



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:46 AM UTC

PDB ID : 5C76 / pdb_00005c76
Title : ATP-driven lipid-linked oligosaccharide flippase PglK in apo-inward facing state (2)
Authors : Perez, C.; Gerber, S.; Locher, K.P.
Deposited on : 2015-06-24
Resolution : 3.94 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
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

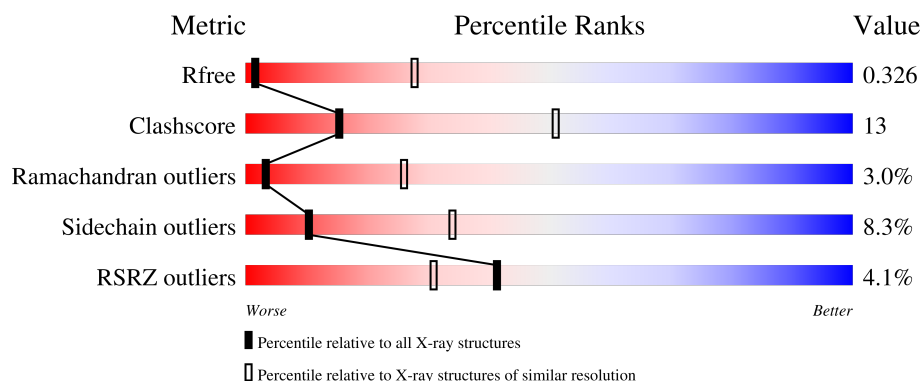
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

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	3% 62% 33% 5%
1	B	564	4% 65% 30% 5%
1	C	564	5% 62% 33% 5%
1	D	564	4% 66% 30%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18228 atoms, of which 0 are hydrogens and 0 are deuteriums.

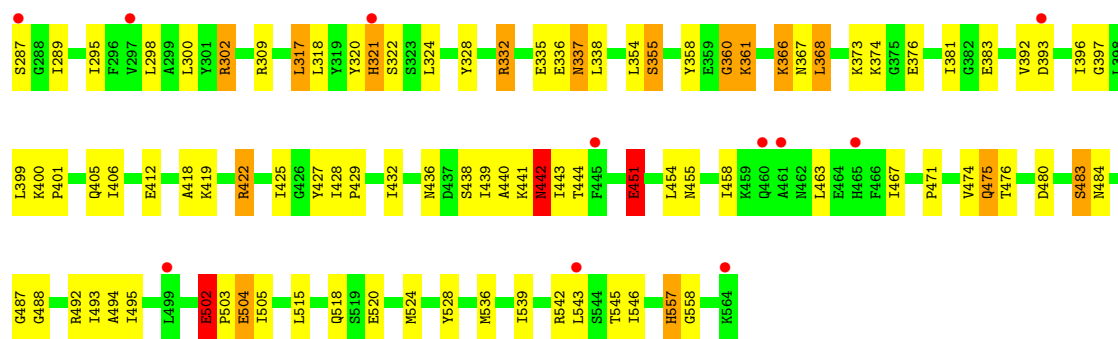
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called WlaB protein.

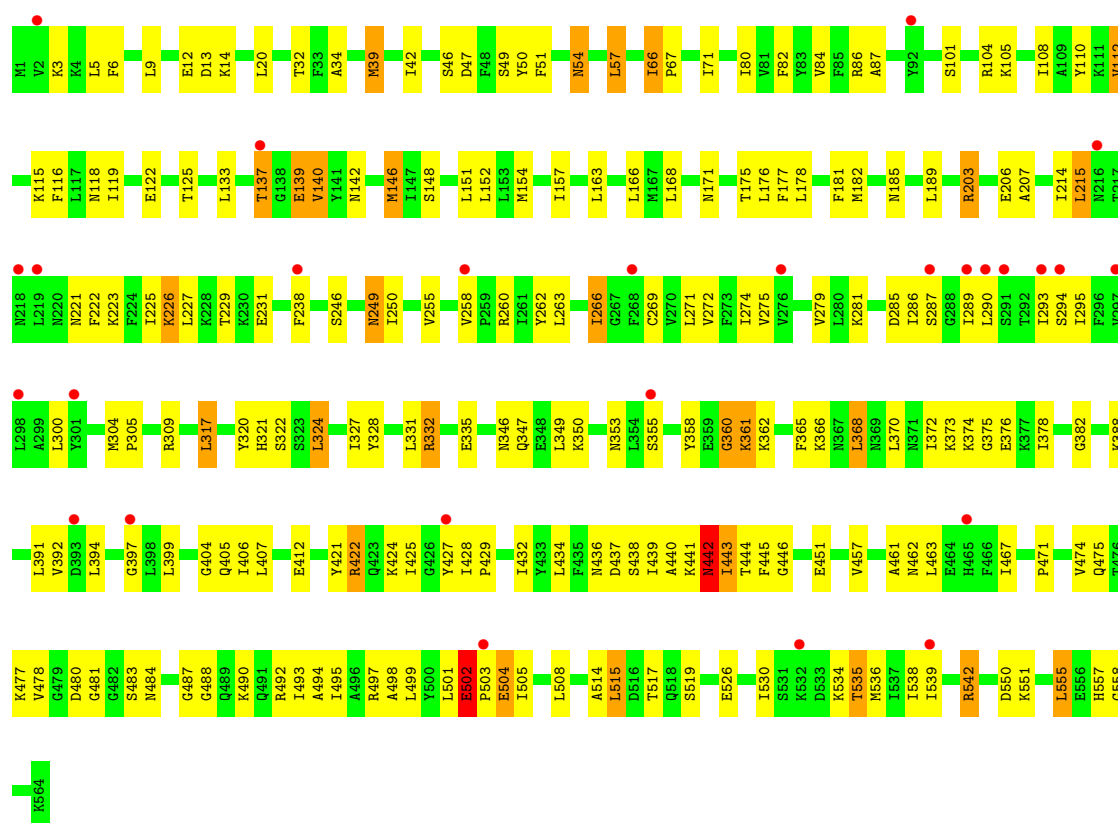
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	B	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	C	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	D	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			

There are 12 discrepancies between the modelled and reference sequences:

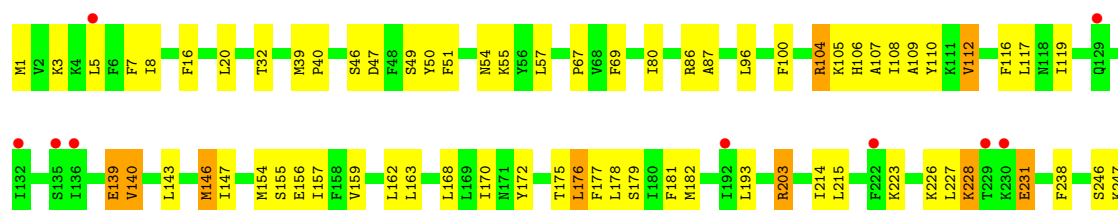
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	conflict	UNP O86150
A	105	LYS	TYR	conflict	UNP O86150
A	510	GLN	GLU	conflict	UNP O86150
B	2	VAL	LEU	conflict	UNP O86150
B	105	LYS	TYR	conflict	UNP O86150
B	510	GLN	GLU	conflict	UNP O86150
C	2	VAL	LEU	conflict	UNP O86150
C	105	LYS	TYR	conflict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

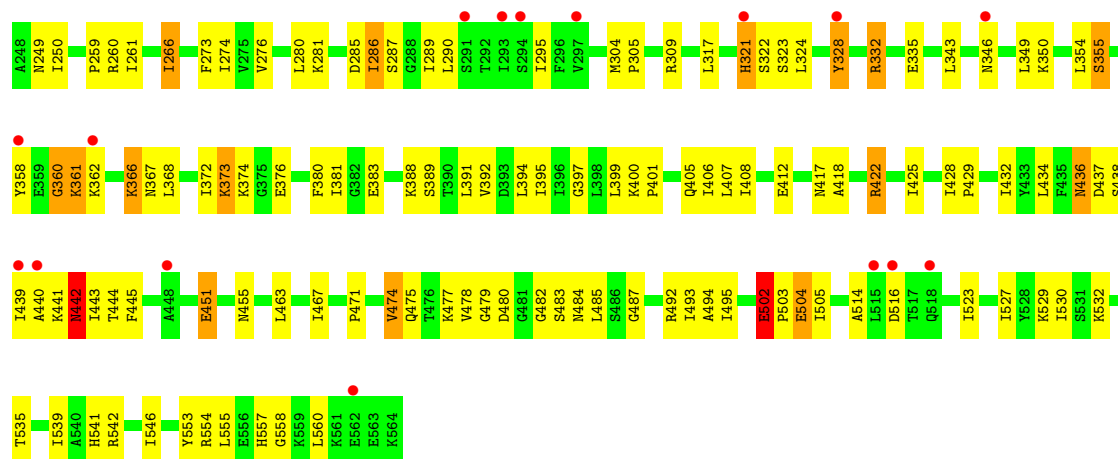


● Molecule 1: WlaB protein



● Molecule 1: WlaB protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.41Å 183.33Å 136.26Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	29.82 – 3.94 29.82 – 3.94	Depositor EDS
% Data completeness (in resolution range)	86.2 (29.82-3.94) 86.1 (29.82-3.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.98Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.275 , 0.329 0.282 , 0.326	Depositor DCC
R_{free} test set	1694 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	166.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18228	wwPDB-VP
Average B, all atoms (Å ²)	208.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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

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	0.35	0/4641	0.81	4/6246 (0.1%)
1	B	0.34	0/4641	0.80	3/6246 (0.0%)
1	C	0.34	0/4641	0.82	3/6246 (0.0%)
1	D	0.32	0/4641	0.81	5/6246 (0.1%)
All	All	0.34	0/18564	0.81	15/24984 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	GLU	CA-C-N	-7.25	110.78	119.84
1	B	502	GLU	C-N-CA	-7.25	110.78	119.84
1	D	502	GLU	CA-C-N	-6.87	111.26	119.84
1	D	502	GLU	C-N-CA	-6.87	111.26	119.84
1	C	502	GLU	CA-C-N	-6.60	111.59	119.84
1	C	502	GLU	C-N-CA	-6.60	111.59	119.84
1	A	272	VAL	N-CA-C	6.34	117.12	110.72
1	C	258	VAL	CB-CA-C	-6.25	107.77	113.70
1	A	502	GLU	CA-C-N	-6.08	112.25	119.84
1	A	502	GLU	C-N-CA	-6.08	112.25	119.84
1	A	397	GLY	N-CA-C	5.46	120.39	113.24
1	B	258	VAL	CB-CA-C	-5.32	108.65	113.70
1	D	8	ILE	N-CA-C	5.30	115.96	110.82
1	D	514	ALA	N-CA-C	-5.24	108.64	114.62
1	D	107	ALA	N-CA-C	5.15	117.29	111.11

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	4557	0	4764	146	0
1	B	4557	0	4764	137	0
1	C	4557	0	4764	139	0
1	D	4557	0	4764	135	0
All	All	18228	0	19056	503	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 13.

All (503) 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:B:520:GLU:OE1	1:B:542:ARG:NH1	2.09	0.85
1:B:503:PRO:HB2	1:B:504:GLU:HG2	1.61	0.82
1:A:425:ILE:HG22	1:A:505:ILE:HB	1.62	0.81
1:C:503:PRO:HB2	1:C:504:GLU:HG2	1.62	0.81
1:C:203:ARG:HH11	1:C:206:GLU:HB3	1.45	0.81
1:D:425:ILE:HG22	1:D:505:ILE:HB	1.61	0.81
1:B:168:LEU:HA	1:B:175:THR:HG21	1.63	0.81
1:A:502:GLU:HB2	1:A:503:PRO:HD3	1.66	0.78
1:A:503:PRO:HB2	1:A:504:GLU:HG2	1.65	0.78
1:C:139:GLU:HB3	1:C:324:LEU:HB3	1.64	0.78
1:D:100:PHE:HA	1:D:104:ARG:HH21	1.50	0.77
1:A:139:GLU:OE2	1:A:324:LEU:HD12	1.86	0.76
1:D:503:PRO:HB2	1:D:504:GLU:HG2	1.67	0.76
1:A:218:ASN:HD21	1:A:237:LEU:HD11	1.50	0.76
1:A:168:LEU:HA	1:A:175:THR:HG21	1.66	0.76
1:C:492:ARG:NH1	1:C:526:GLU:OE1	2.19	0.75
1:B:425:ILE:HG22	1:B:505:ILE:HB	1.68	0.74
1:A:438:SER:O	1:A:440:ALA:N	2.21	0.74
1:B:39:MET:HB2	1:B:295:ILE:HD11	1.70	0.73
1:D:392:VAL:HG21	1:D:539:ILE:HG12	1.71	0.73
1:C:502:GLU:HB2	1:C:503:PRO:HD3	1.71	0.72
1:D:502:GLU:HB2	1:D:503:PRO:HD3	1.72	0.72
1:A:501:LEU:HD11	1:D:228:LYS:HZ1	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:GLU:HB2	1:B:503:PRO:HD3	1.71	0.71
1:A:442:ASN:O	1:A:444:THR:N	2.23	0.71
1:D:442:ASN:O	1:D:444:THR:N	2.25	0.70
1:A:483:SER:OG	1:A:484:ASN:N	2.23	0.70
1:C:392:VAL:HG21	1:C:539:ILE:HG12	1.74	0.70
1:B:400:LYS:NZ	1:D:516:ASP:HB2	2.08	0.69
1:B:392:VAL:HG21	1:B:539:ILE:HG12	1.75	0.68
1:C:438:SER:O	1:C:440:ALA:N	2.26	0.68
1:A:429:PRO:HG2	1:A:432:ILE:HG22	1.74	0.68
1:B:425:ILE:HD11	1:C:227:LEU:HD22	1.76	0.68
1:B:520:GLU:CD	1:B:542:ARG:HH12	2.02	0.67
1:A:45:ALA:HA	1:A:72:ILE:HD12	1.77	0.67
1:D:483:SER:OG	1:D:484:ASN:N	2.21	0.67
1:A:392:VAL:HG21	1:A:539:ILE:HG12	1.76	0.66
1:B:360:GLY:H	1:B:361:LYS:HD2	1.61	0.66
1:C:39:MET:SD	1:C:39:MET:N	2.68	0.66
1:D:388:LYS:NZ	1:D:541:HIS:HA	2.11	0.66
1:B:483:SER:OG	1:B:484:ASN:N	2.21	0.66
1:C:429:PRO:HG2	1:C:432:ILE:HG22	1.78	0.66
1:B:212:PHE:O	1:B:216:ASN:ND2	2.26	0.66
1:A:442:ASN:O	1:A:445:PHE:N	2.26	0.65
1:D:438:SER:O	1:D:440:ALA:N	2.29	0.65
1:C:397:GLY:HA3	1:C:422:ARG:HD2	1.78	0.65
1:A:501:LEU:HD11	1:D:228:LYS:NZ	2.12	0.64
1:D:112:VAL:HG22	1:D:332:ARG:HH22	1.62	0.64
1:A:261:ILE:HG22	1:D:87:ALA:HA	1.78	0.64
1:B:47:ASP:HB3	1:C:286:ILE:HG12	1.80	0.63
1:A:227:LEU:HD22	1:D:425:ILE:HD11	1.80	0.63
1:B:228:LYS:HG2	1:C:501:LEU:HD21	1.80	0.63
1:C:349:LEU:HB2	1:C:372:ILE:HB	1.79	0.63
1:A:66:ILE:HD12	1:A:71:ILE:HG23	1.79	0.63
1:B:438:SER:O	1:B:440:ALA:N	2.32	0.63
1:B:358:TYR:HB2	1:B:361:LYS:HD3	1.81	0.63
1:D:451:GLU:O	1:D:455:ASN:ND2	2.29	0.63
1:A:262:TYR:O	1:A:266:ILE:HG22	1.99	0.62
1:C:425:ILE:HG22	1:C:505:ILE:HB	1.79	0.62
1:D:429:PRO:HG2	1:D:432:ILE:HG22	1.80	0.62
1:B:264:GLU:HB3	1:C:86:ARG:HH12	1.64	0.61
1:B:105:LYS:HD2	1:B:140:VAL:HG12	1.82	0.61
1:C:203:ARG:HH11	1:C:206:GLU:CB	2.13	0.61
1:C:181:PHE:CE2	1:C:266:ILE:HD11	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:HA	1:B:248:ALA:HB1	1.84	0.60
1:D:349:LEU:HB2	1:D:372:ILE:HB	1.82	0.60
1:C:434:LEU:HB2	1:C:481:GLY:HA2	1.84	0.60
1:D:139:GLU:OE2	1:D:324:LEU:HD12	2.02	0.60
1:B:451:GLU:O	1:B:455:ASN:ND2	2.31	0.60
1:A:178:LEU:HD13	1:A:300:LEU:HD11	1.84	0.60
1:B:442:ASN:O	1:B:444:THR:N	2.35	0.60
1:B:528:TYR:OH	1:B:545:THR:O	2.14	0.59
1:A:287:SER:HB2	1:D:286:ILE:HG22	1.85	0.59
1:D:332:ARG:NH1	1:D:332:ARG:HB3	2.17	0.59
1:C:168:LEU:HA	1:C:175:THR:HG21	1.82	0.59
1:C:358:TYR:HB2	1:C:361:LYS:HD3	1.85	0.59
1:D:492:ARG:NH1	1:D:523:ILE:HG12	2.17	0.59
1:B:178:LEU:HD13	1:B:300:LEU:HD11	1.83	0.58
1:C:477:LYS:O	1:C:484:ASN:ND2	2.37	0.58
1:A:441:LYS:HA	1:A:442:ASN:O	2.04	0.58
1:C:397:GLY:C	1:C:422:ARG:HH11	2.12	0.58
1:A:39:MET:HB2	1:A:295:ILE:HD11	1.86	0.58
1:A:317:LEU:O	1:A:321:HIS:NE2	2.36	0.58
1:C:105:LYS:HD2	1:C:140:VAL:HB	1.84	0.58
1:A:100:PHE:HA	1:A:104:ARG:HH21	1.67	0.57
1:A:264:GLU:OE2	1:A:264:GLU:N	2.37	0.57
1:D:285:ASP:O	1:D:287:SER:N	2.36	0.57
1:D:381:ILE:HD11	1:D:546:ILE:HD13	1.87	0.57
1:D:109:ALA:HB2	1:D:140:VAL:HG11	1.86	0.57
1:A:290:LEU:HD13	1:D:290:LEU:HB3	1.86	0.56
1:A:428:ILE:HD13	1:A:495:ILE:HG12	1.88	0.56
1:D:3:LYS:H	1:D:3:LYS:HD3	1.71	0.56
1:D:170:ILE:HD13	1:D:295:ILE:HG21	1.87	0.56
1:D:405:GLN:NE2	1:D:412:GLU:OE1	2.37	0.56
1:A:321:HIS:CG	1:A:322:SER:H	2.23	0.56
1:B:20:LEU:HB3	1:B:151:LEU:HD13	1.87	0.56
1:C:391:LEU:HD12	1:C:555:LEU:HD13	1.86	0.56
1:A:54:ASN:HB3	1:A:57:LEU:HB2	1.87	0.56
1:B:524:MET:HG3	1:B:545:THR:HG22	1.86	0.56
1:D:355:SER:OG	1:D:367:ASN:N	2.35	0.56
1:D:193:LEU:HD13	1:D:259:PRO:HG3	1.86	0.56
1:B:355:SER:OG	1:B:367:ASN:N	2.32	0.56
1:C:457:VAL:O	1:C:461:ALA:N	2.35	0.56
1:C:557:HIS:O	1:C:557:HIS:ND1	2.38	0.55
1:B:39:MET:HA	1:B:42:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:SER:OG	1:C:484:ASN:N	2.23	0.55
1:A:39:MET:HA	1:A:42:ILE:HG22	1.88	0.55
1:A:360:GLY:H	1:A:361:LYS:HD2	1.71	0.55
1:B:108:ILE:O	1:B:112:VAL:HG23	2.06	0.55
1:C:181:PHE:HE2	1:C:266:ILE:HD11	1.72	0.55
1:D:388:LYS:HZ2	1:D:541:HIS:HA	1.70	0.55
1:A:383:GLU:OE1	1:B:557:HIS:N	2.30	0.55
1:C:6:PHE:HD1	1:C:14:LYS:HG2	1.71	0.55
1:A:20:LEU:HB3	1:A:151:LEU:HD13	1.89	0.55
1:A:512:THR:HG22	1:A:541:HIS:CE1	2.42	0.55
1:C:441:LYS:HE2	1:C:446:GLY:HA2	1.88	0.54
1:B:400:LYS:HZ2	1:D:516:ASP:HB2	1.72	0.54
1:A:478:VAL:O	1:A:483:SER:OG	2.25	0.54
1:C:178:LEU:O	1:C:182:MET:HB2	2.08	0.54
1:C:440:ALA:O	1:C:444:THR:N	2.28	0.54
1:A:225:ILE:HG21	1:D:117:LEU:HD22	1.90	0.54
1:A:427:TYR:HE2	1:A:429:PRO:HB3	1.71	0.54
1:B:285:ASP:O	1:B:287:SER:N	2.40	0.54
1:D:223:LYS:O	1:D:227:LEU:HD13	2.07	0.54
1:A:322:SER:C	1:A:324:LEU:H	2.15	0.54
1:D:478:VAL:O	1:D:483:SER:OG	2.26	0.54
1:D:492:ARG:HH12	1:D:523:ILE:HG12	1.72	0.54
1:A:94:PHE:CE2	1:D:260:ARG:NH1	2.77	0.53
1:A:135:SER:HA	1:A:139:GLU:HG2	1.90	0.53
1:B:159:VAL:HG11	1:B:302:ARG:NH2	2.24	0.53
1:B:184:LEU:O	1:B:188:ILE:HG13	2.09	0.53
1:C:108:ILE:O	1:C:112:VAL:HG23	2.09	0.53
1:C:424:LYS:HB2	1:C:504:GLU:HG3	1.90	0.53
1:A:381:ILE:HD11	1:A:546:ILE:HD13	1.90	0.53
1:A:321:HIS:CG	1:A:322:SER:N	2.77	0.53
1:B:381:ILE:HD11	1:B:546:ILE:HD13	1.91	0.53
1:D:273:PHE:HA	1:D:276:VAL:HG22	1.91	0.53
1:D:441:LYS:HA	1:D:442:ASN:O	2.09	0.53
1:A:290:LEU:HB3	1:D:290:LEU:HD13	1.91	0.53
1:B:264:GLU:HB3	1:C:86:ARG:NH1	2.24	0.53
1:B:557:HIS:O	1:B:557:HIS:ND1	2.42	0.52
1:C:332:ARG:HB3	1:C:332:ARG:NH1	2.23	0.52
1:B:429:PRO:HG2	1:B:432:ILE:HG22	1.89	0.52
1:A:384:SER:H	1:A:388:LYS:HE2	1.75	0.52
1:C:405:GLN:NE2	1:C:412:GLU:OE1	2.41	0.52
1:A:214:ILE:HG12	1:A:241:GLN:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:HG22	1:D:287:SER:HB2	1.91	0.52
1:A:424:LYS:HB2	1:A:504:GLU:HG3	1.90	0.52
1:A:427:TYR:CE2	1:A:429:PRO:HB3	2.44	0.52
1:C:49:SER:OG	1:C:50:TYR:N	2.40	0.52
1:C:360:GLY:H	1:C:361:LYS:HD2	1.74	0.52
1:A:226:LYS:NZ	1:D:119:ILE:O	2.40	0.52
1:B:227:LEU:HD22	1:C:425:ILE:HD11	1.92	0.52
1:D:477:LYS:O	1:D:484:ASN:ND2	2.42	0.52
1:A:24:SER:HB3	1:A:155:SER:HB2	1.91	0.52
1:C:178:LEU:HD13	1:C:300:LEU:HD11	1.90	0.52
1:B:432:ILE:HG21	1:B:494:ALA:HB2	1.92	0.51
1:C:285:ASP:O	1:C:287:SER:N	2.43	0.51
1:A:154:MET:O	1:A:157:ILE:HG13	2.11	0.51
1:A:553:TYR:HB3	1:A:560:LEU:HG	1.92	0.51
1:B:400:LYS:HZ1	1:D:516:ASP:HB2	1.75	0.51
1:A:3:LYS:H	1:A:3:LYS:HD3	1.76	0.51
1:B:49:SER:OG	1:B:50:TYR:N	2.42	0.51
1:D:175:THR:O	1:D:179:SER:OG	2.26	0.51
1:D:32:THR:HG22	1:D:163:LEU:HG	1.92	0.51
1:B:393:ASP:OD1	1:C:223:LYS:NZ	2.37	0.51
1:D:178:LEU:O	1:D:182:MET:HB2	2.11	0.51
1:B:210:ASN:O	1:B:214:ILE:HG12	2.10	0.50
1:D:527:ILE:HA	1:D:530:ILE:HG12	1.92	0.50
1:A:285:ASP:O	1:A:287:SER:N	2.42	0.50
1:B:427:TYR:HE2	1:B:429:PRO:HB3	1.75	0.50
1:C:378:ILE:HG22	1:C:551:LYS:HB2	1.92	0.50
1:D:49:SER:C	1:D:51:PHE:H	2.20	0.50
1:A:184:LEU:O	1:A:188:ILE:HG13	2.10	0.50
1:A:328:TYR:HD1	1:A:332:ARG:HD2	1.77	0.50
1:B:46:SER:OG	1:C:286:ILE:O	2.27	0.50
1:B:154:MET:O	1:B:157:ILE:HG13	2.11	0.50
1:C:350:LYS:HB3	1:C:407:LEU:HB2	1.94	0.50
1:A:373:LYS:HB2	1:A:376:GLU:HG3	1.94	0.50
1:A:502:GLU:HB2	1:A:503:PRO:CD	2.39	0.50
1:D:557:HIS:ND1	1:D:557:HIS:O	2.44	0.50
1:C:101:SER:HB3	1:C:148:SER:OG	2.12	0.50
1:D:360:GLY:H	1:D:361:LYS:HD2	1.77	0.50
1:B:139:GLU:CD	1:B:324:LEU:HD12	2.37	0.50
1:B:428:ILE:HD13	1:B:495:ILE:HG12	1.94	0.50
1:D:105:LYS:HD2	1:D:140:VAL:HB	1.92	0.50
1:A:140:VAL:HB	1:A:328:TYR:OH	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ILE:HG21	1:A:494:ALA:HB2	1.94	0.50
1:A:175:THR:O	1:A:179:SER:OG	2.21	0.50
1:B:302:ARG:HH21	1:B:302:ARG:CG	2.24	0.49
1:C:215:LEU:HG	1:C:238:PHE:HE1	1.77	0.49
1:C:508:LEU:HB3	1:C:538:ILE:HG12	1.94	0.49
1:D:146:MET:HE2	1:D:321:HIS:CE1	2.47	0.49
1:A:181:PHE:HE2	1:A:266:ILE:HD11	1.76	0.49
1:D:47:ASP:OD2	1:D:49:SER:HB3	2.12	0.49
1:D:553:TYR:HB3	1:D:560:LEU:HD11	1.95	0.49
1:A:123:LYS:HA	1:A:126:GLN:HG2	1.93	0.49
1:A:396:ILE:HD12	1:D:227:LEU:HD21	1.94	0.49
1:C:66:ILE:HD12	1:C:71:ILE:HG23	1.95	0.49
1:B:261:ILE:HG22	1:C:87:ALA:HA	1.94	0.49
1:C:332:ARG:HB3	1:C:332:ARG:HH11	1.78	0.49
1:A:405:GLN:NE2	1:A:412:GLU:OE1	2.41	0.49
1:B:322:SER:C	1:B:324:LEU:H	2.20	0.49
1:B:442:ASN:ND2	1:B:442:ASN:H	2.10	0.49
1:B:193:LEU:O	1:B:197:ILE:HG12	2.12	0.49
1:C:20:LEU:HB3	1:C:151:LEU:HD13	1.95	0.49
1:A:513:SER:HA	1:A:542:ARG:HH12	1.78	0.48
1:C:146:MET:SD	1:C:317:LEU:HG	2.52	0.48
1:B:366:LYS:HB2	1:B:366:LYS:NZ	2.28	0.48
1:A:187:PHE:O	1:A:191:LYS:HB2	2.14	0.48
1:B:34:ALA:HB2	1:B:86:ARG:CD	2.43	0.48
1:B:117:LEU:O	1:C:226:LYS:NZ	2.46	0.48
1:C:373:LYS:HB2	1:C:376:GLU:HG3	1.95	0.48
1:A:243:GLU:HA	1:A:246:SER:HB3	1.94	0.48
1:B:94:PHE:CZ	1:C:260:ARG:NH1	2.81	0.48
1:D:55:LYS:H	1:D:55:LYS:HD2	1.78	0.48
1:D:322:SER:C	1:D:324:LEU:H	2.22	0.48
1:A:108:ILE:O	1:A:112:VAL:HG23	2.13	0.48
1:B:488:GLY:O	1:B:492:ARG:HG3	2.14	0.48
1:B:524:MET:HE2	1:B:545:THR:HB	1.96	0.48
1:D:391:LEU:HD12	1:D:555:LEU:HD13	1.95	0.48
1:D:529:LYS:HA	1:D:532:LYS:NZ	2.29	0.48
1:B:397:GLY:HA3	1:B:422:ARG:HG3	1.94	0.48
1:B:427:TYR:CE2	1:B:429:PRO:HB3	2.49	0.48
1:C:115:LYS:HE2	1:C:332:ARG:O	2.14	0.48
1:D:373:LYS:HB2	1:D:376:GLU:HG3	1.96	0.48
1:A:275:VAL:O	1:A:279:VAL:HG23	2.14	0.47
1:B:108:ILE:HG23	1:B:328:TYR:OH	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:PHE:CZ	1:D:266:ILE:HD11	2.49	0.47
1:D:442:ASN:O	1:D:445:PHE:N	2.30	0.47
1:B:80:ILE:HG12	1:C:269:CYS:SG	2.54	0.47
1:B:373:LYS:HB2	1:B:376:GLU:HG3	1.96	0.47
1:D:350:LYS:HB3	1:D:407:LEU:HB2	1.95	0.47
1:A:378:ILE:HG22	1:A:551:LYS:HB2	1.96	0.47
1:A:428:ILE:HG12	1:A:495:ILE:HA	1.95	0.47
1:A:133:LEU:O	1:A:137:THR:HG22	2.15	0.47
1:A:382:GLY:HA3	1:A:388:LYS:HD3	1.96	0.47
1:B:102:LYS:HB2	1:C:250:ILE:CG2	2.45	0.47
1:C:438:SER:HB2	1:C:475:GLN:HA	1.96	0.47
1:C:442:ASN:O	1:C:445:PHE:N	2.30	0.47
1:B:32:THR:HG21	1:B:162:LEU:HB2	1.95	0.47
1:C:443:ILE:HA	1:C:497:ARG:HB2	1.96	0.47
1:A:349:LEU:HB2	1:A:372:ILE:HB	1.96	0.47
1:B:262:TYR:O	1:B:266:ILE:HG22	2.14	0.47
1:C:428:ILE:HD13	1:C:495:ILE:HG12	1.97	0.47
1:C:442:ASN:ND2	1:C:442:ASN:H	2.13	0.47
1:D:418:ALA:O	1:D:422:ARG:HD3	2.14	0.47
1:A:94:PHE:CZ	1:D:260:ARG:NH1	2.82	0.47
1:A:115:LYS:NZ	1:A:332:ARG:O	2.44	0.47
1:A:529:LYS:HG2	1:A:532:LYS:NZ	2.29	0.47
1:B:102:LYS:HB2	1:C:250:ILE:HG22	1.97	0.47
1:C:376:GLU:O	1:C:550:ASP:HB2	2.14	0.47
1:D:442:ASN:ND2	1:D:442:ASN:H	2.12	0.47
1:A:49:SER:OG	1:A:50:TYR:N	2.43	0.47
1:A:442:ASN:ND2	1:A:442:ASN:H	2.13	0.47
1:B:396:ILE:HD12	1:C:227:LEU:HD11	1.97	0.47
1:C:437:ASP:OD2	1:C:441:LYS:HG3	2.16	0.46
1:A:528:TYR:OH	1:A:545:THR:O	2.29	0.46
1:C:189:LEU:HD21	1:C:262:TYR:CE1	2.49	0.46
1:C:557:HIS:HA	1:C:558:GLY:HA2	1.57	0.46
1:D:389:SER:HA	1:D:539:ILE:HD13	1.97	0.46
1:A:235:LEU:HB3	1:D:110:TYR:HE1	1.80	0.46
1:A:273:PHE:HA	1:A:276:VAL:HG22	1.96	0.46
1:C:514:ALA:HB2	1:C:542:ARG:HH22	1.80	0.46
1:D:557:HIS:HA	1:D:558:GLY:HA2	1.57	0.46
1:A:328:TYR:O	1:A:332:ARG:HG2	2.16	0.46
1:C:142:ASN:HB3	1:C:320:TYR:HB3	1.97	0.46
1:A:264:GLU:HB3	1:D:86:ARG:NH1	2.30	0.46
1:B:23:PHE:CE2	1:B:96:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HD12	1:B:71:ILE:HD13	1.96	0.46
1:B:118:ASN:HB3	1:B:336:GLU:HB3	1.97	0.46
1:C:54:ASN:HB3	1:C:57:LEU:HB2	1.97	0.46
1:C:185:ASN:O	1:C:189:LEU:HG	2.15	0.46
1:D:428:ILE:HD13	1:D:495:ILE:HG12	1.98	0.46
1:A:376:GLU:O	1:A:550:ASP:HB2	2.15	0.46
1:B:142:ASN:HB3	1:B:320:TYR:HB3	1.97	0.46
1:C:177:PHE:CD1	1:C:274:ILE:HD11	2.50	0.46
1:C:375:GLY:H	1:C:535:THR:HB	1.79	0.46
1:D:358:TYR:HB2	1:D:361:LYS:HD3	1.97	0.46
1:A:239:LYS:HA	1:D:106:HIS:HE1	1.80	0.46
1:A:421:TYR:O	1:A:424:LYS:HG2	2.16	0.46
1:C:346:ASN:HA	1:C:374:LYS:HD2	1.97	0.46
1:D:383:GLU:OE2	1:D:554:ARG:NH2	2.49	0.46
1:C:421:TYR:O	1:C:424:LYS:HG2	2.16	0.46
1:D:355:SER:HA	1:D:366:LYS:H	1.79	0.46
1:A:324:LEU:O	1:A:328:TYR:N	2.45	0.46
1:C:327:ILE:O	1:C:331:LEU:HG	2.16	0.46
1:A:287:SER:O	1:A:291:SER:N	2.44	0.46
1:A:383:GLU:HG3	1:B:383:GLU:HB2	1.98	0.46
1:A:467:ILE:HG21	1:A:474:VAL:HG22	1.97	0.46
1:B:400:LYS:HD2	1:B:401:PRO:HD2	1.98	0.46
1:C:304:MET:HB2	1:C:305:PRO:HD3	1.96	0.46
1:D:529:LYS:HA	1:D:532:LYS:HZ3	1.80	0.46
1:C:365:PHE:HB3	1:C:368:LEU:HD23	1.98	0.45
1:C:481:GLY:O	1:C:490:LYS:HE2	2.15	0.45
1:D:104:ARG:HA	1:D:104:ARG:HD3	1.70	0.45
1:A:499:LEU:HD21	1:A:530:ILE:HD12	1.99	0.45
1:A:513:SER:HA	1:A:542:ARG:NH1	2.31	0.45
1:A:327:ILE:O	1:A:331:LEU:HD23	2.16	0.45
1:A:422:ARG:O	1:A:425:ILE:HG12	2.16	0.45
1:C:353:ASN:O	1:C:404:GLY:HA2	2.16	0.45
1:A:7:PHE:HE2	1:A:332:ARG:HB2	1.82	0.45
1:A:350:LYS:HB3	1:A:407:LEU:HB2	1.99	0.45
1:B:101:SER:HB3	1:B:148:SER:OG	2.17	0.45
1:C:262:TYR:O	1:C:266:ILE:HG22	2.16	0.45
1:B:7:PHE:HE2	1:B:332:ARG:HB2	1.82	0.45
1:B:181:PHE:CE2	1:B:266:ILE:HD11	2.51	0.45
1:B:243:GLU:HA	1:B:246:SER:HB3	1.98	0.45
1:B:422:ARG:O	1:B:425:ILE:HG12	2.17	0.45
1:B:441:LYS:HA	1:B:442:ASN:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LEU:O	1:B:467:ILE:HG12	2.17	0.45
1:D:168:LEU:HA	1:D:175:THR:HG21	1.98	0.45
1:D:328:TYR:HD2	1:D:328:TYR:HA	1.68	0.45
1:A:184:LEU:O	1:A:187:PHE:HB3	2.17	0.45
1:A:350:LYS:O	1:A:407:LEU:N	2.47	0.45
1:B:146:MET:HE2	1:B:321:HIS:CE1	2.51	0.45
1:C:274:ILE:HD13	1:C:274:ILE:HA	1.78	0.45
1:C:275:VAL:O	1:C:279:VAL:HG23	2.16	0.45
1:A:142:ASN:HB2	1:A:324:LEU:HG	1.99	0.45
1:A:391:LEU:HD12	1:A:555:LEU:HD13	2.00	0.44
1:B:8:ILE:HG12	1:B:328:TYR:HE1	1.82	0.44
1:B:228:LYS:HE2	1:B:228:LYS:HB3	1.79	0.44
1:B:335:GLU:H	1:B:335:GLU:CD	2.26	0.44
1:D:181:PHE:CE2	1:D:266:ILE:HD11	2.51	0.44
1:A:235:LEU:HB3	1:D:110:TYR:CE1	2.52	0.44
1:A:87:ALA:HA	1:D:261:ILE:HG22	1.99	0.44
1:A:437:ASP:OD2	1:A:441:LYS:HG3	2.17	0.44
1:D:332:ARG:HB3	1:D:332:ARG:HH11	1.82	0.44
1:C:80:ILE:O	1:C:84:VAL:HG23	2.17	0.44
1:D:155:SER:O	1:D:159:VAL:HG23	2.17	0.44
1:B:104:ARG:HA	1:B:104:ARG:HD3	1.70	0.44
1:B:418:ALA:O	1:B:422:ARG:HD3	2.17	0.44
1:C:271:LEU:HD21	1:C:293:ILE:HD11	1.99	0.44
1:A:302:ARG:O	1:A:305:PRO:HD2	2.17	0.44
1:B:152:LEU:HD22	1:B:156:GLU:HG2	1.99	0.44
1:B:255:VAL:HA	1:B:258:VAL:HG23	2.00	0.44
1:B:502:GLU:HB2	1:B:503:PRO:CD	2.44	0.44
1:A:529:LYS:HA	1:A:532:LYS:NZ	2.32	0.44
1:B:237:LEU:HB3	1:B:241:GLN:HE22	1.82	0.44
1:C:347:GLN:O	1:C:374:LYS:N	2.49	0.44
1:A:101:SER:HB2	1:A:148:SER:OG	2.17	0.44
1:A:279:VAL:HG12	1:D:69:PHE:CZ	2.53	0.44
1:C:463:LEU:O	1:C:467:ILE:HG12	2.18	0.44
1:D:350:LYS:O	1:D:407:LEU:N	2.50	0.44
1:D:434:LEU:HD22	1:D:442:ASN:ND2	2.33	0.44
1:B:80:ILE:HG13	1:C:272:VAL:HB	2.00	0.43
1:B:368:LEU:HD22	1:B:368:LEU:HA	1.89	0.43
1:C:46:SER:HA	1:C:47:ASP:HA	1.84	0.43
1:C:488:GLY:O	1:C:492:ARG:HG3	2.18	0.43
1:A:365:PHE:HB3	1:A:368:LEU:HD23	2.00	0.43
1:C:432:ILE:HG21	1:C:494:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:LYS:HA	1:D:442:ASN:C	2.43	0.43
1:B:121:TYR:HA	1:C:222:PHE:HE2	1.83	0.43
1:B:178:LEU:O	1:B:182:MET:HB2	2.18	0.43
1:D:335:GLU:H	1:D:335:GLU:CD	2.26	0.43
1:A:434:LEU:HD22	1:A:442:ASN:ND2	2.34	0.43
1:C:504:GLU:O	1:C:534:LYS:HB3	2.17	0.43
1:A:90:ASN:HB3	1:D:261:ILE:HD13	2.00	0.43
1:A:332:ARG:HG2	1:A:332:ARG:H	1.61	0.43
1:A:438:SER:HB2	1:A:475:GLN:HA	2.00	0.43
1:B:122:GLU:HA	1:B:125:THR:HG22	2.00	0.43
1:C:478:VAL:O	1:C:483:SER:OG	2.37	0.43
1:C:499:LEU:HD21	1:C:530:ILE:HD12	1.99	0.43
1:D:112:VAL:HG22	1:D:332:ARG:NH2	2.29	0.43
1:D:247:LYS:O	1:D:250:ILE:HG12	2.18	0.43
1:D:177:PHE:CE1	1:D:274:ILE:HD11	2.53	0.43
1:D:397:GLY:HA3	1:D:422:ARG:HG3	2.00	0.43
1:D:482:GLY:HA2	1:D:485:LEU:H	1.83	0.43
1:D:523:ILE:O	1:D:527:ILE:HG13	2.19	0.43
1:A:260:ARG:HG3	1:A:261:ILE:N	2.33	0.43
1:A:365:PHE:HE1	1:A:394:LEU:HD12	1.84	0.43
1:B:119:ILE:HA	1:B:336:GLU:HA	2.01	0.43
1:B:119:ILE:HG13	1:B:335:GLU:O	2.18	0.43
1:D:143:LEU:O	1:D:147:ILE:HG13	2.19	0.43
1:D:463:LEU:O	1:D:467:ILE:HG12	2.18	0.43
1:B:520:GLU:CD	1:B:542:ARG:NH1	2.71	0.43
1:C:502:GLU:HB2	1:C:503:PRO:CD	2.44	0.43
1:C:517:THR:C	1:C:519:SER:H	2.26	0.43
1:A:62:GLU:C	1:A:64:LEU:H	2.27	0.43
1:A:501:LEU:CD1	1:D:228:LYS:HZ1	2.28	0.43
1:B:235:LEU:HD22	1:C:110:TYR:CE1	2.53	0.43
1:D:203:ARG:HE	1:D:203:ARG:HA	1.84	0.42
1:D:343:LEU:HD22	1:D:417:ASN:ND2	2.34	0.42
1:A:322:SER:C	1:A:324:LEU:N	2.77	0.42
1:B:223:LYS:HE3	1:C:427:TYR:OH	2.19	0.42
1:C:39:MET:HE2	1:C:294:SER:OG	2.18	0.42
1:C:365:PHE:HE1	1:C:394:LEU:HD12	1.83	0.42
1:C:428:ILE:HG12	1:C:495:ILE:HA	2.01	0.42
1:A:492:ARG:NH1	1:A:523:ILE:HG12	2.34	0.42
1:B:249:ASN:O	1:B:253:GLU:HB2	2.18	0.42
1:D:432:ILE:HG21	1:D:494:ALA:HB2	2.02	0.42
1:A:106:HIS:HB2	1:D:246:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:VAL:HG21	1:A:500:TYR:HA	2.00	0.42
1:B:146:MET:HG2	1:B:321:HIS:ND1	2.34	0.42
1:B:419:LYS:HG2	1:C:229:THR:HG21	2.01	0.42
1:C:427:TYR:H	1:C:498:ALA:HB1	1.84	0.42
1:A:252:ASN:HA	1:A:255:VAL:HG12	2.01	0.42
1:A:323:SER:O	1:A:324:LEU:HD13	2.19	0.42
1:A:557:HIS:HA	1:A:558:GLY:HA2	1.74	0.42
1:B:32:THR:HG21	1:B:162:LEU:CB	2.50	0.42
1:C:203:ARG:NH1	1:C:207:ALA:N	2.67	0.42
1:C:322:SER:C	1:C:324:LEU:H	2.27	0.42
1:D:154:MET:O	1:D:157:ILE:HG13	2.20	0.42
1:D:156:GLU:HG3	1:D:309:ARG:HD2	2.02	0.42
1:A:6:PHE:HD1	1:A:14:LYS:HG2	1.84	0.42
1:A:450:ASP:O	1:A:452:GLU:N	2.51	0.42
1:B:139:GLU:HB3	1:B:324:LEU:HB3	2.01	0.42
1:B:438:SER:HB2	1:B:475:GLN:HA	2.00	0.42
1:D:391:LEU:O	1:D:395:ILE:HG13	2.20	0.42
1:D:436:ASN:ND2	1:D:479:GLY:O	2.52	0.42
1:B:374:LYS:NZ	1:B:504:GLU:OE1	2.52	0.42
1:B:557:HIS:HA	1:B:558:GLY:HA2	1.54	0.42
1:C:12:GLU:OE1	1:C:12:GLU:N	2.41	0.42
1:C:116:PHE:O	1:C:119:ILE:HG22	2.19	0.42
1:A:69:PHE:HE1	1:D:280:LEU:HD13	1.85	0.42
1:A:181:PHE:HZ	1:A:266:ILE:HG13	1.85	0.42
1:C:34:ALA:HA	1:C:82:PHE:HE2	1.84	0.42
1:C:382:GLY:HA3	1:C:388:LYS:HD3	2.01	0.42
1:A:527:ILE:HA	1:A:530:ILE:HG12	2.01	0.42
1:B:181:PHE:HE2	1:B:266:ILE:HD11	1.84	0.42
1:C:122:GLU:HA	1:C:125:THR:HG22	2.02	0.42
1:D:39:MET:HB3	1:D:40:PRO:HD3	2.01	0.42
1:D:226:LYS:HD3	1:D:226:LYS:HA	1.89	0.42
1:D:346:ASN:HA	1:D:374:LYS:HD2	2.02	0.42
1:D:372:ILE:HD11	1:D:395:ILE:HD13	2.02	0.42
1:B:262:TYR:HD1	1:B:263:LEU:HD22	1.85	0.42
1:C:221:ASN:O	1:C:225:ILE:HG13	2.20	0.42
1:B:177:PHE:CE1	1:B:274:ILE:HD11	2.55	0.41
1:D:7:PHE:HE2	1:D:332:ARG:HG3	1.85	0.41
1:B:108:ILE:HG23	1:B:328:TYR:CZ	2.55	0.41
1:B:185:ASN:OD1	1:B:262:TYR:OH	2.27	0.41
1:B:247:LYS:O	1:B:250:ILE:HG12	2.19	0.41
1:B:438:SER:HA	1:B:476:THR:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LYS:HA	1:C:442:ASN:C	2.45	0.41
1:D:32:THR:HG21	1:D:162:LEU:HB3	2.02	0.41
1:B:214:ILE:HB	1:B:241:GLN:CD	2.45	0.41
1:B:405:GLN:NE2	1:B:412:GLU:OE1	2.53	0.41
1:B:536:MET:HE3	1:B:536:MET:HB2	1.96	0.41
1:C:49:SER:C	1:C:51:PHE:H	2.28	0.41
1:C:492:ARG:HH12	1:C:526:GLU:CD	2.27	0.41
1:A:108:ILE:HG22	1:A:328:TYR:OH	2.21	0.41
1:A:234:VAL:O	1:A:237:LEU:HG	2.21	0.41
1:B:112:VAL:HA	1:B:332:ARG:NH2	2.36	0.41
1:D:231:GLU:H	1:D:231:GLU:HG3	1.67	0.41
1:D:343:LEU:HD23	1:D:408:ILE:HD12	2.02	0.41
1:D:354:LEU:HD22	1:D:394:LEU:HD13	2.02	0.41
1:A:397:GLY:HA3	1:A:422:ARG:HG3	2.03	0.41
1:B:146:MET:SD	1:B:317:LEU:HG	2.61	0.41
1:D:116:PHE:O	1:D:119:ILE:HG22	2.21	0.41
1:A:188:ILE:HA	1:A:192:ILE:HD12	2.02	0.41
1:B:176:LEU:HD13	1:B:176:LEU:HA	1.97	0.41
1:C:171:ASN:O	1:C:175:THR:HG22	2.20	0.41
1:A:116:PHE:O	1:A:119:ILE:HG22	2.21	0.41
1:A:190:VAL:HA	1:A:194:SER:HB3	2.03	0.41
1:B:225:ILE:HG12	1:C:445:PHE:HE2	1.86	0.41
1:B:228:LYS:C	1:B:230:LYS:H	2.29	0.41
1:B:441:LYS:HA	1:B:442:ASN:O	2.20	0.41
1:C:372:ILE:HG12	1:C:378:ILE:HD13	2.03	0.41
1:A:441:LYS:HA	1:A:442:ASN:C	2.46	0.41
1:C:262:TYR:HD1	1:C:263:LEU:HD22	1.84	0.41
1:A:36:SER:C	1:A:38:VAL:H	2.29	0.41
1:B:106:HIS:HB2	1:C:246:SER:HB2	2.03	0.41
1:B:166:LEU:HD22	1:B:170:ILE:HD11	2.03	0.41
1:C:39:MET:HA	1:C:42:ILE:HG22	2.03	0.41
1:C:112:VAL:HG21	1:C:328:TYR:HE1	1.86	0.41
1:C:152:LEU:HD11	1:C:309:ARG:HB3	2.03	0.41
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.91	0.41
1:C:249:ASN:HD22	1:C:249:ASN:C	2.27	0.41
1:D:16:PHE:O	1:D:20:LEU:HD23	2.20	0.41
1:D:47:ASP:C	1:D:49:SER:H	2.29	0.41
1:D:49:SER:OG	1:D:50:TYR:N	2.53	0.41
1:D:304:MET:HB2	1:D:305:PRO:HD3	2.03	0.41
1:D:380:PHE:CE1	1:D:391:LEU:HD13	2.56	0.41
1:D:467:ILE:CG2	1:D:474:VAL:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HG21	1:D:46:SER:HB2	2.03	0.41
1:A:396:ILE:HB	1:A:425:ILE:HD12	2.03	0.41
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.93	0.41
1:B:337:ASN:HD22	1:B:338:LEU:H	1.69	0.41
1:B:454:LEU:O	1:B:458:ILE:HG13	2.20	0.41
1:D:176:LEU:HA	1:D:176:LEU:HD13	1.90	0.41
1:A:110:TYR:HA	1:D:238:PHE:CE2	2.56	0.40
1:A:271:LEU:HD21	1:A:293:ILE:HD11	2.03	0.40
1:A:401:PRO:O	1:C:515:LEU:HD21	2.21	0.40
1:B:100:PHE:HA	1:B:104:ARG:HH21	1.85	0.40
1:B:156:GLU:HG3	1:B:309:ARG:HD2	2.03	0.40
1:B:189:LEU:HD21	1:B:262:TYR:CE1	2.56	0.40
1:B:518:GLN:H	1:B:518:GLN:HG3	1.72	0.40
1:C:32:THR:HG22	1:C:163:LEU:HG	2.02	0.40
1:D:96:LEU:HD23	1:D:96:LEU:HA	1.89	0.40
1:D:260:ARG:HG3	1:D:261:ILE:N	2.36	0.40
1:C:9:LEU:HB3	1:C:13:ASP:HB2	2.03	0.40
1:C:536:MET:HE3	1:C:536:MET:HB2	2.00	0.40
1:A:427:TYR:CZ	1:D:223:LYS:HG2	2.56	0.40
1:C:6:PHE:CD1	1:C:14:LYS:HG2	2.54	0.40
1:C:154:MET:O	1:C:157:ILE:HG13	2.21	0.40
1:D:388:LYS:HZ1	1:D:541:HIS:HA	1.85	0.40
1:D:400:LYS:HA	1:D:401:PRO:HD2	1.96	0.40
1:B:35:ILE:HG23	1:B:298:LEU:HB3	2.03	0.40
1:C:335:GLU:H	1:C:335:GLU:CD	2.29	0.40
1:A:380:PHE:HA	1:A:553:TYR:O	2.21	0.40
1:C:133:LEU:O	1:C:137:THR:HG22	2.21	0.40
1:C:462:ASN:ND2	1:C:492:ARG:HD3	2.36	0.40
1:D:1:MET:HE3	1:D:1:MET:HB3	1.98	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%)	478 (85%)	68 (12%)	16 (3%)	4	27
1	B	562/564 (100%)	478 (85%)	65 (12%)	19 (3%)	3	24
1	C	562/564 (100%)	478 (85%)	69 (12%)	15 (3%)	4	28
1	D	562/564 (100%)	477 (85%)	68 (12%)	17 (3%)	3	26
All	All	2248/2256 (100%)	1911 (85%)	270 (12%)	67 (3%)	3	26

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	HIS
1	A	436	ASN
1	A	439	ILE
1	A	442	ASN
1	A	443	ILE
1	A	502	GLU
1	B	443	ILE
1	B	487	GLY
1	B	502	GLU
1	C	443	ILE
1	C	502	GLU
1	D	443	ILE
1	D	487	GLY
1	D	502	GLU
1	A	67	PRO
1	A	399	LEU
1	A	487	GLY
1	B	67	PRO
1	B	436	ASN
1	B	439	ILE
1	B	442	ASN
1	C	67	PRO
1	C	399	LEU
1	C	436	ASN
1	C	439	ILE
1	C	480	ASP
1	C	487	GLY
1	D	54	ASN
1	D	67	PRO
1	D	436	ASN
1	D	439	ILE
1	D	442	ASN
1	D	480	ASP

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Mol	Chain	Res	Type
1	A	54	ASN
1	A	355	SER
1	A	480	ASP
1	B	54	ASN
1	B	355	SER
1	B	360	GLY
1	B	399	LEU
1	B	471	PRO
1	B	480	ASP
1	C	54	ASN
1	C	321	HIS
1	C	471	PRO
1	D	399	LEU
1	C	355	SER
1	C	442	ASN
1	D	321	HIS
1	D	355	SER
1	D	360	GLY
1	A	360	GLY
1	A	384	SER
1	A	471	PRO
1	B	321	HIS
1	B	354	LEU
1	B	406	ILE
1	B	451	GLU
1	C	360	GLY
1	C	406	ILE
1	D	323	SER
1	D	406	ILE
1	D	471	PRO
1	B	515	LEU
1	A	406	ILE
1	D	286	ILE
1	B	286	ILE

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	505/505 (100%)	458 (91%)	47 (9%)	8	29
1	B	505/505 (100%)	465 (92%)	40 (8%)	11	36
1	C	505/505 (100%)	462 (92%)	43 (8%)	10	33
1	D	505/505 (100%)	467 (92%)	38 (8%)	12	37
All	All	2020/2020 (100%)	1852 (92%)	168 (8%)	10	34

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	LEU
1	A	12	GLU
1	A	48	PHE
1	A	56	TYR
1	A	57	LEU
1	A	58	ILE
1	A	66	ILE
1	A	104	ARG
1	A	112	VAL
1	A	118	ASN
1	A	137	THR
1	A	139	GLU
1	A	146	MET
1	A	172	TYR
1	A	176	LEU
1	A	203	ARG
1	A	214	ILE
1	A	215	LEU
1	A	226	LYS
1	A	249	ASN
1	A	255	VAL
1	A	264	GLU
1	A	266	ILE
1	A	281	LYS
1	A	289	ILE
1	A	301	TYR
1	A	317	LEU
1	A	324	LEU
1	A	328	TYR
1	A	332	ARG
1	A	335	GLU
1	A	361	LYS

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Mol	Chain	Res	Type
1	A	362	LYS
1	A	366	LYS
1	A	368	LEU
1	A	383	GLU
1	A	400	LYS
1	A	422	ARG
1	A	442	ASN
1	A	451	GLU
1	A	474	VAL
1	A	483	SER
1	A	493	ILE
1	A	504	GLU
1	A	543	LEU
1	A	555	LEU
1	B	3	LYS
1	B	5	LEU
1	B	57	LEU
1	B	58	ILE
1	B	66	ILE
1	B	80	ILE
1	B	104	ARG
1	B	112	VAL
1	B	137	THR
1	B	139	GLU
1	B	146	MET
1	B	152	LEU
1	B	172	TYR
1	B	176	LEU
1	B	203	ARG
1	B	214	ILE
1	B	215	LEU
1	B	226	LYS
1	B	255	VAL
1	B	266	ILE
1	B	278	LEU
1	B	281	LYS
1	B	289	ILE
1	B	302	ARG
1	B	317	LEU
1	B	332	ARG
1	B	337	ASN
1	B	361	LYS

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Mol	Chain	Res	Type
1	B	366	LYS
1	B	368	LEU
1	B	422	ARG
1	B	442	ASN
1	B	451	GLU
1	B	474	VAL
1	B	475	GLN
1	B	483	SER
1	B	493	ILE
1	B	504	GLU
1	B	543	LEU
1	B	557	HIS
1	C	3	LYS
1	C	5	LEU
1	C	39	MET
1	C	57	LEU
1	C	66	ILE
1	C	104	ARG
1	C	112	VAL
1	C	118	ASN
1	C	137	THR
1	C	139	GLU
1	C	140	VAL
1	C	146	MET
1	C	176	LEU
1	C	203	ARG
1	C	214	ILE
1	C	215	LEU
1	C	226	LYS
1	C	231	GLU
1	C	249	ASN
1	C	255	VAL
1	C	266	ILE
1	C	281	LYS
1	C	289	ILE
1	C	290	LEU
1	C	295	ILE
1	C	317	LEU
1	C	324	LEU
1	C	332	ARG
1	C	361	LYS
1	C	362	LYS

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Mol	Chain	Res	Type
1	C	366	LYS
1	C	368	LEU
1	C	370	LEU
1	C	422	ARG
1	C	442	ASN
1	C	451	GLU
1	C	474	VAL
1	C	493	ILE
1	C	504	GLU
1	C	515	LEU
1	C	535	THR
1	C	542	ARG
1	C	555	LEU
1	D	5	LEU
1	D	57	LEU
1	D	80	ILE
1	D	104	ARG
1	D	108	ILE
1	D	112	VAL
1	D	139	GLU
1	D	140	VAL
1	D	146	MET
1	D	172	TYR
1	D	176	LEU
1	D	203	ARG
1	D	214	ILE
1	D	215	LEU
1	D	228	LYS
1	D	231	GLU
1	D	249	ASN
1	D	266	ILE
1	D	281	LYS
1	D	289	ILE
1	D	317	LEU
1	D	328	TYR
1	D	332	ARG
1	D	361	LYS
1	D	362	LYS
1	D	366	LYS
1	D	368	LEU
1	D	373	LYS
1	D	422	ARG

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Mol	Chain	Res	Type
1	D	437	ASP
1	D	442	ASN
1	D	451	GLU
1	D	474	VAL
1	D	475	GLN
1	D	493	ILE
1	D	504	GLU
1	D	535	THR
1	D	542	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	218	ASN
1	A	249	ASN
1	A	315	HIS
1	A	411	GLN
1	A	420	ASN
1	A	462	ASN
1	B	241	GLN
1	B	315	HIS
1	B	329	GLN
1	B	367	ASN
1	B	436	ASN
1	C	54	ASN
1	C	95	HIS
1	C	126	GLN
1	C	315	HIS
1	C	367	ASN
1	C	411	GLN
1	C	420	ASN
1	D	54	ASN
1	D	185	ASN
1	D	220	ASN
1	D	329	GLN
1	D	367	ASN
1	D	411	GLN

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](#)

There are no ligands in this entry.

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%)	0.13	17 (3%)	52	37	122, 177, 272, 322	0
1	B	564/564 (100%)	0.21	23 (4%)	41	31	156, 204, 285, 320	0
1	C	564/564 (100%)	0.30	27 (4%)	35	28	139, 215, 288, 326	0
1	D	564/564 (100%)	0.25	25 (4%)	39	29	127, 218, 286, 328	0
All	All	2256/2256 (100%)	0.22	92 (4%)	41	31	122, 202, 284, 328	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	HIS	6.3
1	C	297	VAL	6.2
1	C	293	ILE	5.9
1	C	291	SER	5.9
1	B	5	LEU	5.8
1	A	561	LYS	5.5
1	B	6	PHE	5.0
1	C	92	TYR	4.9
1	A	464	GLU	4.8
1	C	290	LEU	4.8
1	C	289	ILE	4.6
1	C	294	SER	4.6
1	D	321	HIS	4.5
1	D	297	VAL	4.4
1	D	518	GLN	4.2
1	B	212	PHE	4.2
1	B	17	LEU	4.2
1	C	287	SER	4.2
1	A	253	GLU	4.1
1	A	335	GLU	4.1
1	C	137	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	516	ASP	4.0
1	D	294	SER	3.9
1	D	5	LEU	3.9
1	B	460	GLN	3.8
1	A	382	GLY	3.8
1	D	328	TYR	3.8
1	C	276	VAL	3.8
1	B	90	ASN	3.6
1	A	52	ASP	3.6
1	B	287	SER	3.6
1	A	549	CYS	3.5
1	A	290	LEU	3.5
1	B	277	PHE	3.4
1	C	216	ASN	3.4
1	D	129	GLN	3.3
1	D	135	SER	3.3
1	B	461	ALA	3.3
1	B	278	LEU	3.2
1	B	543	LEU	3.2
1	A	449	VAL	3.0
1	B	393	ASP	3.0
1	D	293	ILE	3.0
1	C	238	PHE	3.0
1	C	539	ILE	2.8
1	D	192	ILE	2.8
1	C	268	PHE	2.8
1	D	562	GLU	2.8
1	B	35	ILE	2.7
1	D	136	ILE	2.7
1	B	465	HIS	2.7
1	B	13	ASP	2.6
1	A	562	GLU	2.6
1	C	218	ASN	2.6
1	C	465	HIS	2.6
1	A	297	VAL	2.6
1	B	222	PHE	2.5
1	C	427	TYR	2.5
1	A	105	LYS	2.5
1	D	132	ILE	2.5
1	B	564	LYS	2.4
1	C	219	LEU	2.4
1	D	439	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	440	ALA	2.4
1	B	297	VAL	2.4
1	A	129	GLN	2.4
1	D	448	ALA	2.4
1	C	532	LYS	2.4
1	B	445	PHE	2.3
1	D	346	ASN	2.3
1	D	515	LEU	2.3
1	A	2	VAL	2.3
1	D	230	LYS	2.3
1	C	2	VAL	2.3
1	C	298	LEU	2.2
1	C	397	GLY	2.2
1	D	222	PHE	2.1
1	D	362	LYS	2.1
1	A	236	SER	2.1
1	C	393	ASP	2.1
1	B	499	LEU	2.1
1	A	564	LYS	2.1
1	C	355	SER	2.1
1	D	358	TYR	2.1
1	C	301	TYR	2.0
1	D	291	SER	2.0
1	C	258	VAL	2.0
1	A	400	LYS	2.0
1	B	286	ILE	2.0
1	D	229	THR	2.0
1	C	503	PRO	2.0
1	B	16	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.