C	193	ARG
1	C	195	GLU
1	C	204	SER
1	C	205	ASN
1	C	219	ILE
1	C	220	GLN
1	C	230	VAL
1	C	231	LEU
1	C	235	VAL
1	C	236	ILE
1	C	239	LEU
1	C	244	GLU
1	C	275	SER
1	C	302	LEU
1	C	304	ASP
1	C	307	ASP
1	C	308	GLU
1	C	312	ASP
1	C	315	LEU
1	D	27	THR
1	D	31	VAL
1	D	33	VAL
1	D	46	LEU
1	D	59	LEU
1	D	65	THR
1	D	70	THR
1	D	71	SER
1	D	78	LEU
1	D	98	SER
1	D	100	GLU
1	D	104	LEU
1	D	106	ARG
1	D	112	LEU
1	D	119	LEU
1	D	121	SER
1	D	125	ASN
1	D	126	LEU
1	D	133	GLU
1	D	141	ARG
1	D	150	SER
1	D	211	ARG

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Mol	Chain	Res	Type
1	D	215	SER
1	D	220	GLN
1	D	230	VAL
1	D	239	LEU
1	D	276	ILE
1	D	290	LEU
1	D	301	PHE
1	D	302	LEU
1	D	306	VAL
1	D	308	GLU
1	D	310	SER
1	D	317	SER
1	E	3	LEU
1	E	21	ARG
1	E	27	THR
1	E	28	SER
1	E	31	VAL
1	E	33	VAL
1	E	46	LEU
1	E	57	LYS
1	E	60	LEU
1	E	61	LYS
1	E	64	ASP
1	E	67	VAL
1	E	78	LEU
1	E	85	ARG
1	E	90	VAL
1	E	93	MET
1	E	95	ASP
1	E	101	ARG
1	E	104	LEU
1	E	112	LEU
1	E	114	LEU
1	E	119	LEU
1	E	121	SER
1	E	122	LYS
1	E	127	ILE
1	E	129	ASP
1	E	131	LEU
1	E	139	ARG
1	E	141	ARG
1	E	142	GLN

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Mol	Chain	Res	Type
1	E	195	GLU
1	E	205	ASN
1	E	213	GLU
1	E	215	SER
1	E	220	GLN
1	E	225	ASN
1	E	230	VAL
1	E	233	ARG
1	E	235	VAL
1	E	239	LEU
1	E	254	LEU
1	E	257	GLU
1	E	264	ILE
1	E	282	GLU
1	E	296	ARG
1	E	299	SER
1	E	302	LEU
1	E	308	GLU
1	E	311	ASP
1	E	315	LEU
1	E	317	SER
1	F	3	LEU
1	F	6	SER
1	F	21	ARG
1	F	31	VAL
1	F	33	VAL
1	F	41	SER
1	F	46	LEU
1	F	48	LEU
1	F	61	LYS
1	F	65	THR
1	F	67	VAL
1	F	71	SER
1	F	74	VAL
1	F	78	LEU
1	F	96	THR
1	F	99	VAL
1	F	102	ARG
1	F	104	LEU
1	F	106	ARG
1	F	112	LEU
1	F	119	LEU

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Mol	Chain	Res	Type
1	F	121	SER
1	F	126	LEU
1	F	130	GLU
1	F	131	LEU
1	F	134	LYS
1	F	139	ARG
1	F	193	ARG
1	F	204	SER
1	F	220	GLN
1	F	230	VAL
1	F	235	VAL
1	F	239	LEU
1	F	244	GLU
1	F	248	ARG
1	F	254	LEU
1	F	278	GLU
1	F	300	THR
1	F	301	PHE
1	F	302	LEU
1	F	308	GLU
1	F	310	SER
1	F	312	ASP
1	F	317	SER
1	G	3	LEU
1	G	7	ILE
1	G	17	VAL
1	G	18	ARG
1	G	27	THR
1	G	28	SER
1	G	31	VAL
1	G	33	VAL
1	G	41	SER
1	G	46	LEU
1	G	48	LEU
1	G	57	LYS
1	G	61	LYS
1	G	65	THR
1	G	67	VAL
1	G	71	SER
1	G	78	LEU
1	G	85	ARG
1	G	88	ARG

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Mol	Chain	Res	Type
1	G	99	VAL
1	G	102	ARG
1	G	104	LEU
1	G	105	ILE
1	G	106	ARG
1	G	119	LEU
1	G	121	SER
1	G	122	LYS
1	G	126	LEU
1	G	193	ARG
1	G	202	GLU
1	G	215	SER
1	G	218	GLN
1	G	227	VAL
1	G	230	VAL
1	G	235	VAL
1	G	252	ARG
1	G	275	SER
1	G	298	LEU
1	G	300	THR
1	G	301	PHE
1	G	302	LEU
1	G	308	GLU
1	G	315	LEU
1	G	318	LEU
1	H	3	LEU
1	H	25	GLU
1	H	27	THR
1	H	28	SER
1	H	46	LEU
1	H	48	LEU
1	H	50	VAL
1	H	59	LEU
1	H	65	THR
1	H	67	VAL
1	H	69	CYS
1	H	71	SER
1	H	78	LEU
1	H	92	VAL
1	H	93	MET
1	H	95	ASP
1	H	101	ARG

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Mol	Chain	Res	Type
1	H	102	ARG
1	H	103	LYS
1	H	104	LEU
1	H	106	ARG
1	H	111	LYS
1	H	112	LEU
1	H	114	LEU
1	H	122	LYS
1	H	126	LEU
1	H	131	LEU
1	H	133	GLU
1	H	134	LYS
1	H	139	ARG
1	H	141	ARG
1	H	142	GLN
1	H	195	GLU
1	H	202	GLU
1	H	235	VAL
1	H	243	ASP
1	H	245	VAL
1	H	251	SER
1	H	265	SER
1	H	278	GLU
1	H	296	ARG
1	H	298	LEU
1	H	302	LEU
1	H	304	ASP
1	H	307	ASP
1	H	310	SER
1	H	317	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	171	HIS
1	B	5	ASN
1	C	171	HIS
1	C	217	HIS
1	D	125	ASN
1	E	171	HIS
1	E	218	GLN

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Mol	Chain	Res	Type
1	F	5	ASN
1	F	20	GLN
1	F	125	ASN
1	F	171	HIS
1	F	220	GLN
1	G	20	GLN
1	G	171	HIS
1	H	20	GLN
1	H	73	ASN
1	H	125	ASN
1	H	142	GLN
1	H	171	HIS

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	PLP	D	401	1	15,15,16	2.12	6 (40%)	21,22,23	1.46	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	C	401	1	15,15,16	2.19	7 (46%)	21,22,23	1.50	5 (23%)
2	PLP	F	401	1	15,15,16	2.19	7 (46%)	21,22,23	1.49	5 (23%)
2	PLP	G	401	1	15,15,16	2.12	6 (40%)	21,22,23	1.49	5 (23%)
2	PLP	H	401	1	15,15,16	2.13	6 (40%)	21,22,23	1.50	5 (23%)
2	PLP	A	401	1	15,15,16	2.15	7 (46%)	21,22,23	1.42	4 (19%)
2	PLP	B	401	1	15,15,16	2.12	6 (40%)	21,22,23	1.47	5 (23%)
2	PLP	E	401	1	15,15,16	2.22	6 (40%)	21,22,23	1.47	5 (23%)

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	PLP	D	401	1	-	0/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	F	401	1	-	0/6/6/8	0/1/1/1
2	PLP	G	401	1	-	0/6/6/8	0/1/1/1
2	PLP	H	401	1	-	0/6/6/8	0/1/1/1
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
2	PLP	E	401	1	-	0/6/6/8	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	PLP	C3-C2	-4.20	1.36	1.41
2	G	401	PLP	C2-N1	4.02	1.41	1.33
2	D	401	PLP	C2-N1	3.93	1.40	1.33
2	H	401	PLP	C2-N1	3.90	1.40	1.33
2	A	401	PLP	C4A-C4	3.89	1.59	1.51
2	E	401	PLP	C4A-C4	3.88	1.59	1.51
2	C	401	PLP	C4A-C4	3.87	1.59	1.51
2	C	401	PLP	C2-N1	3.84	1.40	1.33
2	F	401	PLP	C4A-C4	3.83	1.59	1.51
2	E	401	PLP	C2-N1	3.77	1.40	1.33
2	C	401	PLP	C3-C2	-3.76	1.37	1.41
2	F	401	PLP	C2-N1	3.73	1.40	1.33
2	A	401	PLP	C3-C2	-3.71	1.37	1.41
2	H	401	PLP	C4A-C4	3.71	1.59	1.51
2	G	401	PLP	C4A-C4	3.69	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C3-C2	-3.68	1.37	1.41
2	B	401	PLP	C2-N1	3.67	1.40	1.33
2	H	401	PLP	C3-C2	-3.65	1.37	1.41
2	A	401	PLP	C2-N1	3.63	1.40	1.33
2	B	401	PLP	C4A-C4	3.62	1.58	1.51
2	D	401	PLP	C4A-C4	3.52	1.58	1.51
2	D	401	PLP	C3-C2	-3.49	1.37	1.41
2	G	401	PLP	C3-C2	-3.47	1.37	1.41
2	F	401	PLP	C3-C2	-3.42	1.37	1.41
2	F	401	PLP	C5-C4	2.83	1.43	1.40
2	D	401	PLP	C6-C5	-2.81	1.32	1.37
2	F	401	PLP	C6-C5	-2.80	1.32	1.37
2	B	401	PLP	C6-C5	-2.80	1.32	1.37
2	G	401	PLP	C6-C5	-2.78	1.32	1.37
2	E	401	PLP	C6-C5	-2.77	1.32	1.37
2	A	401	PLP	C6-C5	-2.74	1.32	1.37
2	C	401	PLP	C6-C5	-2.69	1.32	1.37
2	H	401	PLP	C6-C5	-2.58	1.32	1.37
2	D	401	PLP	P-O3P	-2.35	1.46	1.54
2	D	401	PLP	P-O2P	-2.35	1.46	1.54
2	E	401	PLP	P-O3P	-2.30	1.46	1.54
2	C	401	PLP	P-O2P	-2.29	1.46	1.54
2	B	401	PLP	P-O2P	-2.28	1.46	1.54
2	H	401	PLP	P-O2P	-2.25	1.46	1.54
2	C	401	PLP	C5-C4	2.24	1.43	1.40
2	F	401	PLP	P-O3P	-2.23	1.46	1.54
2	F	401	PLP	P-O2P	-2.22	1.46	1.54
2	B	401	PLP	P-O3P	-2.22	1.46	1.54
2	E	401	PLP	P-O2P	-2.21	1.46	1.54
2	C	401	PLP	P-O3P	-2.20	1.46	1.54
2	A	401	PLP	C5-C4	2.20	1.43	1.40
2	A	401	PLP	P-O3P	-2.19	1.46	1.54
2	H	401	PLP	P-O3P	-2.17	1.46	1.54
2	G	401	PLP	P-O2P	-2.15	1.46	1.54
2	G	401	PLP	P-O3P	-2.14	1.46	1.54
2	A	401	PLP	P-O2P	-2.11	1.47	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PLP	C3-C2-N1	-3.03	117.14	120.96
2	F	401	PLP	C3-C2-N1	-2.99	117.19	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	PLP	C3-C2-N1	-2.96	117.23	120.96
2	E	401	PLP	O4P-C5A-C5	2.96	114.90	109.36
2	H	401	PLP	O4P-C5A-C5	2.95	114.89	109.36
2	C	401	PLP	C3-C2-N1	-2.92	117.28	120.96
2	D	401	PLP	C3-C2-N1	-2.89	117.32	120.96
2	E	401	PLP	C3-C2-N1	-2.88	117.32	120.96
2	A	401	PLP	C3-C2-N1	-2.88	117.33	120.96
2	C	401	PLP	O4P-C5A-C5	2.88	114.75	109.36
2	H	401	PLP	C3-C2-N1	-2.86	117.35	120.96
2	F	401	PLP	C6-N1-C2	2.84	124.36	119.20
2	B	401	PLP	C6-N1-C2	2.81	124.29	119.20
2	G	401	PLP	O4P-C5A-C5	2.77	114.54	109.36
2	C	401	PLP	C6-N1-C2	2.74	124.17	119.20
2	D	401	PLP	C6-N1-C2	2.69	124.08	119.20
2	H	401	PLP	C6-N1-C2	2.67	124.05	119.20
2	A	401	PLP	O4P-C5A-C5	2.64	114.30	109.36
2	G	401	PLP	C6-N1-C2	2.63	123.96	119.20
2	A	401	PLP	C6-N1-C2	2.62	123.94	119.20
2	E	401	PLP	C6-N1-C2	2.59	123.90	119.20
2	F	401	PLP	O4P-C5A-C5	2.51	114.07	109.36
2	B	401	PLP	O4P-C5A-C5	2.44	113.93	109.36
2	D	401	PLP	C5-C6-N1	-2.41	119.92	123.83
2	H	401	PLP	C5-C6-N1	-2.38	119.97	123.83
2	C	401	PLP	C5-C6-N1	-2.32	120.06	123.83
2	G	401	PLP	C5-C6-N1	-2.26	120.16	123.83
2	E	401	PLP	C5-C6-N1	-2.22	120.22	123.83
2	B	401	PLP	C5-C6-N1	-2.20	120.25	123.83
2	F	401	PLP	C5-C6-N1	-2.20	120.25	123.83
2	H	401	PLP	C2A-C2-N1	2.20	121.78	117.64
2	F	401	PLP	C5A-C5-C6	-2.19	115.78	119.36
2	A	401	PLP	C5-C6-N1	-2.13	120.36	123.83
2	D	401	PLP	O4P-C5A-C5	2.11	113.31	109.36
2	C	401	PLP	C2A-C2-N1	2.09	121.58	117.64
2	E	401	PLP	C2A-C2-N1	2.09	121.58	117.64
2	G	401	PLP	C2A-C2-N1	2.08	121.55	117.64
2	B	401	PLP	C2A-C2-N1	2.06	121.52	117.64
2	D	401	PLP	C6-C5-C4	2.00	119.74	118.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	316/332 (95%)	0.06	6 (1%) 66 67	23, 44, 86, 102	0
1	B	319/332 (96%)	0.13	12 (3%) 44 44	26, 46, 102, 114	0
1	C	317/332 (95%)	0.10	6 (1%) 66 67	22, 48, 89, 110	0
1	D	316/332 (95%)	-0.02	11 (3%) 47 47	22, 39, 97, 119	0
1	E	317/332 (95%)	0.45	16 (5%) 34 33	23, 52, 106, 126	0
1	F	316/332 (95%)	-0.00	5 (1%) 70 71	23, 41, 80, 93	0
1	G	317/332 (95%)	0.23	6 (1%) 66 67	27, 49, 90, 107	0
1	H	316/332 (95%)	0.36	24 (7%) 20 18	27, 47, 111, 132	0
All	All	2534/2656 (95%)	0.16	86 (3%) 48 48	22, 46, 99, 132	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	119	LEU	5.3
1	D	94	GLY	4.4
1	H	120	GLY	4.4
1	B	96	THR	4.3
1	A	317	SER	4.0
1	C	305	GLY	3.8
1	H	116	PRO	3.7
1	E	113	VAL	3.6
1	E	121	SER	3.5
1	D	119	LEU	3.5
1	H	121	SER	3.4
1	H	114	LEU	3.3
1	H	313	ALA	3.2
1	H	69	CYS	3.1
1	B	320	THR	3.1
1	H	94	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	318	LEU	3.1
1	B	119	LEU	3.0
1	G	306	VAL	3.0
1	D	317	SER	2.9
1	A	99	VAL	2.9
1	B	127	ILE	2.9
1	E	118	HIS	2.8
1	B	114	LEU	2.8
1	E	112	LEU	2.8
1	B	113	VAL	2.8
1	H	309	GLY	2.8
1	D	118	HIS	2.8
1	D	69	CYS	2.7
1	H	91	ALA	2.7
1	H	97	TYR	2.7
1	F	120	GLY	2.7
1	C	306	VAL	2.6
1	C	318	LEU	2.6
1	F	124	GLY	2.6
1	D	313	ALA	2.6
1	E	93	MET	2.6
1	H	99	VAL	2.6
1	E	128	ALA	2.5
1	E	313	ALA	2.5
1	G	315	LEU	2.5
1	B	126	LEU	2.5
1	H	118	HIS	2.5
1	D	93	MET	2.4
1	B	95	ASP	2.4
1	E	311	ASP	2.4
1	E	94	GLY	2.4
1	E	98	SER	2.4
1	F	121	SER	2.4
1	E	302	LEU	2.4
1	H	315	LEU	2.4
1	D	97	TYR	2.3
1	E	120	GLY	2.3
1	A	124	GLY	2.3
1	H	71	SER	2.3
1	G	112	LEU	2.2
1	H	306	VAL	2.3
1	G	225	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2	PRO	2.2
1	H	93	MET	2.2
1	A	27	THR	2.2
1	E	314	TRP	2.2
1	E	90	VAL	2.2
1	D	91	ALA	2.2
1	H	317	SER	2.2
1	C	314	TRP	2.1
1	B	227	VAL	2.1
1	H	113	VAL	2.1
1	H	115	PHE	2.1
1	D	310	SER	2.1
1	C	97	TYR	2.1
1	D	306	VAL	2.1
1	F	118	HIS	2.1
1	H	92	VAL	2.1
1	H	303	PHE	2.1
1	G	307	ASP	2.1
1	C	218	GLN	2.1
1	B	123	GLY	2.1
1	H	70	THR	2.1
1	A	316	ALA	2.1
1	A	306	VAL	2.1
1	H	96	THR	2.0
1	B	128	ALA	2.0
1	E	279	HIS	2.0
1	E	225	ASN	2.0
1	F	125	ASN	2.0

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(Å ²)	Q<0.9
2	PLP	B	401	15/16	0.95	0.08	31,38,41,41	0
2	PLP	C	401	15/16	0.96	0.07	37,42,45,46	0
2	PLP	G	401	15/16	0.96	0.07	36,39,43,46	0
2	PLP	H	401	15/16	0.96	0.07	36,41,43,43	0
2	PLP	E	401	15/16	0.97	0.07	43,45,48,49	0
2	PLP	F	401	15/16	0.98	0.05	27,30,33,34	0
2	PLP	D	401	15/16	0.98	0.06	28,32,34,34	0
2	PLP	A	401	15/16	0.98	0.05	30,34,36,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.