



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:17 PM UTC

PDB ID : 5C78 / pdb_00005c78
Title : ATP-driven lipid-linked oligosaccharide flippase PglK in apo-inward state (1)
Authors : Perez, C.; Locher, K.P.
Deposited on : 2015-06-24
Resolution : 2.90 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

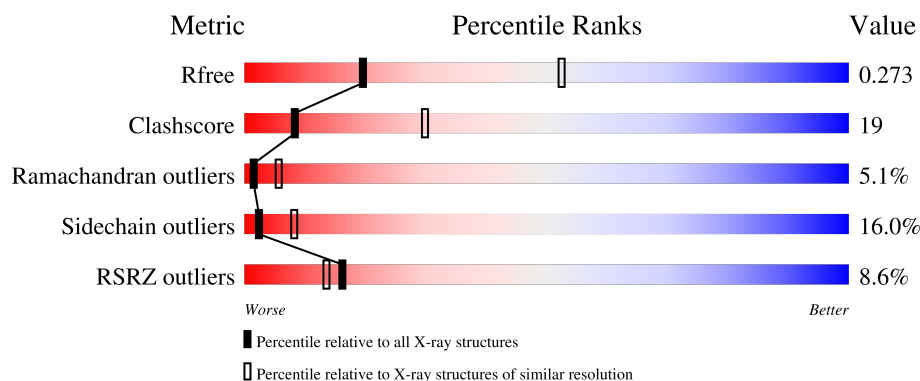
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	564	8% 52% 37% 10% .
1	B	564	10% 53% 35% 10% .
1	C	564	8% 52% 37% 10% .
1	D	564	9% 51% 35% 12% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18423 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.

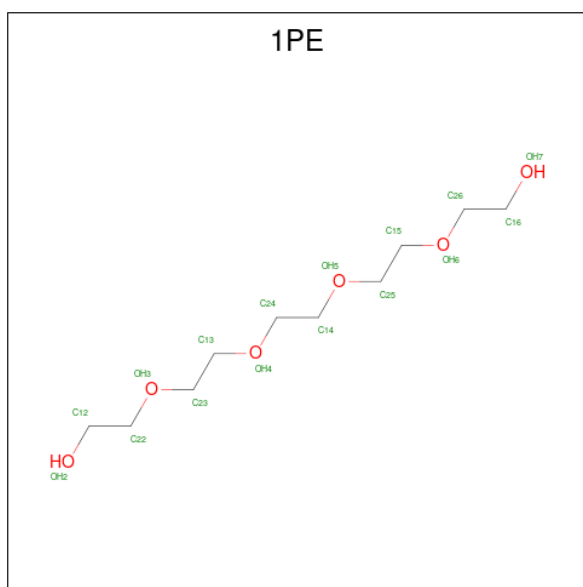
- Molecule 1 is a protein called ATP-driven flippase PglK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	B	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	C	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	D	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	conflict	UNP O86150
A	105	LYS	TYR	conflict	UNP O86150
A	510	GLN	GLU	conflict	UNP O86150
B	2	VAL	LEU	conflict	UNP O86150
B	105	LYS	TYR	conflict	UNP O86150
B	510	GLN	GLU	conflict	UNP O86150
C	2	VAL	LEU	conflict	UNP O86150
C	105	LYS	TYR	conflict	UNP O86150
C	510	GLN	GLU	conflict	UNP O86150
D	2	VAL	LEU	conflict	UNP O86150
D	105	LYS	TYR	conflict	UNP O86150
D	510	GLN	GLU	conflict	UNP O86150

- Molecule 2 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	10	6		
2	B	1	Total	C	O	0	0
			16	10	6		
2	B	1	Total	C	O	0	0
			16	10	6		
2	C	1	Total	C	O	0	0
			16	10	6		
2	D	1	Total	C	O	0	0
			16	10	6		

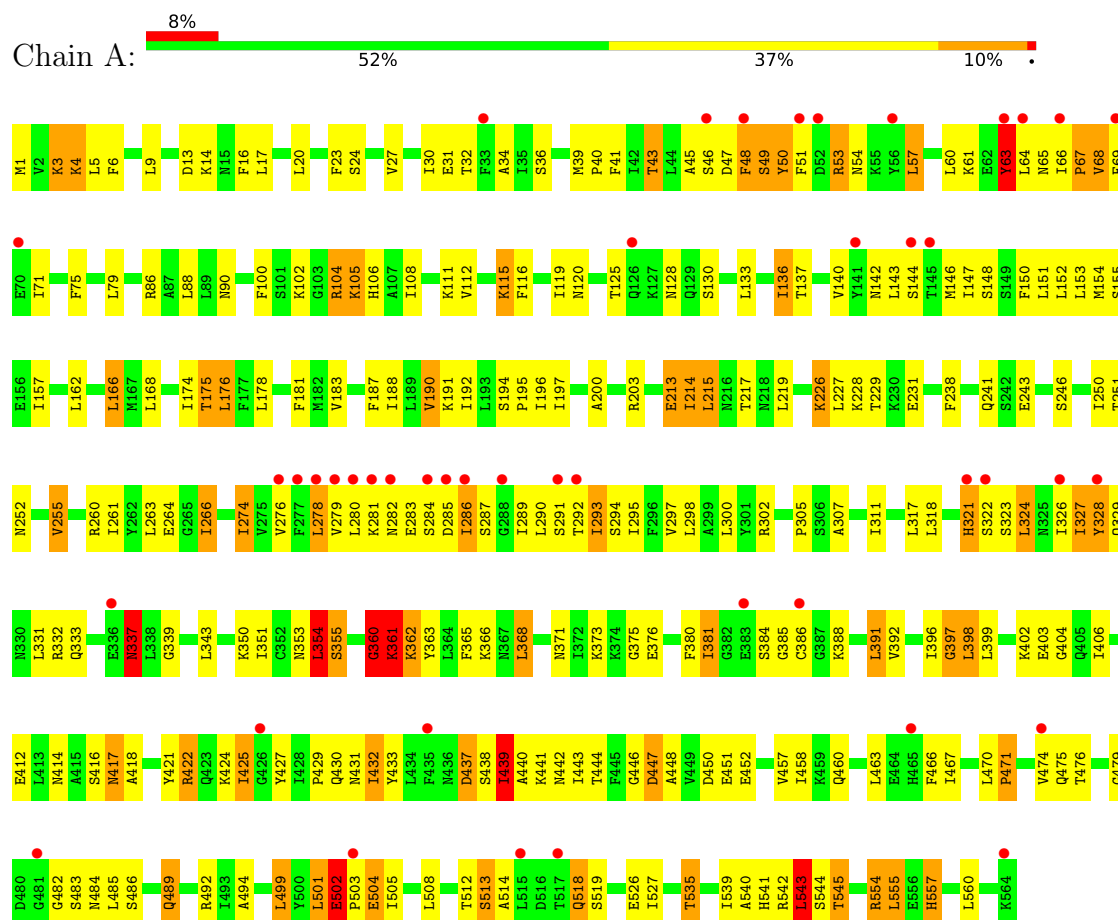
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	26	Total	O	0	0
			26	26		
3	C	27	Total	O	0	0
			27	27		
3	D	35	Total	O	0	0
			35	35		

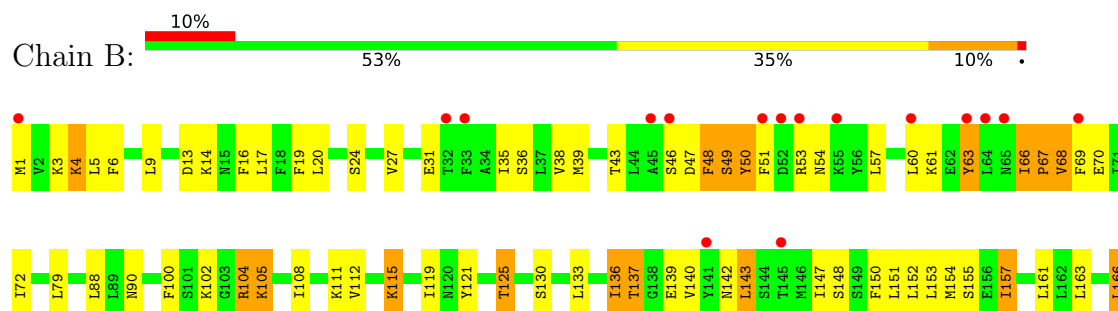
3 Residue-property plots

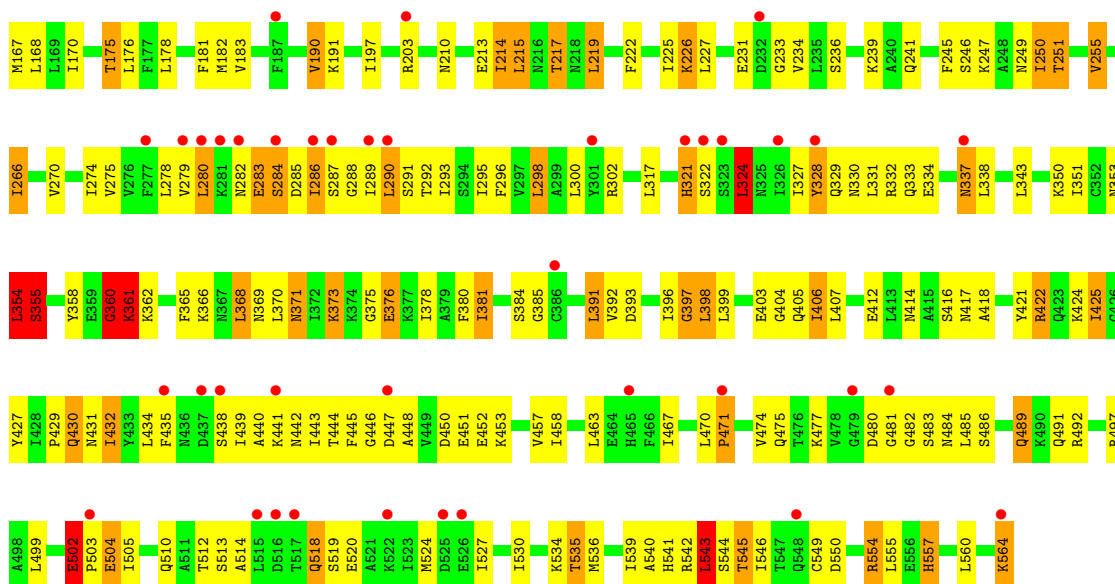
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP-driven flippase PgIK

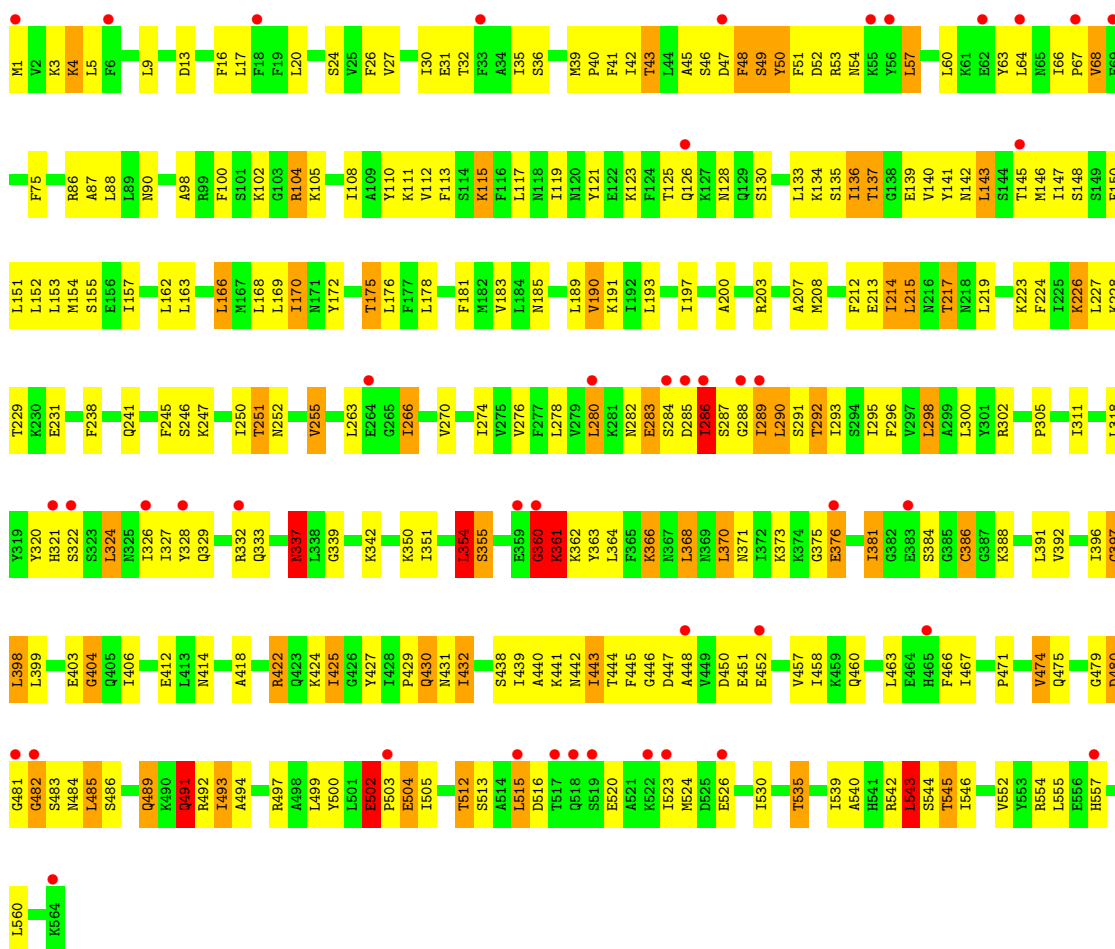


• Molecule 1: ATP-driven flippase PgIK





• Molecule 1: ATP-driven flippase PgIK



• Molecule 1: ATP-driven flippase PgIK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.60Å 114.42Å 145.59Å 68.44° 73.27° 68.67°	Depositor
Resolution (Å)	27.93 – 2.90 27.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	87.2 (27.93-2.90) 87.1 (27.93-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.232 , 0.267 0.240 , 0.273	Depositor DCC
R_{free} test set	5179 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18423	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: 1PE

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	0.69	1/4641 (0.0%)	1.08	16/6246 (0.3%)
1	B	0.68	0/4641	1.07	14/6246 (0.2%)
1	C	0.70	0/4641	1.08	21/6246 (0.3%)
1	D	0.72	1/4641 (0.0%)	1.11	16/6246 (0.3%)
All	All	0.70	2/18564 (0.0%)	1.09	67/24984 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	TYR	CA-C	-7.56	1.45	1.52
1	D	328	TYR	CA-C	-5.34	1.47	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	VAL	N-CA-C	-8.98	104.40	113.47
1	D	545	THR	N-CA-C	-8.88	101.78	114.12
1	A	279	VAL	N-CA-C	-8.59	104.80	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	397	GLY	N-CA-C	8.13	121.93	112.50
1	A	397	GLY	N-CA-C	7.53	121.24	112.50
1	B	545	THR	N-CA-C	-7.49	103.70	114.12
1	D	481	GLY	N-CA-C	-7.23	103.52	112.77
1	D	543	LEU	N-CA-C	-7.23	95.41	110.80
1	C	481	GLY	N-CA-C	-7.20	103.72	113.37
1	D	397	GLY	N-CA-C	7.20	120.85	112.50
1	B	397	GLY	N-CA-C	7.17	120.82	112.50
1	B	543	LEU	N-CA-C	-7.13	95.62	110.80
1	D	333	GLN	N-CA-C	-6.92	104.58	113.16
1	B	514	ALA	N-CA-C	-6.79	106.88	114.62
1	A	514	ALA	N-CA-C	-6.75	106.93	114.62
1	B	360	GLY	CA-C-N	6.65	133.68	121.70
1	B	360	GLY	C-N-CA	6.65	133.68	121.70
1	B	324	LEU	N-CA-C	6.54	119.38	111.40
1	A	543	LEU	N-CA-C	-6.49	96.97	110.80
1	A	354	LEU	N-CA-C	6.33	117.87	110.97
1	C	545	THR	N-CA-C	-6.25	105.43	114.12
1	B	333	GLN	N-CA-C	-6.24	105.43	113.16
1	D	282	ASN	CA-C-N	6.12	132.72	121.70
1	D	282	ASN	C-N-CA	6.12	132.72	121.70
1	A	63	TYR	N-CA-C	-6.11	105.79	113.18
1	A	45	ALA	N-CA-C	-6.09	105.84	113.20
1	A	339	GLY	N-CA-C	6.03	120.27	112.18
1	A	360	GLY	CA-C-N	6.01	132.51	121.70
1	A	360	GLY	C-N-CA	6.01	132.51	121.70
1	C	360	GLY	CA-C-N	6.00	132.49	121.70
1	C	360	GLY	C-N-CA	6.00	132.49	121.70
1	C	441	LYS	N-CA-C	-5.94	99.05	108.73
1	C	354	LEU	N-CA-C	5.89	117.39	110.97
1	D	118	ASN	N-CA-C	5.87	120.44	113.28
1	A	437	ASP	N-CA-C	5.82	115.53	107.73
1	C	425	ILE	N-CA-C	5.77	116.43	108.12
1	A	333	GLN	N-CA-C	-5.74	106.05	113.16
1	C	63	TYR	N-CA-C	-5.72	106.25	113.18
1	C	543	LEU	N-CA-C	-5.72	98.62	110.80
1	D	425	ILE	N-CA-C	5.69	116.32	108.12
1	A	105	LYS	N-CA-C	-5.69	104.98	111.07
1	B	63	TYR	N-CA-C	-5.67	106.36	113.28
1	C	45	ALA	N-CA-C	-5.66	106.33	113.18
1	B	385	GLY	N-CA-C	-5.64	106.97	115.32
1	A	385	GLY	N-CA-C	-5.63	106.99	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	386	CYS	N-CA-C	-5.54	106.48	113.18
1	D	482	GLY	N-CA-C	-5.54	100.05	113.18
1	C	170	ILE	N-CA-C	5.52	116.15	110.36
1	C	339	GLY	N-CA-C	5.48	118.90	111.72
1	D	360	GLY	CA-C-N	5.43	131.48	121.70
1	D	360	GLY	C-N-CA	5.43	131.48	121.70
1	C	482	GLY	N-CA-C	-5.41	100.36	113.18
1	D	354	LEU	N-CA-C	5.41	116.86	110.97
1	C	376	GLU	N-CA-C	5.39	118.08	111.82
1	C	342	LYS	N-CA-C	5.37	118.68	110.36
1	C	491	GLN	N-CA-C	5.36	116.81	111.07
1	A	545	THR	N-CA-C	-5.29	106.76	114.12
1	B	328	TYR	N-CA-C	-5.27	105.97	112.72
1	C	364	LEU	N-CA-C	-5.22	106.75	113.23
1	B	354	LEU	N-CA-C	5.17	117.33	111.02
1	C	333	GLN	N-CA-C	-5.14	106.85	113.02
1	D	339	GLY	N-CA-C	5.12	118.43	111.72
1	A	501	LEU	N-CA-C	-5.11	105.89	111.82
1	C	404	GLY	N-CA-C	5.11	121.77	112.27
1	D	105	LYS	N-CA-C	-5.05	105.67	111.07
1	B	287	SER	N-CA-C	-5.04	105.97	111.82
1	B	481	GLY	N-CA-C	-5.02	106.34	112.77

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	502	GLU	Peptide
1	B	502	GLU	Peptide
1	C	502	GLU	Peptide
1	D	502	GLU	Peptide

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	4557	0	4764	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4557	0	4764	193	0
1	C	4557	0	4764	185	0
1	D	4557	0	4764	198	0
2	A	16	0	22	0	0
2	B	32	0	44	1	0
2	C	16	0	22	1	0
2	D	16	0	22	1	0
3	A	27	0	0	0	0
3	B	26	0	0	1	0
3	C	27	0	0	0	0
3	D	35	0	0	5	0
All	All	18423	0	19166	719	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 19.

All (719) 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:4:LYS:HG3	1:A:329:GLN:HG3	1.44	1.00
1:C:4:LYS:HG3	1:C:329:GLN:HG3	1.45	0.98
1:B:4:LYS:HG3	1:B:329:GLN:HG3	1.46	0.98
1:D:4:LYS:HG3	1:D:329:GLN:HG3	1.48	0.95
1:B:119:ILE:O	1:C:226:LYS:NZ	2.00	0.94
1:A:425:ILE:HG22	1:A:505:ILE:HB	1.48	0.94
1:D:425:ILE:HG22	1:D:505:ILE:HB	1.50	0.93
1:C:425:ILE:HG22	1:C:505:ILE:HB	1.48	0.93
1:C:355:SER:HB2	1:C:403:GLU:HB2	1.48	0.93
1:D:355:SER:HB2	1:D:403:GLU:HB2	1.52	0.92
1:B:425:ILE:HG22	1:B:505:ILE:HB	1.53	0.90
1:C:214:ILE:HD11	1:C:238:PHE:HA	1.57	0.87
1:A:486:SER:OG	1:A:489:GLN:NE2	2.09	0.86
1:A:49:SER:O	1:A:51:PHE:N	2.08	0.85
1:B:49:SER:O	1:B:51:PHE:N	2.10	0.84
1:D:49:SER:O	1:D:51:PHE:N	2.12	0.83
1:A:375:GLY:H	1:A:535:THR:HB	1.43	0.83
1:D:520:GLU:OE2	1:D:542:ARG:NH1	2.11	0.83
1:A:438:SER:O	1:A:440:ALA:N	2.13	0.82
1:A:215:LEU:HD21	1:D:136:ILE:HD11	1.63	0.81
1:A:397:GLY:HA3	1:A:422:ARG:HD2	1.63	0.80
1:B:397:GLY:HA3	1:B:422:ARG:HD2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:SER:O	1:C:440:ALA:N	2.16	0.79
1:B:412:GLU:HG2	1:B:414:ASN:HD22	1.46	0.79
1:B:48:PHE:HE1	1:B:68:VAL:HB	1.46	0.79
1:D:375:GLY:H	1:D:535:THR:HB	1.48	0.78
1:B:51:PHE:HB3	1:B:61:LYS:HG3	1.66	0.78
1:C:450:ASP:O	1:C:452:GLU:N	2.16	0.78
1:C:49:SER:O	1:C:51:PHE:N	2.17	0.77
1:B:438:SER:O	1:B:440:ALA:N	2.18	0.76
1:A:188:ILE:HA	1:A:192:ILE:HD12	1.67	0.76
1:D:438:SER:O	1:D:440:ALA:N	2.18	0.76
1:B:227:LEU:HD22	1:C:425:ILE:HD11	1.67	0.75
1:D:1:MET:HA	1:D:4:LYS:HD3	1.69	0.75
1:A:492:ARG:NH1	1:A:526:GLU:OE1	2.20	0.74
1:B:503:PRO:HB2	1:B:504:GLU:HG2	1.69	0.73
1:C:502:GLU:HB2	1:C:503:PRO:HD3	1.69	0.73
1:C:486:SER:OG	1:C:489:GLN:OE1	2.05	0.73
1:D:335:GLU:H	1:D:335:GLU:CD	1.96	0.73
1:D:412:GLU:HG2	1:D:414:ASN:HD22	1.53	0.73
1:D:430:GLN:HG2	1:D:491:GLN:HE22	1.54	0.73
1:B:360:GLY:HA3	1:B:361:LYS:HB2	1.69	0.73
1:B:286:ILE:HG21	1:C:286:ILE:HD12	1.69	0.73
1:A:555:LEU:HB2	1:A:560:LEU:HD12	1.70	0.72
1:A:13:ASP:OD1	1:A:104:ARG:NH1	2.23	0.72
1:A:427:TYR:HE2	1:A:429:PRO:HB3	1.54	0.72
1:D:450:ASP:O	1:D:452:GLU:N	2.23	0.72
1:B:48:PHE:CE1	1:B:68:VAL:HB	2.24	0.72
1:D:503:PRO:HB2	1:D:504:GLU:HG2	1.70	0.72
1:A:250:ILE:HG22	1:D:102:LYS:HB2	1.73	0.71
1:C:1:MET:HA	1:C:4:LYS:HD3	1.72	0.71
1:A:291:SER:O	1:A:294:SER:OG	2.09	0.71
1:D:424:LYS:HB2	1:D:504:GLU:HG3	1.72	0.71
1:B:350:LYS:HA	1:B:371:ASN:HB3	1.73	0.70
1:C:197:ILE:HD13	1:C:255:VAL:HG13	1.72	0.70
1:A:414:ASN:OD1	1:A:416:SER:OG	2.10	0.70
1:B:450:ASP:O	1:B:452:GLU:N	2.25	0.70
1:B:424:LYS:HB2	1:B:504:GLU:HG3	1.73	0.70
1:B:375:GLY:H	1:B:535:THR:HB	1.57	0.69
1:C:111:LYS:HB3	1:C:332:ARG:HH12	1.57	0.69
1:D:430:GLN:N	3:D:701:HOH:O	2.10	0.69
1:D:502:GLU:HB2	1:D:503:PRO:HD3	1.73	0.69
1:B:250:ILE:HG22	1:C:102:LYS:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASN:O	1:B:444:THR:N	2.26	0.68
1:A:36:SER:HB3	1:A:166:LEU:HD11	1.74	0.68
1:C:555:LEU:HB2	1:C:560:LEU:HD12	1.75	0.68
1:C:427:TYR:HE2	1:C:429:PRO:HB3	1.59	0.67
1:D:19:PHE:HE1	1:D:23:PHE:HD2	1.42	0.67
1:D:290:LEU:HA	1:D:293:ILE:HG22	1.75	0.67
1:D:430:GLN:HG2	1:D:491:GLN:NE2	2.09	0.67
1:C:492:ARG:NH1	1:C:526:GLU:OE1	2.27	0.67
1:C:442:ASN:O	1:C:445:PHE:N	2.19	0.67
1:D:397:GLY:HA3	1:D:422:ARG:HD2	1.76	0.66
1:C:112:VAL:HG12	1:C:136:ILE:HG22	1.77	0.66
1:C:503:PRO:HB2	1:C:504:GLU:HG2	1.76	0.66
1:D:442:ASN:O	1:D:444:THR:N	2.29	0.66
1:A:227:LEU:HD22	1:D:425:ILE:HD11	1.78	0.65
1:A:328:TYR:O	1:A:332:ARG:HG2	1.96	0.65
1:D:115:LYS:HD2	1:D:334:GLU:HB3	1.78	0.65
1:A:9:LEU:HD22	1:A:13:ASP:HB3	1.79	0.65
1:A:518:GLN:OE1	1:A:519:SER:N	2.23	0.65
1:D:178:LEU:HD13	1:D:300:LEU:HD11	1.79	0.65
1:D:492:ARG:NH1	1:D:526:GLU:OE1	2.30	0.65
1:A:108:ILE:O	1:A:112:VAL:HG23	1.97	0.65
1:C:115:LYS:HG2	1:C:332:ARG:HA	1.79	0.65
1:D:146:MET:SD	1:D:321:HIS:ND1	2.67	0.65
1:B:502:GLU:HB2	1:B:503:PRO:HD3	1.79	0.64
1:C:427:TYR:CE2	1:C:429:PRO:HB3	2.32	0.64
1:D:427:TYR:HE2	1:D:429:PRO:HB3	1.60	0.64
1:B:69:PHE:HE2	1:C:282:ASN:HD22	1.45	0.64
1:C:146:MET:SD	1:C:321:HIS:ND1	2.66	0.64
1:A:20:LEU:HB3	1:A:151:LEU:HD13	1.79	0.64
1:D:197:ILE:HD13	1:D:255:VAL:HG13	1.80	0.64
1:D:427:TYR:CE2	1:D:429:PRO:HB3	2.34	0.64
1:C:375:GLY:H	1:C:535:THR:HB	1.63	0.63
1:C:190:VAL:HG13	1:C:191:LYS:HG2	1.80	0.63
1:D:518:GLN:CD	1:D:518:GLN:H	2.05	0.63
1:A:354:LEU:HA	1:A:404:GLY:HA3	1.81	0.63
1:A:424:LYS:HB2	1:A:504:GLU:HG3	1.80	0.63
1:B:328:TYR:O	1:B:332:ARG:HG2	1.99	0.63
1:A:285:ASP:O	1:A:287:SER:N	2.32	0.63
1:A:503:PRO:HB2	1:A:504:GLU:HG2	1.79	0.63
1:B:215:LEU:HD13	1:C:133:LEU:HD11	1.80	0.63
1:A:243:GLU:HG3	1:D:106:HIS:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:HG2	1:A:414:ASN:HD22	1.63	0.63
1:A:102:LYS:HB2	1:D:250:ILE:HG22	1.81	0.62
1:A:112:VAL:HG22	1:A:332:ARG:HH21	1.64	0.62
1:A:140:VAL:HG22	1:A:328:TYR:OH	2.00	0.62
1:A:355:SER:HB2	1:A:403:GLU:HB2	1.81	0.62
1:A:392:VAL:HG21	1:A:539:ILE:HG12	1.82	0.62
1:B:139:GLU:O	1:B:328:TYR:OH	2.17	0.62
1:D:9:LEU:HD22	1:D:13:ASP:HB3	1.81	0.62
1:D:115:LYS:HG2	1:D:332:ARG:HA	1.81	0.62
1:A:450:ASP:O	1:A:452:GLU:N	2.32	0.62
1:B:36:SER:HB3	1:B:166:LEU:HD11	1.81	0.62
1:B:520:GLU:OE1	1:B:542:ARG:NH1	2.32	0.62
1:B:1:MET:HA	1:B:4:LYS:HD3	1.80	0.62
1:C:397:GLY:HA3	1:C:422:ARG:HD2	1.81	0.62
1:A:200:ALA:HB1	1:A:252:ASN:HA	1.82	0.61
1:A:486:SER:HG	1:A:489:GLN:HE22	1.42	0.61
1:B:16:PHE:CD2	1:B:100:PHE:HD1	2.18	0.61
1:C:354:LEU:HA	1:C:404:GLY:HA3	1.81	0.61
1:B:197:ILE:HD13	1:B:255:VAL:HG13	1.82	0.61
1:B:181:PHE:HZ	1:B:266:ILE:HG13	1.66	0.61
1:A:427:TYR:CE2	1:A:429:PRO:HB3	2.36	0.61
1:A:502:GLU:HB2	1:A:503:PRO:HD3	1.83	0.61
1:C:139:GLU:O	1:C:328:TYR:OH	2.18	0.61
1:D:214:ILE:HD11	1:D:238:PHE:HA	1.83	0.61
1:D:458:ILE:HG23	1:D:463:LEU:HB2	1.82	0.61
1:A:136:ILE:HD11	1:D:215:LEU:HD11	1.82	0.60
1:A:39:MET:HE1	1:A:292:THR:HG22	1.83	0.60
1:D:48:PHE:HE1	1:D:68:VAL:HB	1.66	0.60
1:A:360:GLY:CA	1:A:361:LYS:HB2	2.31	0.60
1:D:153:LEU:O	1:D:157:ILE:HG23	2.00	0.60
1:A:48:PHE:HE1	1:A:68:VAL:HB	1.67	0.60
1:C:20:LEU:HB3	1:C:151:LEU:HD13	1.83	0.60
1:B:435:PHE:H	1:B:442:ASN:HD21	1.49	0.60
1:A:354:LEU:HB2	1:A:368:LEU:HB3	1.82	0.59
1:C:181:PHE:HZ	1:C:266:ILE:HG13	1.66	0.59
1:C:282:ASN:O	1:C:283:GLU:HB2	2.01	0.59
1:C:412:GLU:HG2	1:C:414:ASN:HD22	1.67	0.59
1:A:283:GLU:O	1:A:285:ASP:N	2.35	0.59
1:D:200:ALA:HB1	1:D:252:ASN:HA	1.84	0.59
1:D:492:ARG:NH1	1:D:523:ILE:HG12	2.17	0.59
1:C:438:SER:HB2	1:C:475:GLN:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG12	1:A:136:ILE:HG22	1.85	0.59
1:B:543:LEU:O	1:B:545:THR:N	2.35	0.59
1:D:51:PHE:CE1	1:D:57:LEU:HD12	2.37	0.59
1:A:168:LEU:HA	1:A:175:THR:HG21	1.85	0.59
1:B:175:THR:HG22	1:B:296:PHE:HZ	1.67	0.59
1:C:178:LEU:HD13	1:C:300:LEU:HD11	1.85	0.59
1:D:108:ILE:O	1:D:112:VAL:HG23	2.03	0.59
1:C:424:LYS:HB2	1:C:504:GLU:HG3	1.84	0.59
1:A:281:LYS:O	1:A:283:GLU:N	2.36	0.58
1:B:284:SER:C	1:B:286:ILE:H	2.11	0.58
1:B:368:LEU:HD11	1:B:560:LEU:HD22	1.84	0.58
1:C:418:ALA:O	1:C:422:ARG:HD3	2.03	0.58
1:C:457:VAL:HG21	1:C:500:TYR:HA	1.84	0.58
1:B:354:LEU:HB2	1:B:368:LEU:HB3	1.86	0.58
1:B:421:TYR:O	1:B:424:LYS:HG2	2.02	0.58
1:A:31:GLU:HG3	1:A:302:ARG:HH22	1.68	0.58
1:C:350:LYS:HA	1:C:371:ASN:HB3	1.85	0.58
1:D:143:LEU:O	1:D:147:ILE:HG13	2.04	0.58
1:B:557:HIS:O	1:B:557:HIS:ND1	2.36	0.57
1:B:136:ILE:HD11	1:C:215:LEU:HD21	1.85	0.57
1:D:35:ILE:HG23	1:D:298:LEU:HB3	1.85	0.57
1:D:375:GLY:N	1:D:535:THR:HB	2.18	0.57
1:A:49:SER:OG	1:A:53:ARG:NE	2.38	0.57
1:C:142:ASN:HD22	1:C:324:LEU:HD21	1.69	0.57
1:C:392:VAL:O	1:C:396:ILE:HG12	2.04	0.57
1:C:432:ILE:HD13	1:C:494:ALA:HB2	1.85	0.57
1:B:360:GLY:CA	1:B:361:LYS:HB2	2.34	0.57
1:A:326:ILE:C	1:A:328:TYR:H	2.13	0.57
1:D:392:VAL:O	1:D:396:ILE:HG12	2.04	0.57
1:A:215:LEU:HD13	1:D:133:LEU:HD11	1.85	0.57
1:A:100:PHE:HE2	1:A:147:ILE:HG21	1.70	0.57
1:D:328:TYR:O	1:D:332:ARG:HG2	2.05	0.57
1:B:102:LYS:HB2	1:C:250:ILE:HG22	1.87	0.57
1:D:482:GLY:HA2	1:D:483:SER:HB3	1.87	0.57
1:C:51:PHE:CE1	1:C:57:LEU:HD12	2.39	0.57
1:A:142:ASN:HB2	1:A:324:LEU:HG	1.87	0.56
1:A:388:LYS:NZ	1:A:540:ALA:O	2.31	0.56
1:B:520:GLU:CD	1:B:542:ARG:HH12	2.13	0.56
1:C:16:PHE:CD2	1:C:100:PHE:HD1	2.23	0.56
1:C:502:GLU:HB2	1:C:503:PRO:CD	2.34	0.56
1:D:418:ALA:O	1:D:422:ARG:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PHE:CD2	1:A:100:PHE:HD1	2.23	0.56
1:A:197:ILE:HD13	1:A:255:VAL:HG13	1.88	0.56
1:A:442:ASN:H	1:A:442:ASN:ND2	2.03	0.56
1:A:479:GLY:O	1:A:483:SER:HB3	2.05	0.56
1:B:49:SER:OG	1:B:50:TYR:N	2.37	0.56
1:B:543:LEU:C	1:B:545:THR:H	2.14	0.56
1:C:141:TYR:O	1:C:145:THR:HG22	2.05	0.56
1:D:20:LEU:HB3	1:D:151:LEU:HD13	1.86	0.56
1:A:174:ILE:HD11	1:A:278:LEU:HD22	1.86	0.56
1:A:34:ALA:HB2	1:A:86:ARG:HD3	1.85	0.56
1:C:247:LYS:O	1:C:251:THR:HG23	2.06	0.56
1:A:41:PHE:HD1	1:A:75:PHE:HD2	1.52	0.56
1:D:392:VAL:HG21	1:D:539:ILE:HG12	1.87	0.56
1:B:418:ALA:O	1:B:422:ARG:HD3	2.06	0.56
1:B:483:SER:OG	1:B:484:ASN:N	2.32	0.56
1:A:512:THR:HG22	1:A:541:HIS:CD2	2.42	0.55
1:C:392:VAL:HG21	1:C:539:ILE:HG12	1.88	0.55
1:D:66:ILE:HB	1:D:70:GLU:HB2	1.87	0.55
1:D:105:LYS:HA	1:D:140:VAL:HG12	1.89	0.55
1:A:447:ASP:OD2	1:D:228:LYS:NZ	2.30	0.55
1:C:429:PRO:O	1:C:431:ASN:N	2.40	0.55
1:C:360:GLY:CA	1:C:361:LYS:HB2	2.36	0.55
1:D:485:LEU:HD21	1:D:493:ILE:HD12	1.88	0.55
1:B:181:PHE:CZ	1:B:266:ILE:HG13	2.42	0.54
1:D:555:LEU:HB2	1:D:560:LEU:HD12	1.88	0.54
1:D:429:PRO:O	1:D:431:ASN:N	2.40	0.54
1:C:351:ILE:HG13	1:C:370:LEU:HG	1.89	0.54
1:D:4:LYS:CG	1:D:329:GLN:HG3	2.32	0.54
1:D:111:LYS:HB3	1:D:332:ARG:HH12	1.73	0.54
1:D:343:LEU:HD22	1:D:417:ASN:ND2	2.22	0.54
1:A:360:GLY:HA3	1:A:361:LYS:HB2	1.88	0.54
1:A:375:GLY:N	1:A:535:THR:HB	2.20	0.54
1:A:285:ASP:HB3	1:A:289:ILE:H	1.73	0.54
1:A:24:SER:HB3	1:A:155:SER:HB2	1.90	0.54
1:A:368:LEU:HD11	1:A:560:LEU:HD22	1.90	0.54
1:D:39:MET:HE2	1:D:295:ILE:HG13	1.89	0.54
1:D:373:LYS:HB2	1:D:376:GLU:HG3	1.90	0.54
1:A:146:MET:SD	1:A:321:HIS:ND1	2.77	0.54
1:A:41:PHE:HD1	1:A:75:PHE:CD2	2.26	0.53
1:C:520:GLU:CD	1:C:542:ARG:HH12	2.17	0.53
1:D:16:PHE:CD2	1:D:100:PHE:HD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LEU:HA	1:D:404:GLY:HA3	1.89	0.53
1:B:355:SER:HB2	1:B:403:GLU:HB2	1.89	0.53
1:B:414:ASN:OD1	1:B:416:SER:OG	2.25	0.53
1:C:466:PHE:CE1	1:C:489:GLN:HG2	2.43	0.53
1:C:482:GLY:HA2	1:C:483:SER:OG	2.07	0.53
1:D:453:LYS:HD3	1:D:500:TYR:O	2.08	0.53
1:A:442:ASN:H	1:A:442:ASN:HD22	1.54	0.53
1:B:283:GLU:O	1:B:285:ASP:N	2.41	0.53
1:B:427:TYR:HE2	1:B:429:PRO:HB3	1.73	0.53
1:C:285:ASP:O	1:C:288:GLY:N	2.41	0.53
1:C:442:ASN:H	1:C:442:ASN:ND2	2.06	0.53
1:D:133:LEU:O	1:D:137:THR:HB	2.09	0.53
1:B:215:LEU:HD21	1:C:136:ILE:HD11	1.89	0.53
1:B:427:TYR:CE2	1:B:429:PRO:HB3	2.44	0.53
1:D:48:PHE:CE1	1:D:68:VAL:HB	2.44	0.53
1:C:112:VAL:CG1	1:C:136:ILE:HG22	2.38	0.53
1:A:429:PRO:O	1:A:431:ASN:N	2.42	0.53
1:B:360:GLY:HA3	1:B:361:LYS:CB	2.39	0.53
1:B:442:ASN:O	1:B:445:PHE:N	2.23	0.53
1:A:446:GLY:O	1:A:448:ALA:N	2.42	0.53
1:B:143:LEU:O	1:B:147:ILE:HG13	2.09	0.53
1:C:354:LEU:O	1:C:404:GLY:N	2.42	0.53
1:D:543:LEU:O	1:D:545:THR:N	2.42	0.53
1:C:483:SER:OG	1:C:484:ASN:N	2.33	0.53
1:D:323:SER:O	1:D:327:ILE:HG13	2.08	0.53
1:B:24:SER:HB3	1:B:155:SER:HB2	1.90	0.52
1:B:429:PRO:O	1:B:431:ASN:N	2.42	0.52
1:C:24:SER:HB3	1:C:155:SER:HB2	1.91	0.52
1:C:388:LYS:NZ	1:C:540:ALA:O	2.42	0.52
1:A:380:PHE:CE1	1:A:391:LEU:HD13	2.44	0.52
1:B:178:LEU:HD13	1:B:300:LEU:HD11	1.90	0.52
1:B:215:LEU:HD13	1:C:133:LEU:CD1	2.39	0.52
1:D:111:LYS:CB	1:D:332:ARG:HH22	2.22	0.52
1:A:48:PHE:CE1	1:A:68:VAL:HB	2.44	0.52
1:B:213:GLU:O	1:B:217:THR:HG23	2.09	0.52
1:B:438:SER:HB2	1:B:475:GLN:HA	1.90	0.52
1:B:482:GLY:HA2	1:B:483:SER:OG	2.10	0.52
1:B:285:ASP:CG	1:B:288:GLY:HA3	2.35	0.52
1:C:36:SER:HB3	1:C:166:LEU:HD11	1.92	0.52
1:A:63:TYR:O	1:A:65:ASN:N	2.43	0.52
1:D:368:LEU:HD11	1:D:560:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:VAL:HG22	1:D:499:LEU:HB3	1.91	0.52
1:A:381:ILE:HG21	1:A:554:ARG:NH1	2.25	0.52
1:C:286:ILE:O	1:C:289:ILE:HG23	2.10	0.52
1:C:355:SER:CB	1:C:403:GLU:HB2	2.31	0.52
1:B:9:LEU:HD22	1:B:13:ASP:HB3	1.92	0.52
1:D:197:ILE:HD12	1:D:256:ALA:HA	1.92	0.52
1:B:20:LEU:HB3	1:B:151:LEU:HD13	1.91	0.51
1:C:48:PHE:HE1	1:C:68:VAL:HB	1.76	0.51
1:A:421:TYR:O	1:A:424:LYS:HG2	2.11	0.51
1:B:290:LEU:HD23	1:C:42:ILE:HD11	1.92	0.51
1:C:320:TYR:HA	1:C:324:LEU:HD23	1.92	0.51
1:A:40:PRO:HA	1:A:43:THR:HG22	1.91	0.51
1:C:442:ASN:H	1:C:442:ASN:HD22	1.57	0.51
1:C:543:LEU:C	1:C:545:THR:H	2.18	0.51
1:A:543:LEU:O	1:A:545:THR:N	2.43	0.51
1:D:111:LYS:HB3	1:D:332:ARG:HH22	1.75	0.51
1:B:392:VAL:HG21	1:B:539:ILE:HG12	1.92	0.51
1:A:106:HIS:CE1	1:D:243:GLU:HG3	2.46	0.51
1:A:47:ASP:OD2	1:A:49:SER:HB3	2.11	0.51
1:B:286:ILE:HG22	1:C:287:SER:HB2	1.91	0.51
1:D:279:VAL:HA	1:D:282:ASN:OD1	2.10	0.51
1:A:442:ASN:O	1:A:444:THR:N	2.43	0.51
1:A:501:LEU:HD23	3:D:707:HOH:O	2.10	0.51
1:C:360:GLY:HA3	1:C:361:LYS:HB2	1.93	0.51
1:D:40:PRO:HA	1:D:43:THR:HG22	1.93	0.51
1:D:502:GLU:HB2	1:D:503:PRO:CD	2.40	0.51
1:C:486:SER:H	1:C:489:GLN:NE2	2.09	0.51
1:D:167:MET:C	1:D:175:THR:HG21	2.35	0.51
1:D:339:GLY:HA3	1:D:415:ALA:O	2.11	0.51
1:D:354:LEU:HB2	1:D:368:LEU:HB3	1.93	0.51
1:B:290:LEU:HD13	1:B:290:LEU:O	2.11	0.50
1:A:31:GLU:HG3	1:A:302:ARG:NH2	2.26	0.50
1:B:13:ASP:CG	1:B:104:ARG:HD2	2.36	0.50
1:B:175:THR:HG22	1:B:296:PHE:CZ	2.44	0.50
1:A:418:ALA:O	1:A:422:ARG:HD3	2.12	0.50
1:D:360:GLY:CA	1:D:361:LYS:HB2	2.41	0.50
1:A:30:ILE:HG22	1:A:86:ARG:HG3	1.92	0.50
1:C:200:ALA:HB1	1:C:252:ASN:HA	1.94	0.50
1:C:446:GLY:O	1:C:448:ALA:N	2.44	0.50
1:D:167:MET:HE2	1:D:175:THR:HB	1.93	0.50
1:B:150:PHE:CZ	1:B:154:MET:HE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:PHE:HE2	1:C:121:TYR:HA	1.75	0.50
1:D:309:ARG:O	1:D:313:SER:HB3	2.12	0.50
1:B:121:TYR:O	1:B:125:THR:HB	2.10	0.50
1:C:153:LEU:O	1:C:157:ILE:HG23	2.11	0.50
1:A:181:PHE:HZ	1:A:266:ILE:HD12	1.76	0.50
1:B:111:LYS:HB3	1:B:332:ARG:HH22	1.77	0.50
1:B:292:THR:O	1:B:296:PHE:HD2	1.95	0.50
1:A:362:LYS:HD2	1:A:362:LYS:O	2.11	0.50
1:C:24:SER:O	1:C:27:VAL:HG22	2.12	0.50
1:C:512:THR:O	1:C:513:SER:OG	2.29	0.50
1:A:51:PHE:CE1	1:A:57:LEU:HD12	2.47	0.50
1:A:437:ASP:CG	1:A:438:SER:H	2.20	0.50
1:C:328:TYR:O	1:C:332:ARG:HG2	2.12	0.50
1:A:214:ILE:HD11	1:A:238:PHE:HA	1.95	0.49
1:C:32:THR:HG21	1:C:162:LEU:CB	2.42	0.49
1:C:35:ILE:HG23	1:C:298:LEU:HB3	1.94	0.49
1:D:442:ASN:HD22	1:D:442:ASN:H	1.60	0.49
1:B:354:LEU:HA	1:B:404:GLY:HA3	1.92	0.49
1:B:540:ALA:HB2	1:B:546:ILE:HG21	1.93	0.49
1:C:458:ILE:HG23	1:C:463:LEU:HB2	1.94	0.49
1:D:479:GLY:O	1:D:480:ASP:HB2	2.12	0.49
1:B:112:VAL:CG1	1:B:136:ILE:HG22	2.43	0.49
1:B:112:VAL:HG12	1:B:136:ILE:HG22	1.94	0.49
1:A:142:ASN:CB	1:A:324:LEU:HG	2.42	0.49
1:B:463:LEU:O	1:B:467:ILE:HG12	2.12	0.49
1:B:35:ILE:HG23	1:B:298:LEU:HB3	1.94	0.49
1:B:542:ARG:O	1:B:543:LEU:HB2	2.12	0.49
1:D:175:THR:HG22	1:D:296:PHE:CZ	2.47	0.49
1:C:207:ALA:HB1	1:C:245:PHE:HA	1.94	0.49
1:B:486:SER:H	1:B:489:GLN:NE2	2.11	0.49
1:C:150:PHE:CZ	1:C:154:MET:HE3	2.47	0.49
1:C:479:GLY:O	1:C:480:ASP:HB2	2.12	0.49
1:D:304:MET:HB2	1:D:305:PRO:HD3	1.93	0.49
1:B:512:THR:HG22	1:B:541:HIS:CD2	2.48	0.49
1:B:6:PHE:CD1	1:B:14:LYS:HG2	2.48	0.48
1:B:112:VAL:HG22	1:B:332:ARG:HH21	1.78	0.48
1:B:405:GLN:CD	1:B:407:LEU:HD21	2.38	0.48
1:D:140:VAL:N	1:D:328:TYR:OH	2.46	0.48
1:B:425:ILE:HD11	1:C:227:LEU:HD22	1.95	0.48
1:C:520:GLU:O	1:C:524:MET:HG2	2.13	0.48
1:D:290:LEU:HA	1:D:293:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:LEU:C	1:D:545:THR:H	2.20	0.48
1:A:396:ILE:HB	1:A:425:ILE:HD12	1.95	0.48
1:A:466:PHE:CE1	1:A:489:GLN:HG2	2.48	0.48
1:B:497:ARG:HD3	1:C:224:PHE:CZ	2.49	0.48
3:B:717:HOH:O	1:C:87:ALA:HA	2.14	0.48
1:D:142:ASN:HD22	1:D:324:LEU:HD21	1.78	0.48
1:A:392:VAL:HG11	1:A:539:ILE:HD11	1.96	0.48
1:B:380:PHE:CE1	1:B:391:LEU:HD13	2.49	0.48
1:A:427:TYR:CZ	1:D:223:LYS:HE3	2.49	0.47
1:A:463:LEU:O	1:A:467:ILE:HG12	2.14	0.47
1:C:119:ILE:HD11	1:C:123:LYS:HD3	1.95	0.47
1:C:128:ASN:OD1	1:C:128:ASN:N	2.36	0.47
1:D:233:GLY:O	1:D:236:SER:HB3	2.14	0.47
1:D:442:ASN:H	1:D:442:ASN:ND2	2.12	0.47
1:A:133:LEU:HD12	1:D:215:LEU:HD13	1.96	0.47
1:A:433:TYR:CD2	1:D:220:ASN:HB3	2.49	0.47
1:B:337:ASN:O	1:B:338:LEU:HG	2.14	0.47
1:D:134:LYS:O	1:D:139:GLU:HG2	2.14	0.47
1:B:108:ILE:O	1:B:112:VAL:HG23	2.15	0.47
1:B:373:LYS:HB2	1:B:376:GLU:HG3	1.96	0.47
1:D:350:LYS:HA	1:D:371:ASN:HB3	1.96	0.47
1:D:412:GLU:HG2	1:D:414:ASN:ND2	2.25	0.47
1:A:266:ILE:HD13	1:A:266:ILE:HA	1.66	0.47
1:B:381:ILE:HD13	1:B:381:ILE:HA	1.67	0.47
1:C:41:PHE:HD1	1:C:75:PHE:HD2	1.62	0.47
1:C:133:LEU:O	1:C:137:THR:HB	2.15	0.47
1:C:190:VAL:CG1	1:C:191:LYS:HG2	2.42	0.47
1:D:36:SER:HB3	1:D:166:LEU:HD11	1.95	0.47
1:D:207:ALA:HB1	1:D:245:PHE:HA	1.96	0.47
1:D:181:PHE:HZ	1:D:266:ILE:HG13	1.80	0.47
1:A:432:ILE:HG13	1:A:433:TYR:N	2.28	0.47
1:B:227:LEU:HD23	1:C:398:LEU:HD21	1.96	0.47
1:D:396:ILE:HB	1:D:425:ILE:CD1	2.44	0.47
1:B:266:ILE:HD12	1:B:266:ILE:HA	1.77	0.47
1:B:343:LEU:HD22	1:B:417:ASN:ND2	2.29	0.47
1:D:228:LYS:O	1:D:229:THR:HB	2.15	0.47
1:A:128:ASN:OD1	1:A:128:ASN:N	2.45	0.47
1:A:3:LYS:H	1:A:3:LYS:HD3	1.80	0.47
1:B:119:ILE:HD13	1:B:119:ILE:HG21	1.69	0.47
1:B:458:ILE:HG23	1:B:463:LEU:HB2	1.97	0.47
1:B:477:LYS:O	1:B:484:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:THR:O	1:D:513:SER:OG	2.31	0.47
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.65	0.46
1:B:412:GLU:HG2	1:B:414:ASN:ND2	2.24	0.46
1:D:273:PHE:HA	1:D:276:VAL:HG12	1.97	0.46
1:D:278:LEU:HD22	1:D:278:LEU:HA	1.58	0.46
1:D:441:LYS:HA	1:D:442:ASN:O	2.15	0.46
1:D:450:ASP:HB3	1:D:453:LYS:HB3	1.98	0.46
1:A:116:PHE:O	1:A:119:ILE:HG12	2.16	0.46
1:A:501:LEU:O	1:A:503:PRO:HD3	2.14	0.46
1:D:438:SER:HB2	1:D:475:GLN:HA	1.97	0.46
1:B:133:LEU:O	1:B:137:THR:HB	2.15	0.46
1:C:443:ILE:HA	1:C:497:ARG:HB2	1.98	0.46
1:C:492:ARG:NH1	1:C:523:ILE:HG12	2.30	0.46
1:D:13:ASP:OD1	1:D:104:ARG:NH1	2.48	0.46
1:D:324:LEU:HD13	1:D:324:LEU:HA	1.67	0.46
1:A:438:SER:HB2	1:A:475:GLN:HA	1.96	0.46
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.62	0.46
1:B:104:ARG:HA	1:B:104:ARG:HD3	1.65	0.46
1:B:226:LYS:NZ	1:C:119:ILE:O	2.47	0.46
1:B:247:LYS:O	1:B:251:THR:HG23	2.16	0.46
1:B:368:LEU:HD12	1:B:369:ASN:H	1.79	0.46
1:D:49:SER:OG	1:D:53:ARG:NH2	2.48	0.46
1:A:293:ILE:O	1:A:297:VAL:HG23	2.15	0.46
1:D:457:VAL:HG21	1:D:500:TYR:HA	1.98	0.46
1:D:503:PRO:HA	1:D:534:LYS:HE3	1.98	0.46
1:C:170:ILE:HD12	1:C:295:ILE:HG21	1.98	0.46
1:C:292:THR:O	1:C:296:PHE:HD2	1.99	0.46
1:D:524:MET:HE2	1:D:545:THR:O	2.15	0.46
1:A:112:VAL:CG1	1:A:136:ILE:HG22	2.44	0.46
1:C:146:MET:SD	1:C:321:HIS:HA	2.55	0.46
1:D:6:PHE:HD1	1:D:14:LYS:HG2	1.80	0.46
1:D:24:SER:HB3	1:D:155:SER:HB2	1.98	0.46
1:B:210:ASN:O	1:B:214:ILE:HG22	2.15	0.46
1:B:392:VAL:O	1:B:396:ILE:HG12	2.15	0.46
1:A:153:LEU:O	1:A:157:ILE:HG23	2.16	0.46
1:A:432:ILE:HD13	1:A:494:ALA:HB2	1.98	0.46
1:B:225:ILE:HD13	1:B:234:VAL:HG21	1.98	0.46
1:B:527:ILE:HG23	1:B:536:MET:HE1	1.98	0.46
1:D:19:PHE:CD1	1:D:19:PHE:C	2.93	0.46
1:D:66:ILE:HG22	1:D:70:GLU:OE1	2.16	0.46
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LYS:HE3	1:B:504:GLU:OE2	2.17	0.45
1:C:134:LYS:O	1:C:139:GLU:HG2	2.16	0.45
1:C:485:LEU:HD21	1:C:493:ILE:HD12	1.98	0.45
1:D:128:ASN:OD1	1:D:128:ASN:N	2.37	0.45
1:C:515:LEU:HA	1:C:516:ASP:HA	1.75	0.45
1:D:196:ILE:HG22	1:D:255:VAL:HG21	1.98	0.45
1:A:398:LEU:HD21	1:D:227:LEU:HD23	1.97	0.45
1:B:31:GLU:HG3	1:B:302:ARG:HH22	1.81	0.45
1:B:358:TYR:O	1:B:360:GLY:N	2.50	0.45
1:A:286:ILE:HG22	1:D:287:SER:HB2	1.99	0.45
1:C:289:ILE:HD13	1:C:290:LEU:N	2.31	0.45
1:C:398:LEU:H	1:C:398:LEU:HG	1.21	0.45
1:D:557:HIS:O	1:D:557:HIS:ND1	2.48	0.45
1:A:119:ILE:O	1:D:226:LYS:NZ	2.49	0.45
1:A:196:ILE:HG22	1:A:255:VAL:HG21	1.98	0.45
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.74	0.45
1:A:542:ARG:O	1:A:543:LEU:HB2	2.17	0.45
1:A:543:LEU:C	1:A:545:THR:H	2.25	0.45
1:B:233:GLY:O	1:B:236:SER:HB3	2.16	0.45
1:D:405:GLN:CD	1:D:407:LEU:HD21	2.41	0.45
1:A:67:PRO:HB2	1:A:68:VAL:H	1.63	0.45
1:B:286:ILE:HA	1:C:46:SER:HB2	1.99	0.45
1:A:213:GLU:HG2	3:D:715:HOH:O	2.17	0.45
1:A:307:ALA:O	1:A:311:ILE:HG12	2.17	0.45
1:A:329:GLN:C	1:A:331:LEU:H	2.25	0.45
1:C:396:ILE:HB	1:C:425:ILE:CD1	2.47	0.45
1:D:37:LEU:HD23	1:D:37:LEU:HA	1.80	0.45
1:D:126:GLN:HB3	3:D:724:HOH:O	2.17	0.45
1:D:152:LEU:HD11	1:D:309:ARG:HD3	1.98	0.45
1:D:262:TYR:CD1	1:D:263:LEU:HD13	2.52	0.45
1:D:150:PHE:CZ	1:D:154:MET:HE3	2.52	0.45
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.83	0.45
1:A:24:SER:O	1:A:27:VAL:HG22	2.17	0.45
1:A:302:ARG:O	1:A:305:PRO:HD2	2.17	0.45
1:A:463:LEU:HD21	1:A:492:ARG:HB2	1.99	0.45
1:B:376:GLU:O	1:B:550:ASP:HB2	2.17	0.45
1:D:542:ARG:HB2	1:D:543:LEU:O	2.16	0.44
1:A:46:SER:HA	1:A:47:ASP:HA	1.71	0.44
1:A:168:LEU:HA	1:A:168:LEU:HD23	1.85	0.44
1:A:323:SER:O	1:A:327:ILE:HG13	2.17	0.44
1:B:39:MET:SD	1:B:291:SER:HB3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:HD12	1:B:295:ILE:HG21	1.98	0.44
1:B:510:GLN:OE1	1:B:541:HIS:N	2.36	0.44
1:C:13:ASP:CG	1:C:104:ARG:HD2	2.42	0.44
1:C:41:PHE:HB2	1:C:75:PHE:HE2	1.82	0.44
1:D:266:ILE:HA	1:D:266:ILE:HD12	1.64	0.44
1:D:505:ILE:HA	1:D:535:THR:O	2.17	0.44
1:A:260:ARG:HG3	1:A:261:ILE:N	2.32	0.44
1:B:137:THR:HG21	1:C:212:PHE:CZ	2.52	0.44
1:B:72:ILE:HD13	1:B:72:ILE:HA	1.85	0.44
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.84	0.44
1:C:246:SER:O	1:C:250:ILE:HG23	2.17	0.44
1:A:32:THR:HG21	1:A:162:LEU:CB	2.47	0.44
1:B:38:VAL:HG21	1:B:298:LEU:HD21	1.99	0.44
1:D:116:PHE:O	1:D:119:ILE:HG12	2.16	0.44
1:D:386:CYS:SG	1:D:556:GLU:HA	2.58	0.44
1:A:215:LEU:HD11	1:D:136:ILE:HD11	2.00	0.44
1:A:427:TYR:OH	1:D:223:LYS:HE3	2.18	0.44
1:B:24:SER:O	1:B:27:VAL:HG22	2.18	0.44
1:B:108:ILE:HB	1:B:140:VAL:HG13	2.00	0.44
1:B:289:ILE:HG13	1:B:290:LEU:N	2.33	0.44
1:B:405:GLN:O	1:B:406:ILE:HB	2.18	0.44
1:B:453:LYS:HE2	1:B:502:GLU:OE1	2.17	0.44
1:D:318:LEU:HD23	1:D:318:LEU:HA	1.71	0.44
1:A:190:VAL:CG1	1:A:191:LYS:HG2	2.47	0.44
1:A:424:LYS:HE3	1:A:504:GLU:OE2	2.18	0.44
1:B:153:LEU:O	1:B:157:ILE:HG23	2.17	0.44
1:B:245:PHE:O	1:B:249:ASN:HB2	2.17	0.44
1:B:432:ILE:HD11	1:B:434:LEU:HG	1.99	0.44
1:D:108:ILE:HB	1:D:140:VAL:HG13	2.00	0.44
1:D:425:ILE:HD13	1:D:425:ILE:HG21	1.78	0.44
1:A:112:VAL:CG2	1:A:332:ARG:HH21	2.28	0.44
1:B:46:SER:HA	1:B:47:ASP:HA	1.71	0.44
1:B:167:MET:HE3	1:B:296:PHE:CE1	2.53	0.44
1:C:178:LEU:HD23	1:C:178:LEU:HA	1.74	0.44
1:C:368:LEU:HD11	1:C:560:LEU:HD13	1.99	0.44
1:D:139:GLU:CD	1:D:324:LEU:HD11	2.42	0.44
1:D:139:GLU:OE2	1:D:324:LEU:HD11	2.17	0.44
1:A:482:GLY:HA2	1:A:484:ASN:N	2.33	0.43
1:B:430:GLN:HG2	1:B:491:GLN:OE1	2.18	0.43
1:B:549:CYS:O	1:B:564:LYS:NZ	2.38	0.43
1:C:381:ILE:O	1:C:554:ARG:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:ASN:O	1:D:445:PHE:N	2.31	0.43
1:A:150:PHE:CZ	1:A:154:MET:HE3	2.53	0.43
1:A:246:SER:O	1:A:250:ILE:HG23	2.18	0.43
1:D:492:ARG:HH12	1:D:523:ILE:HG12	1.83	0.43
1:A:350:LYS:HA	1:A:371:ASN:HB3	2.00	0.43
1:B:19:PHE:CD1	1:B:19:PHE:C	2.96	0.43
2:B:602:1PE:H161	2:B:602:1PE:H151	1.55	0.43
1:C:9:LEU:HD22	1:C:13:ASP:HB3	2.00	0.43
1:C:543:LEU:O	1:C:544:SER:OG	2.34	0.43
1:D:30:ILE:HG22	1:D:86:ARG:HG3	1.99	0.43
1:D:193:LEU:HA	1:D:193:LEU:HD23	1.67	0.43
1:D:329:GLN:C	1:D:331:LEU:H	2.26	0.43
1:D:421:TYR:O	1:D:424:LYS:HG2	2.18	0.43
1:A:39:MET:HE2	1:A:295:ILE:HG13	2.00	0.43
1:A:111:LYS:C	1:A:332:ARG:HH22	2.27	0.43
1:C:113:PHE:CZ	1:C:117:LEU:HD11	2.53	0.43
1:D:41:PHE:HD1	1:D:75:PHE:CD2	2.36	0.43
1:D:359:GLU:HG3	2:D:601:1PE:H121	2.00	0.43
1:A:187:PHE:CE1	1:A:192:ILE:HD11	2.54	0.43
1:B:142:ASN:HB2	1:B:324:LEU:HG	2.00	0.43
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.64	0.43
1:B:284:SER:C	1:B:286:ILE:N	2.77	0.43
1:C:442:ASN:O	1:C:444:THR:N	2.51	0.43
1:B:67:PRO:HB2	1:B:68:VAL:H	1.64	0.43
1:C:13:ASP:OD1	1:C:104:ARG:NH1	2.51	0.43
1:C:142:ASN:CB	1:C:324:LEU:HG	2.48	0.43
1:C:324:LEU:HA	1:C:324:LEU:HD13	1.71	0.43
1:A:178:LEU:HD13	1:A:300:LEU:HD11	2.01	0.43
1:C:381:ILE:HD11	1:C:546:ILE:HD13	2.01	0.43
1:D:172:TYR:CE1	1:D:173:LYS:HG3	2.53	0.43
1:D:417:ASN:OD1	1:D:417:ASN:N	2.45	0.43
1:B:66:ILE:HB	1:B:70:GLU:HB2	2.01	0.43
1:B:381:ILE:HG21	1:B:554:ARG:NH1	2.33	0.43
1:C:32:THR:HG22	1:C:163:LEU:HG	2.01	0.43
1:A:68:VAL:HG12	1:A:71:ILE:HG21	2.00	0.43
1:A:188:ILE:O	1:A:192:ILE:HB	2.18	0.43
1:B:290:LEU:HD22	1:B:290:LEU:HA	1.79	0.43
1:B:502:GLU:HB2	1:B:503:PRO:CD	2.49	0.43
1:C:48:PHE:CE1	1:C:68:VAL:HB	2.54	0.43
1:C:228:LYS:O	1:C:229:THR:HB	2.19	0.43
1:D:352:CYS:HA	1:D:369:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:SER:CB	1:D:403:GLU:HB2	2.38	0.43
1:C:355:SER:HB3	1:C:363:TYR:CD1	2.54	0.43
1:D:271:LEU:HD21	1:D:293:ILE:CD1	2.49	0.43
1:A:360:GLY:HA3	1:A:361:LYS:CB	2.49	0.42
1:A:439:ILE:HG22	1:A:476:THR:O	2.18	0.42
1:C:123:LYS:O	1:C:126:GLN:HG2	2.18	0.42
1:C:142:ASN:HB2	1:C:324:LEU:HG	2.01	0.42
1:C:208:MET:HB2	1:C:245:PHE:CE2	2.54	0.42
1:C:318:LEU:HD23	1:C:318:LEU:HA	1.83	0.42
1:C:397:GLY:O	2:C:601:1PE:H262	2.18	0.42
1:A:458:ILE:HG23	1:A:463:LEU:HB2	2.01	0.42
1:B:115:LYS:HE3	1:B:334:GLU:O	2.19	0.42
1:C:133:LEU:HD12	1:C:133:LEU:HA	1.80	0.42
1:C:168:LEU:HA	1:C:175:THR:HG21	2.01	0.42
1:A:120:ASN:HB3	1:A:337:ASN:ND2	2.34	0.42
1:A:194:SER:N	1:A:195:PRO:HD2	2.35	0.42
1:A:260:ARG:O	1:A:264:GLU:HG3	2.19	0.42
1:C:175:THR:HG22	1:C:296:PHE:HZ	1.83	0.42
1:C:460:GLN:HB3	1:C:499:LEU:HD23	2.00	0.42
1:D:274:ILE:O	1:D:278:LEU:HB2	2.20	0.42
1:B:105:LYS:HA	1:B:140:VAL:HG12	2.01	0.42
1:B:368:LEU:HD12	1:B:369:ASN:N	2.34	0.42
1:D:354:LEU:CB	1:D:368:LEU:HB3	2.50	0.42
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.71	0.42
1:B:225:ILE:HG12	1:C:445:PHE:HE2	1.85	0.42
1:B:354:LEU:HA	1:B:354:LEU:HD23	1.72	0.42
1:B:417:ASN:OD1	1:B:417:ASN:N	2.51	0.42
1:B:524:MET:HE2	1:B:545:THR:O	2.20	0.42
1:D:133:LEU:HD12	1:D:133:LEU:HA	1.76	0.42
1:A:51:PHE:HB3	1:A:61:LYS:HG3	2.01	0.42
1:A:140:VAL:HA	1:A:328:TYR:OH	2.18	0.42
1:A:217:THR:HG21	1:D:435:PHE:HB3	2.00	0.42
1:A:343:LEU:HD22	1:A:417:ASN:ND2	2.34	0.42
1:B:111:LYS:C	1:B:332:ARG:HH22	2.27	0.42
1:B:190:VAL:CG1	1:B:191:LYS:HG2	2.49	0.42
1:B:393:ASP:O	1:B:398:LEU:O	2.38	0.42
1:C:49:SER:OG	1:C:50:TYR:N	2.51	0.42
1:D:440:ALA:O	1:D:444:THR:HG23	2.20	0.42
1:A:274:ILE:HD13	1:A:274:ILE:HA	1.70	0.42
1:A:354:LEU:HA	1:A:354:LEU:HD23	1.75	0.42
1:A:441:LYS:HA	1:A:442:ASN:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:HA	1:A:471:PRO:HD3	1.94	0.42
1:B:226:LYS:HE3	1:C:337:ASN:OD1	2.19	0.42
1:B:503:PRO:HA	1:B:534:LYS:HE3	2.01	0.42
1:C:360:GLY:HA3	1:C:361:LYS:CB	2.50	0.42
1:D:178:LEU:HD23	1:D:178:LEU:HA	1.82	0.42
1:D:260:ARG:O	1:D:264:GLU:HG3	2.20	0.42
1:A:508:LEU:HD22	1:A:527:ILE:HD13	2.00	0.42
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.89	0.42
1:B:282:ASN:O	1:B:283:GLU:HB2	2.20	0.42
1:B:564:LYS:HE2	1:B:564:LYS:HB3	1.77	0.42
1:C:213:GLU:O	1:C:217:THR:HG23	2.20	0.42
1:D:405:GLN:NE2	1:D:407:LEU:HD21	2.35	0.42
1:A:115:LYS:HG3	1:A:332:ARG:HA	2.01	0.42
1:A:354:LEU:O	1:A:404:GLY:N	2.53	0.42
1:B:100:PHE:HE2	1:B:147:ILE:HG21	1.85	0.42
1:C:105:LYS:HA	1:C:140:VAL:HG12	2.00	0.42
1:C:108:ILE:O	1:C:112:VAL:HG23	2.19	0.42
1:C:189:LEU:HD23	1:C:193:LEU:HD12	2.01	0.42
1:C:276:VAL:O	1:C:280:LEU:HB2	2.19	0.42
1:D:247:LYS:O	1:D:251:THR:HG23	2.19	0.42
1:A:1:MET:HA	1:A:4:LYS:HD3	2.02	0.42
1:B:39:MET:HB2	1:B:295:ILE:HD11	2.02	0.42
1:B:142:ASN:CB	1:B:324:LEU:HG	2.50	0.42
1:C:168:LEU:HA	1:C:168:LEU:HD23	1.85	0.42
1:C:311:ILE:HD12	1:C:311:ILE:HG23	1.82	0.42
1:C:326:ILE:O	1:C:328:TYR:N	2.53	0.42
1:D:298:LEU:HA	1:D:298:LEU:HD12	1.80	0.42
1:A:397:GLY:C	1:A:422:ARG:HH11	2.28	0.41
1:C:41:PHE:HD1	1:C:75:PHE:CD2	2.37	0.41
1:A:228:LYS:O	1:A:229:THR:HB	2.19	0.41
1:B:215:LEU:HD22	1:B:219:LEU:HD22	2.01	0.41
1:B:227:LEU:CD2	1:C:398:LEU:HD21	2.50	0.41
1:B:324:LEU:HD13	1:B:324:LEU:HA	1.75	0.41
1:C:39:MET:HE2	1:C:295:ILE:HG13	2.02	0.41
1:C:425:ILE:HD13	1:C:425:ILE:HG21	1.80	0.41
1:D:326:ILE:C	1:D:328:TYR:H	2.27	0.41
1:D:355:SER:O	1:D:402:LYS:HB2	2.19	0.41
1:A:111:LYS:HB3	1:A:332:ARG:HH12	1.84	0.41
1:A:226:LYS:HE3	1:D:337:ASN:OD1	2.20	0.41
1:A:360:GLY:N	1:A:361:LYS:HB2	2.35	0.41
1:A:502:GLU:HB2	1:A:503:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:HD11	1:C:215:LEU:HD13	2.03	0.41
1:B:329:GLN:C	1:B:331:LEU:H	2.28	0.41
1:B:470:LEU:HA	1:B:471:PRO:HD3	1.87	0.41
1:B:543:LEU:C	1:B:545:THR:N	2.75	0.41
1:C:26:PHE:O	1:C:30:ILE:HG12	2.20	0.41
1:C:40:PRO:HA	1:C:43:THR:HG22	2.01	0.41
1:C:135:SER:HA	1:C:139:GLU:HG3	2.02	0.41
1:C:555:LEU:HB2	1:C:560:LEU:CD1	2.47	0.41
1:A:176:LEU:HD22	1:A:176:LEU:HA	1.84	0.41
1:A:190:VAL:HG13	1:A:191:LYS:HG2	2.01	0.41
1:A:365:PHE:CG	1:A:368:LEU:HD23	2.55	0.41
1:C:302:ARG:O	1:C:305:PRO:HD2	2.21	0.41
1:D:24:SER:O	1:D:27:VAL:HG22	2.21	0.41
1:D:271:LEU:HD21	1:D:293:ILE:HD11	2.01	0.41
1:D:398:LEU:H	1:D:398:LEU:HG	1.33	0.41
1:A:105:LYS:HA	1:A:140:VAL:HG12	2.02	0.41
1:A:214:ILE:HD11	1:A:238:PHE:CA	2.50	0.41
1:A:512:THR:O	1:A:513:SER:OG	2.27	0.41
1:B:275:VAL:O	1:B:279:VAL:HG22	2.20	0.41
1:B:351:ILE:HG23	1:B:354:LEU:HG	2.03	0.41
1:A:49:SER:OG	1:A:50:TYR:N	2.52	0.41
1:B:168:LEU:HA	1:B:175:THR:HG21	2.03	0.41
1:D:194:SER:N	1:D:195:PRO:HD2	2.35	0.41
1:A:381:ILE:HD13	1:A:381:ILE:HA	1.85	0.41
1:A:438:SER:O	1:A:438:SER:OG	2.35	0.41
1:B:446:GLY:O	1:B:448:ALA:N	2.54	0.41
1:C:98:ALA:O	1:C:102:LYS:HG2	2.21	0.41
1:D:354:LEU:O	1:D:404:GLY:N	2.53	0.41
1:A:227:LEU:CD2	1:D:398:LEU:HD21	2.50	0.41
1:A:363:TYR:OH	1:A:402:LYS:HD2	2.20	0.41
1:D:483:SER:HG	1:D:484:ASN:H	1.67	0.41
1:A:6:PHE:CD1	1:A:14:LYS:HG2	2.56	0.41
1:A:276:VAL:HG21	1:D:76:GLY:HA3	2.03	0.41
1:B:222:PHE:CE2	1:B:226:LYS:HG3	2.56	0.41
1:B:463:LEU:HD21	1:B:492:ARG:HB2	2.03	0.41
1:B:510:GLN:CD	1:B:540:ALA:HA	2.46	0.41
1:C:4:LYS:CG	1:C:329:GLN:HG3	2.33	0.41
1:C:32:THR:HG21	1:C:162:LEU:HB2	2.02	0.41
1:C:50:TYR:C	1:C:52:ASP:H	2.28	0.41
1:D:219:LEU:HA	1:D:219:LEU:HD12	1.82	0.41
1:D:480:ASP:OD2	1:D:481:GLY:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:HIS:O	1:A:557:HIS:ND1	2.52	0.41
1:B:321:HIS:O	1:B:324:LEU:N	2.54	0.41
1:B:518:GLN:OE1	1:B:519:SER:N	2.54	0.41
1:C:546:ILE:HD12	1:C:552:VAL:HG21	2.02	0.41
1:D:189:LEU:HD23	1:D:189:LEU:HA	1.86	0.41
1:D:285:ASP:O	1:D:289:ILE:HG12	2.20	0.41
1:D:538:ILE:HD12	1:D:549:CYS:SG	2.60	0.41
1:A:460:GLN:HB3	1:A:499:LEU:HD23	2.03	0.40
1:C:31:GLU:OE2	1:C:86:ARG:HD2	2.20	0.40
1:C:46:SER:HA	1:C:47:ASP:HA	1.70	0.40
1:C:430:GLN:HG2	1:C:491:GLN:OE1	2.21	0.40
1:C:467:ILE:HG21	1:C:474:VAL:HG22	2.04	0.40
1:C:543:LEU:C	1:C:545:THR:N	2.79	0.40
1:D:381:ILE:O	1:D:554:ARG:HA	2.21	0.40
1:A:482:GLY:HA2	1:A:483:SER:HB3	2.03	0.40
1:B:441:LYS:HA	1:B:442:ASN:C	2.46	0.40
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.95	0.40
1:C:39:MET:SD	1:C:291:SER:HB3	2.62	0.40
1:D:23:PHE:O	1:D:27:VAL:HG13	2.21	0.40
1:D:491:GLN:O	1:D:495:ILE:HG13	2.21	0.40
1:A:391:LEU:HD12	1:A:555:LEU:HD13	2.02	0.40
1:B:239:LYS:HB2	1:C:110:TYR:CE1	2.56	0.40
1:B:250:ILE:HG22	1:C:102:LYS:CB	2.49	0.40
1:B:280:LEU:HD22	1:B:280:LEU:HA	1.94	0.40
1:B:427:TYR:CZ	1:C:223:LYS:HE3	2.57	0.40
1:C:172:TYR:HA	1:C:175:THR:HG23	2.03	0.40
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.86	0.40
1:D:180:ILE:HD13	1:D:180:ILE:HA	1.88	0.40
1:A:23:PHE:HD1	1:A:23:PHE:O	2.05	0.40
1:B:111:LYS:CB	1:B:332:ARG:HH22	2.35	0.40
1:B:338:LEU:HD23	1:B:338:LEU:HA	1.87	0.40
1:B:365:PHE:CD1	1:B:368:LEU:HD23	2.57	0.40
1:C:104:ARG:HD3	1:C:104:ARG:HA	1.78	0.40
1:C:119:ILE:HD13	1:C:119:ILE:HG21	1.87	0.40
1:C:143:LEU:O	1:C:147:ILE:HG13	2.21	0.40
1:D:125:THR:HG22	3:D:724:HOH:O	2.22	0.40
1:D:274:ILE:HD13	1:D:274:ILE:HA	1.79	0.40
1:D:527:ILE:HA	1:D:530:ILE:HG12	2.02	0.40
1:B:246:SER:O	1:B:250:ILE:HG23	2.20	0.40
1:C:266:ILE:HA	1:C:266:ILE:HD12	1.74	0.40
1:D:293:ILE:HD13	1:D:293:ILE:HG21	1.70	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	562/564 (100%)	475 (84%)	58 (10%)	29 (5%)	1	5
1	B	562/564 (100%)	475 (84%)	57 (10%)	30 (5%)	1	5
1	C	562/564 (100%)	473 (84%)	62 (11%)	27 (5%)	2	7
1	D	562/564 (100%)	476 (85%)	57 (10%)	29 (5%)	1	5
All	All	2248/2256 (100%)	1899 (84%)	234 (10%)	115 (5%)	1	6

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	50	TYR
1	A	67	PRO
1	A	282	ASN
1	A	284	SER
1	A	286	ILE
1	A	361	LYS
1	A	366	LYS
1	A	439	ILE
1	A	443	ILE
1	A	447	ASP
1	A	451	GLU
1	A	502	GLU
1	A	543	LEU
1	A	557	HIS
1	B	49	SER
1	B	50	TYR
1	B	67	PRO
1	B	283	GLU
1	B	284	SER

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Mol	Chain	Res	Type
1	B	337	ASN
1	B	355	SER
1	B	361	LYS
1	B	439	ILE
1	B	443	ILE
1	B	447	ASP
1	B	451	GLU
1	B	480	ASP
1	B	502	GLU
1	B	543	LEU
1	B	557	HIS
1	C	49	SER
1	C	283	GLU
1	C	355	SER
1	C	361	LYS
1	C	439	ILE
1	C	443	ILE
1	C	447	ASP
1	C	451	GLU
1	C	480	ASP
1	C	502	GLU
1	C	543	LEU
1	D	49	SER
1	D	50	TYR
1	D	284	SER
1	D	355	SER
1	D	361	LYS
1	D	439	ILE
1	D	443	ILE
1	D	447	ASP
1	D	451	GLU
1	D	480	ASP
1	D	502	GLU
1	D	543	LEU
1	D	557	HIS
1	A	54	ASN
1	A	327	ILE
1	A	337	ASN
1	A	355	SER
1	A	471	PRO
1	B	360	GLY
1	B	366	LYS

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Mol	Chain	Res	Type
1	C	50	TYR
1	C	54	ASN
1	C	67	PRO
1	C	284	SER
1	C	286	ILE
1	C	327	ILE
1	C	337	ASN
1	C	360	GLY
1	C	515	LEU
1	C	557	HIS
1	D	54	ASN
1	D	67	PRO
1	D	286	ILE
1	D	327	ILE
1	D	337	ASN
1	D	360	GLY
1	D	384	SER
1	A	360	GLY
1	B	286	ILE
1	B	544	SER
1	C	366	LYS
1	D	285	ASP
1	D	366	LYS
1	D	399	LEU
1	A	64	LEU
1	A	321	HIS
1	A	384	SER
1	A	399	LEU
1	B	54	ASN
1	B	384	SER
1	C	384	SER
1	C	399	LEU
1	D	430	GLN
1	D	442	ASN
1	A	406	ILE
1	A	544	SER
1	B	321	HIS
1	B	399	LEU
1	B	430	GLN
1	C	430	GLN
1	D	406	ILE
1	A	430	GLN

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Mol	Chain	Res	Type
1	A	513	SER
1	B	330	ASN
1	B	406	ILE
1	B	471	PRO
1	B	513	SER
1	C	406	ILE
1	C	471	PRO
1	D	321	HIS
1	D	471	PRO
1	B	327	ILE
1	D	503	PRO

5.3.2 Protein sidechains [i](#)

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	505/505 (100%)	425 (84%)	80 (16%)	2	8
1	B	505/505 (100%)	422 (84%)	83 (16%)	2	8
1	C	505/505 (100%)	426 (84%)	79 (16%)	2	9
1	D	505/505 (100%)	424 (84%)	81 (16%)	2	8
All	All	2020/2020 (100%)	1697 (84%)	323 (16%)	2	8

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	LYS
1	A	5	LEU
1	A	17	LEU
1	A	43	THR
1	A	48	PHE
1	A	53	ARG
1	A	57	LEU
1	A	60	LEU
1	A	63	TYR

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Mol	Chain	Res	Type
1	A	66	ILE
1	A	68	VAL
1	A	69	PHE
1	A	79	LEU
1	A	88	LEU
1	A	90	ASN
1	A	104	ARG
1	A	115	LYS
1	A	125	THR
1	A	130	SER
1	A	136	ILE
1	A	137	THR
1	A	143	LEU
1	A	144	SER
1	A	148	SER
1	A	152	LEU
1	A	166	LEU
1	A	175	THR
1	A	176	LEU
1	A	183	VAL
1	A	190	VAL
1	A	203	ARG
1	A	213	GLU
1	A	214	ILE
1	A	215	LEU
1	A	219	LEU
1	A	226	LYS
1	A	231	GLU
1	A	241	GLN
1	A	251	THR
1	A	255	VAL
1	A	263	LEU
1	A	266	ILE
1	A	274	ILE
1	A	278	LEU
1	A	280	LEU
1	A	293	ILE
1	A	298	LEU
1	A	317	LEU
1	A	322	SER
1	A	324	LEU
1	A	337	ASN

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Mol	Chain	Res	Type
1	A	351	ILE
1	A	353	ASN
1	A	354	LEU
1	A	361	LYS
1	A	362	LYS
1	A	368	LEU
1	A	373	LYS
1	A	376	GLU
1	A	381	ILE
1	A	386	CYS
1	A	391	LEU
1	A	398	LEU
1	A	417	ASN
1	A	422	ARG
1	A	425	ILE
1	A	432	ILE
1	A	439	ILE
1	A	457	VAL
1	A	474	VAL
1	A	485	LEU
1	A	489	GLN
1	A	499	LEU
1	A	504	GLU
1	A	518	GLN
1	A	535	THR
1	A	543	LEU
1	A	554	ARG
1	A	555	LEU
1	B	3	LYS
1	B	4	LYS
1	B	5	LEU
1	B	17	LEU
1	B	43	THR
1	B	48	PHE
1	B	53	ARG
1	B	57	LEU
1	B	60	LEU
1	B	63	TYR
1	B	66	ILE
1	B	68	VAL
1	B	88	LEU
1	B	90	ASN

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Mol	Chain	Res	Type
1	B	104	ARG
1	B	105	LYS
1	B	115	LYS
1	B	125	THR
1	B	130	SER
1	B	136	ILE
1	B	137	THR
1	B	143	LEU
1	B	148	SER
1	B	152	LEU
1	B	157	ILE
1	B	166	LEU
1	B	175	THR
1	B	176	LEU
1	B	182	MET
1	B	183	VAL
1	B	190	VAL
1	B	203	ARG
1	B	214	ILE
1	B	215	LEU
1	B	217	THR
1	B	219	LEU
1	B	226	LYS
1	B	231	GLU
1	B	241	GLN
1	B	250	ILE
1	B	251	THR
1	B	255	VAL
1	B	266	ILE
1	B	270	VAL
1	B	274	ILE
1	B	278	LEU
1	B	280	LEU
1	B	290	LEU
1	B	293	ILE
1	B	298	LEU
1	B	317	LEU
1	B	322	SER
1	B	324	LEU
1	B	353	ASN
1	B	354	LEU
1	B	355	SER

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Mol	Chain	Res	Type
1	B	361	LYS
1	B	362	LYS
1	B	368	LEU
1	B	370	LEU
1	B	371	ASN
1	B	373	LYS
1	B	376	GLU
1	B	378	ILE
1	B	381	ILE
1	B	391	LEU
1	B	398	LEU
1	B	422	ARG
1	B	425	ILE
1	B	432	ILE
1	B	457	VAL
1	B	474	VAL
1	B	485	LEU
1	B	489	GLN
1	B	499	LEU
1	B	504	GLU
1	B	518	GLN
1	B	530	ILE
1	B	535	THR
1	B	543	LEU
1	B	554	ARG
1	B	555	LEU
1	B	564	LYS
1	C	3	LYS
1	C	4	LYS
1	C	5	LEU
1	C	17	LEU
1	C	43	THR
1	C	48	PHE
1	C	53	ARG
1	C	57	LEU
1	C	60	LEU
1	C	64	LEU
1	C	66	ILE
1	C	68	VAL
1	C	88	LEU
1	C	90	ASN
1	C	104	ARG

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Mol	Chain	Res	Type
1	C	115	LYS
1	C	125	THR
1	C	130	SER
1	C	136	ILE
1	C	137	THR
1	C	143	LEU
1	C	148	SER
1	C	152	LEU
1	C	166	LEU
1	C	169	LEU
1	C	175	THR
1	C	176	LEU
1	C	183	VAL
1	C	185	ASN
1	C	190	VAL
1	C	203	ARG
1	C	214	ILE
1	C	215	LEU
1	C	217	THR
1	C	219	LEU
1	C	226	LYS
1	C	231	GLU
1	C	241	GLN
1	C	251	THR
1	C	255	VAL
1	C	263	LEU
1	C	266	ILE
1	C	270	VAL
1	C	274	ILE
1	C	278	LEU
1	C	280	LEU
1	C	286	ILE
1	C	289	ILE
1	C	290	LEU
1	C	292	THR
1	C	293	ILE
1	C	298	LEU
1	C	322	SER
1	C	324	LEU
1	C	337	ASN
1	C	354	LEU
1	C	361	LYS

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Mol	Chain	Res	Type
1	C	362	LYS
1	C	366	LYS
1	C	368	LEU
1	C	370	LEU
1	C	373	LYS
1	C	376	GLU
1	C	381	ILE
1	C	386	CYS
1	C	391	LEU
1	C	398	LEU
1	C	422	ARG
1	C	432	ILE
1	C	474	VAL
1	C	485	LEU
1	C	489	GLN
1	C	491	GLN
1	C	493	ILE
1	C	504	GLU
1	C	512	THR
1	C	530	ILE
1	C	535	THR
1	C	543	LEU
1	D	3	LYS
1	D	4	LYS
1	D	5	LEU
1	D	17	LEU
1	D	19	PHE
1	D	43	THR
1	D	48	PHE
1	D	57	LEU
1	D	58	ILE
1	D	60	LEU
1	D	64	LEU
1	D	66	ILE
1	D	68	VAL
1	D	69	PHE
1	D	88	LEU
1	D	90	ASN
1	D	104	ARG
1	D	125	THR
1	D	128	ASN
1	D	130	SER

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Mol	Chain	Res	Type
1	D	136	ILE
1	D	137	THR
1	D	143	LEU
1	D	145	THR
1	D	148	SER
1	D	152	LEU
1	D	157	ILE
1	D	166	LEU
1	D	169	LEU
1	D	175	THR
1	D	183	VAL
1	D	190	VAL
1	D	203	ARG
1	D	214	ILE
1	D	215	LEU
1	D	217	THR
1	D	219	LEU
1	D	226	LYS
1	D	231	GLU
1	D	241	GLN
1	D	251	THR
1	D	255	VAL
1	D	263	LEU
1	D	266	ILE
1	D	270	VAL
1	D	274	ILE
1	D	278	LEU
1	D	280	LEU
1	D	293	ILE
1	D	298	LEU
1	D	313	SER
1	D	322	SER
1	D	324	LEU
1	D	337	ASN
1	D	354	LEU
1	D	361	LYS
1	D	362	LYS
1	D	366	LYS
1	D	368	LEU
1	D	369	ASN
1	D	370	LEU
1	D	373	LYS

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Mol	Chain	Res	Type
1	D	376	GLU
1	D	381	ILE
1	D	386	CYS
1	D	391	LEU
1	D	398	LEU
1	D	417	ASN
1	D	422	ARG
1	D	457	VAL
1	D	474	VAL
1	D	485	LEU
1	D	486	SER
1	D	489	GLN
1	D	504	GLU
1	D	517	THR
1	D	535	THR
1	D	542	ARG
1	D	543	LEU
1	D	554	ARG
1	D	555	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	A	337	ASN
1	A	420	ASN
1	A	489	GLN
1	B	90	ASN
1	B	252	ASN
1	B	367	ASN
1	B	541	HIS
1	C	118	ASN
1	C	315	HIS
1	C	436	ASN
1	D	54	ASN
1	D	129	GLN
1	D	353	ASN
1	D	367	ASN
1	D	369	ASN
1	D	405	GLN
1	D	462	ASN
1	D	491	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	1PE	C	601	-	15,15,15	1.06	0	14,14,14	0.69	0
2	1PE	D	601	-	15,15,15	1.04	0	14,14,14	0.74	0
2	1PE	A	601	-	15,15,15	1.16	0	14,14,14	0.67	0
2	1PE	B	602	-	15,15,15	0.93	0	14,14,14	0.43	0
2	1PE	B	601	-	15,15,15	1.06	0	14,14,14	0.58	0

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	1PE	C	601	-	-	7/13/13/13	-
2	1PE	D	601	-	-	10/13/13/13	-
2	1PE	A	601	-	-	6/13/13/13	-
2	1PE	B	602	-	-	8/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1PE	B	601	-	-	10/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	602	1PE	C24-C14-OH5-C25
2	B	602	1PE	C16-C26-OH6-C15
2	A	601	1PE	OH6-C15-C25-OH5
2	B	602	1PE	OH2-C12-C22-OH3
2	D	601	1PE	OH6-C15-C25-OH5
2	B	601	1PE	OH6-C15-C25-OH5
2	D	601	1PE	OH5-C14-C24-OH4
2	D	601	1PE	C15-C25-OH5-C14
2	B	602	1PE	OH5-C14-C24-OH4
2	B	602	1PE	OH7-C16-C26-OH6
2	C	601	1PE	OH7-C16-C26-OH6
2	A	601	1PE	OH4-C13-C23-OH3
2	C	601	1PE	OH4-C13-C23-OH3
2	B	601	1PE	OH7-C16-C26-OH6
2	D	601	1PE	OH7-C16-C26-OH6
2	B	601	1PE	OH2-C12-C22-OH3
2	A	601	1PE	C15-C25-OH5-C14
2	A	601	1PE	C12-C22-OH3-C23
2	B	601	1PE	C13-C23-OH3-C22
2	A	601	1PE	C16-C26-OH6-C15
2	B	601	1PE	C25-C15-OH6-C26
2	D	601	1PE	C23-C13-OH4-C24
2	B	601	1PE	C24-C14-OH5-C25
2	B	602	1PE	C15-C25-OH5-C14
2	D	601	1PE	C25-C15-OH6-C26
2	C	601	1PE	C23-C13-OH4-C24
2	D	601	1PE	C16-C26-OH6-C15
2	D	601	1PE	C12-C22-OH3-C23
2	C	601	1PE	C14-C24-OH4-C13
2	B	602	1PE	C14-C24-OH4-C13
2	B	601	1PE	C15-C25-OH5-C14
2	B	602	1PE	C23-C13-OH4-C24
2	C	601	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
2	D	601	1PE	C14-C24-OH4-C13
2	C	601	1PE	C13-C23-OH3-C22
2	B	601	1PE	C16-C26-OH6-C15
2	A	601	1PE	OH2-C12-C22-OH3
2	B	601	1PE	C14-C24-OH4-C13
2	B	601	1PE	C12-C22-OH3-C23
2	C	601	1PE	C12-C22-OH3-C23
2	D	601	1PE	OH4-C13-C23-OH3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	1PE	1	0
2	D	601	1PE	1	0
2	B	602	1PE	1	0

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	564/564 (100%)	0.41	44 (7%)	19 16	34, 71, 144, 270	0
1	B	564/564 (100%)	0.38	55 (9%)	13 11	32, 74, 151, 231	0
1	C	564/564 (100%)	0.40	44 (7%)	19 16	36, 74, 149, 283	0
1	D	564/564 (100%)	0.34	51 (9%)	15 13	28, 70, 149, 261	0
All	All	2256/2256 (100%)	0.38	194 (8%)	16 13	28, 72, 150, 283	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	286	ILE	8.9
1	C	286	ILE	8.6
1	A	564	LYS	7.3
1	A	286	ILE	7.3
1	B	286	ILE	7.2
1	D	321	HIS	7.1
1	D	282	ASN	6.9
1	A	282	ASN	5.7
1	C	321	HIS	5.5
1	C	522	LYS	5.5
1	B	69	PHE	5.5
1	B	564	LYS	5.3
1	A	279	VAL	5.3
1	C	284	SER	5.2
1	A	321	HIS	5.2
1	A	69	PHE	5.1
1	D	69	PHE	5.1
1	C	523	ILE	5.1
1	D	557	HIS	4.9
1	A	284	SER	4.9
1	B	284	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	232	ASP	4.7
1	C	328	TYR	4.6
1	A	515	LEU	4.6
1	D	503	PRO	4.6
1	C	517	THR	4.6
1	C	481	GLY	4.6
1	D	515	LEU	4.4
1	C	326	ILE	4.4
1	B	328	TYR	4.3
1	D	279	VAL	4.3
1	C	564	LYS	4.2
1	B	481	GLY	4.2
1	B	321	HIS	4.2
1	B	438	SER	4.2
1	D	323	SER	4.2
1	D	277	PHE	4.2
1	A	277	PHE	4.1
1	D	322	SER	4.0
1	C	69	PHE	4.0
1	B	46	SER	3.9
1	D	301	TYR	3.9
1	D	66	ILE	3.9
1	C	448	ALA	3.8
1	C	322	SER	3.8
1	B	326	ILE	3.8
1	A	291	SER	3.7
1	D	320	TYR	3.7
1	B	287	SER	3.6
1	C	465	HIS	3.6
1	D	383	GLU	3.6
1	D	288	GLY	3.6
1	D	280	LEU	3.5
1	B	141	TYR	3.5
1	C	332	ARG	3.5
1	B	386	CYS	3.5
1	A	322	SER	3.5
1	C	452	GLU	3.5
1	B	322	SER	3.5
1	C	18	PHE	3.4
1	D	289	ILE	3.4
1	A	276	VAL	3.4
1	D	276	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	64	LEU	3.3
1	C	360	GLY	3.3
1	C	518	GLN	3.3
1	C	383	GLU	3.2
1	D	319	TYR	3.2
1	A	517	THR	3.2
1	A	383	GLU	3.2
1	B	64	LEU	3.2
1	D	284	SER	3.1
1	B	517	THR	3.1
1	A	328	TYR	3.1
1	C	55	LYS	3.1
1	B	203	ARG	3.1
1	D	480	ASP	3.1
1	D	60	LEU	3.1
1	B	65	ASN	3.0
1	C	519	SER	3.0
1	D	513	SER	3.0
1	A	336	GLU	3.0
1	C	62	GLU	3.0
1	A	326	ILE	2.9
1	A	64	LEU	2.9
1	A	285	ASP	2.9
1	D	65	ASN	2.9
1	C	1	MET	2.9
1	D	533	ASP	2.9
1	A	292	THR	2.9
1	C	126	GLN	2.8
1	B	281	LYS	2.8
1	B	525	ASP	2.8
1	C	67	PRO	2.8
1	D	564	LYS	2.8
1	B	60	LEU	2.8
1	B	290	LEU	2.8
1	B	548	GLN	2.8
1	A	66	ILE	2.8
1	D	290	LEU	2.8
1	B	45	ALA	2.7
1	B	289	ILE	2.7
1	B	515	LEU	2.7
1	B	145	THR	2.7
1	B	435	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	141	TYR	2.7
1	B	465	HIS	2.7
1	B	280	LEU	2.7
1	C	515	LEU	2.7
1	D	511	ALA	2.7
1	B	1	MET	2.7
1	D	1	MET	2.7
1	A	63	TYR	2.7
1	C	289	ILE	2.6
1	A	280	LEU	2.6
1	B	55	LYS	2.6
1	A	144	SER	2.6
1	B	51	PHE	2.6
1	B	516	ASP	2.6
1	D	481	GLY	2.6
1	A	145	THR	2.6
1	D	136	ILE	2.6
1	C	280	LEU	2.5
1	D	285	ASP	2.5
1	C	503	PRO	2.5
1	C	56	TYR	2.5
1	B	32	THR	2.5
1	D	283	GLU	2.5
1	A	281	LYS	2.5
1	B	437	ASP	2.5
1	D	235	LEU	2.5
1	A	435	PHE	2.5
1	C	482	GLY	2.4
1	A	51	PHE	2.4
1	C	526	GLU	2.4
1	D	465	HIS	2.4
1	B	187	PHE	2.4
1	C	33	PHE	2.4
1	A	503	PRO	2.4
1	B	282	ASN	2.4
1	D	48	PHE	2.4
1	D	63	TYR	2.4
1	D	328	TYR	2.4
1	C	557	HIS	2.4
1	A	474	VAL	2.3
1	B	33	PHE	2.3
1	C	6	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	70	GLU	2.3
1	A	278	LEU	2.3
1	C	376	GLU	2.3
1	D	291	SER	2.3
1	B	503	PRO	2.3
1	B	277	PHE	2.3
1	B	337	ASN	2.3
1	C	264	GLU	2.3
1	B	447	ASP	2.3
1	B	53	ARG	2.3
1	A	288	GLY	2.3
1	B	52	ASP	2.2
1	D	447	ASP	2.2
1	B	63	TYR	2.2
1	A	33	PHE	2.2
1	A	48	PHE	2.2
1	A	52	ASP	2.2
1	B	471	PRO	2.2
1	B	526	GLU	2.2
1	A	465	HIS	2.2
1	D	281	LYS	2.2
1	C	288	GLY	2.1
1	D	426	GLY	2.1
1	C	359	GLU	2.1
1	D	304	MET	2.1
1	D	62	GLU	2.1
1	D	472	GLN	2.1
1	B	522	LYS	2.1
1	D	482	GLY	2.1
1	C	145	THR	2.1
1	B	301	TYR	2.1
1	D	56	TYR	2.1
1	A	46	SER	2.1
1	D	28	SER	2.1
1	A	126	GLN	2.1
1	B	279	VAL	2.1
1	C	285	ASP	2.1
1	D	512	THR	2.1
1	B	441	LYS	2.0
1	D	459	LYS	2.0
1	A	481	GLY	2.0
1	A	56	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	323	SER	2.0
1	A	386	CYS	2.0
1	A	426	GLY	2.0
1	B	479	GLY	2.0
1	C	47	ASP	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	1PE	B	602	16/16	0.77	0.15	117,119,121,121	0
2	1PE	C	601	16/16	0.88	0.17	62,63,65,66	0
2	1PE	D	601	16/16	0.89	0.17	62,65,68,70	0
2	1PE	A	601	16/16	0.91	0.13	50,51,53,53	0
2	1PE	B	601	16/16	0.95	0.09	45,46,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.