



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:43 PM UTC

PDB ID : 3LN7 / pdb_00003ln7
Title : Crystal structure of a bifunctional glutathione synthetase from *Pasteurella multocida*
Authors : Stout, J.; Vergauwen, B.; Savvides, S.N.
Deposited on : 2010-02-02
Resolution : 3.20 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

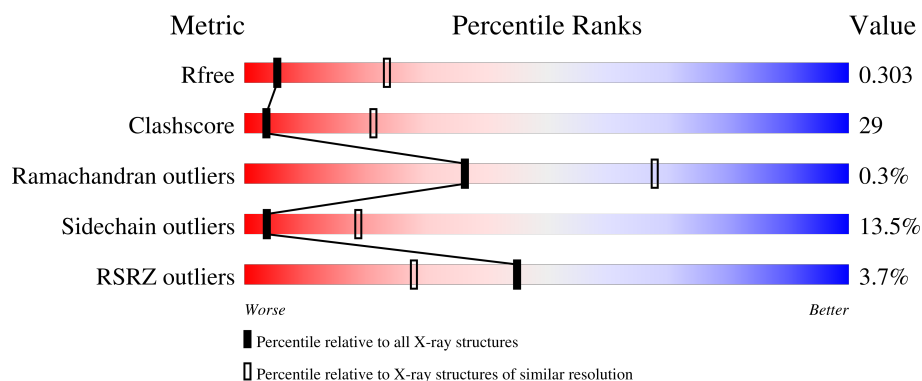
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	757	3% 53% 40% 5%
1	B	757	4% 53% 38% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10601 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 Glutathione biosynthesis bifunctional protein gshAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	Se	0	1	0
			5402	3467	912	1003	2	18			
1	B	729	Total	C	N	O	S	Se	0	0	0
			5199	3329	871	980	2	17			



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.24Å 87.07Å 145.98Å 90.00° 126.53° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-3.20) 97.0 (20.00-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.22Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.275 , 0.314 0.270 , 0.303	Depositor DCC
R_{free} test set	1671 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	0.89	0/5491	1.15	26/7456 (0.3%)
1	B	0.86	0/5280	1.15	19/7177 (0.3%)
All	All	0.88	0/10771	1.15	45/14633 (0.3%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	729	MSE	N-CA-C	9.34	121.54	111.36
1	A	491	VAL	CB-CA-C	-9.02	100.20	112.02
1	B	710	GLN	CA-C-N	8.69	128.73	119.78
1	B	710	GLN	C-N-CA	8.69	128.73	119.78
1	A	269	GLY	N-CA-C	-8.54	102.69	115.32
1	B	106	LEU	CA-C-N	7.98	127.93	120.03
1	B	106	LEU	C-N-CA	7.98	127.93	120.03
1	A	229	ASP	N-CA-C	7.19	114.60	108.13
1	B	434	SER	N-CA-C	-7.04	103.53	111.07
1	B	350	GLU	N-CA-C	-6.79	103.88	111.28
1	A	292	ASN	CA-C-N	6.48	126.10	119.56
1	A	292	ASN	C-N-CA	6.48	126.10	119.56
1	B	750	LYS	N-CA-C	-6.46	104.31	111.36
1	A	119	ASN	CA-C-N	6.44	125.86	118.85
1	A	119	ASN	C-N-CA	6.44	125.86	118.85
1	B	98	PHE	CA-C-N	6.16	125.89	119.05
1	B	98	PHE	C-N-CA	6.16	125.89	119.05
1	A	213	GLY	N-CA-C	-6.12	106.88	115.32
1	B	595	VAL	CA-C-N	6.11	126.07	119.78
1	B	595	VAL	C-N-CA	6.11	126.07	119.78
1	A	679	MSE	CG-SE-CE	6.11	112.36	98.92
1	A	663	ASN	N-CA-C	6.07	121.50	112.94
1	A	595	VAL	CA-C-N	5.96	126.27	119.83
1	A	595	VAL	C-N-CA	5.96	126.27	119.83
1	B	163	GLU	N-CA-C	5.90	117.71	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ALA	N-CA-C	-5.74	105.02	111.28
1	B	60	GLU	N-CA-C	-5.72	104.41	111.33
1	B	156	ARG	N-CA-C	-5.64	105.13	111.28
1	B	250	VAL	N-CA-C	-5.59	104.92	110.62
1	B	547	GLY	N-CA-C	5.38	125.93	113.18
1	A	332	ARG	CG-CD-NE	5.37	123.80	112.00
1	A	654	LYS	N-CA-C	5.27	117.07	110.91
1	A	726	PHE	CA-C-N	-5.19	117.14	122.85
1	A	726	PHE	C-N-CA	-5.19	117.14	122.85
1	A	735	PHE	CA-C-N	-5.19	114.64	120.14
1	A	735	PHE	C-N-CA	-5.19	114.64	120.14
1	B	221	SER	N-CA-C	-5.18	105.76	111.71
1	A	73	LEU	N-CA-C	-5.15	106.10	112.38
1	B	690	ILE	CB-CA-C	-5.14	105.12	112.22
1	A	434	SER	N-CA-C	-5.10	104.99	111.11
1	A	311	ALA	N-CA-C	-5.07	105.64	111.07
1	A	469	TYR	N-CA-C	5.06	116.85	108.20
1	A	271	LYS	N-CA-C	-5.04	105.68	111.07
1	A	229	ASP	CA-C-N	5.03	124.33	118.85
1	A	229	ASP	C-N-CA	5.03	124.33	118.85

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	5402	0	4799	303	0
1	B	5199	0	4516	289	0
All	All	10601	0	9315	584	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 29.

All (584) 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:679:MSE:HE3	1:A:708:LEU:HD23	1.46	0.97
1:A:647:THR:H	1:A:650:SER:HB3	1.31	0.93
1:A:730:MSE:HE3	1:A:745:THR:HG22	1.51	0.93
1:A:30:VAL:HG22	1:A:36:ILE:HA	1.57	0.85
1:B:238:SER:HB3	1:B:241:LYS:HB2	1.58	0.84
1:A:679:MSE:HG3	1:A:680:HIS:N	1.92	0.83
1:B:729:MSE:SE	1:B:732:MSE:HB2	2.27	0.83
1:B:102:MSE:HE3	1:B:103:PRO:HD2	1.60	0.82
1:B:220:ARG:HG3	1:B:221:SER:H	1.46	0.80
1:A:466:HIS:HD2	1:A:753:PHE:CE2	2.00	0.80
1:A:5:HIS:HB2	1:A:316:TRP:O	1.84	0.77
1:B:691:THR:HG22	1:B:699:CYS:SG	2.25	0.77
1:A:187:TRP:HA	1:A:333:LEU:HD12	1.67	0.77
1:A:594:ARG:O	1:A:664:SER:HB2	1.85	0.75
1:B:312:LEU:HB2	1:B:361:MSE:HE1	1.68	0.75
1:A:679:MSE:CE	1:A:708:LEU:HA	2.17	0.75
1:A:73:LEU:HD12	1:A:73:LEU:H	1.52	0.73
1:B:102:MSE:HE3	1:B:102:MSE:HA	1.70	0.73
1:A:632:ALA:O	1:A:637:GLU:HG2	1.87	0.73
1:B:234:VAL:HG12	1:B:235:SER:N	2.03	0.72
1:A:601:GLY:HA3	1:A:652:PRO:HB2	1.70	0.72
1:B:428:PHE:HB3	1:B:431:MSE:HG3	1.72	0.72
1:A:601:GLY:CA	1:A:652:PRO:HB2	2.20	0.71
1:A:602:ASP:HA	1:A:655:ASP:H	1.55	0.71
1:A:459:LEU:HD23	1:A:461:LEU:HD11	1.71	0.71
1:B:247:GLU:CD	1:B:274:ARG:NH2	2.49	0.70
1:A:442:VAL:HG11	1:A:449:THR:HB	1.72	0.70
1:A:466:HIS:HD2	1:A:753:PHE:CD2	2.08	0.70
1:A:588:THR:HG21	1:A:684:LYS:HB3	1.73	0.70
1:B:220:ARG:HG3	1:B:221:SER:N	2.06	0.70
1:A:198:THR:O	1:A:198:THR:HG22	1.90	0.69
1:B:178:MSE:HE3	1:B:284:LEU:HD12	1.75	0.69
1:B:729:MSE:HG3	1:B:730:MSE:N	2.06	0.69
1:B:235:SER:O	1:B:242:TYR:HB2	1.92	0.69
1:B:81:SER:HA	1:B:297:TYR:CE1	2.28	0.69
1:B:146:ASN:HD22	1:B:146:ASN:N	1.91	0.69
1:B:729:MSE:HG3	1:B:730:MSE:H	1.57	0.69
1:B:30:VAL:HG11	1:B:98:PHE:HB2	1.73	0.69
1:A:736:PRO:HB2	1:A:739:GLY:H	1.58	0.68
1:B:145:TYR:HB3	1:B:289:PHE:CE1	2.28	0.68
1:A:301:LEU:O	1:A:305:LYS:HG3	1.94	0.68
1:A:605:HIS:HB3	1:A:609:GLU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:HG23	1:A:588:THR:O	1.93	0.68
1:B:239:VAL:O	1:B:243:VAL:HG23	1.93	0.68
1:A:600:VAL:HG12	1:A:602:ASP:H	1.57	0.68
1:B:706:PRO:HD2	1:B:718:SER:O	1.93	0.68
1:A:186:GLN:HG3	1:A:333:LEU:HD13	1.75	0.68
1:A:651:ILE:HG22	1:A:651:ILE:O	1.94	0.68
1:A:647:THR:N	1:A:650:SER:HB3	2.08	0.67
1:A:153:LEU:HG	1:A:154:ILE:N	2.10	0.67
1:A:603:SER:O	1:A:604:VAL:HB	1.93	0.67
1:B:456:ASP:OD1	1:B:471:LYS:HE3	1.93	0.67
1:A:660:LEU:O	1:A:661:ARG:HG2	1.95	0.67
1:B:234:VAL:HG12	1:B:235:SER:H	1.56	0.67
1:A:185:TYR:CD1	1:A:354:VAL:HG21	2.30	0.67
1:A:617:HIS:ND1	1:A:618:PRO:HD2	2.10	0.66
1:A:143:ILE:CD1	1:A:299:ILE:HB	2.25	0.66
1:B:178:MSE:HE3	1:B:284:LEU:CD1	2.26	0.66
1:A:421:ARG:HD2	1:A:421:ARG:N	2.09	0.66
1:A:679:MSE:HE2	1:A:708:LEU:HA	1.78	0.66
1:B:698:VAL:HG12	1:B:698:VAL:O	1.95	0.66
1:A:65:LEU:HD23	1:A:83:ILE:HG22	1.78	0.66
1:A:723:GLU:HG2	1:A:724:ALA:N	2.10	0.66
1:B:198:THR:HG22	1:B:199:VAL:N	2.11	0.66
1:B:620:ARG:NH1	1:B:629:LYS:O	2.28	0.65
1:A:73:LEU:HD13	1:A:305:LYS:HE2	1.78	0.65
1:A:25:LYS:HG3	1:A:291:LEU:HD21	1.77	0.65
1:B:102:MSE:HG2	1:B:196:THR:HG22	1.77	0.65
1:A:194:ALA:HB3	1:A:390:ALA:HB2	1.78	0.65
1:A:730:MSE:CE	1:A:745:THR:HG22	2.26	0.65
1:A:461:LEU:N	1:A:461:LEU:HD12	2.11	0.65
1:B:592:LEU:HD11	1:B:672:SER:HB2	1.79	0.65
1:A:38:THR:HG22	1:A:38:THR:O	1.95	0.65
1:B:25:LYS:HE3	1:B:297:TYR:O	1.96	0.65
1:B:600:VAL:HG12	1:B:602:ASP:H	1.63	0.64
1:B:723:GLU:HG2	1:B:724:ALA:H	1.62	0.64
1:A:751:MSE:HG3	1:A:751:MSE:O	1.96	0.64
1:B:647:THR:HG22	1:B:649:ASP:H	1.63	0.64
1:A:483:SER:HB2	1:A:484:PRO:HD3	1.79	0.64
1:B:754:PRO:HD2	1:B:755:GLU:OE1	1.98	0.63
1:B:540:GLY:HA2	1:B:560:ILE:HG13	1.80	0.63
1:A:617:HIS:NE2	1:A:619:LEU:HD13	2.14	0.63
1:A:195:ALA:HB3	1:A:290:ASP:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LYS:HG2	1:A:272:LYS:H	1.63	0.63
1:A:441:ASP:OD1	1:A:743:ARG:NH1	2.32	0.63
1:A:183:LEU:O	1:A:186:GLN:HG2	1.98	0.63
1:A:723:GLU:HG2	1:A:724:ALA:H	1.64	0.63
1:B:349:VAL:HG23	1:B:350:GLU:N	2.12	0.63
1:B:431:MSE:HE3	1:B:439:LEU:HD11	1.80	0.62
1:A:604:VAL:HG12	1:A:604:VAL:O	1.97	0.62
1:B:646:LEU:HD22	1:B:658:VAL:HG11	1.80	0.62
1:B:730:MSE:HA	1:B:744:LEU:HD12	1.81	0.62
1:A:183:LEU:HD23	1:A:186:GLN:NE2	2.15	0.62
1:A:355:LEU:HD22	1:A:375:VAL:HG13	1.81	0.62
1:A:540:GLY:HA2	1:A:560:ILE:HG22	1.81	0.62
1:B:483:SER:CB	1:B:484:PRO:HD3	2.30	0.62
1:A:582:PHE:CE1	1:A:728:PRO:HB2	2.35	0.62
1:B:704:ILE:O	1:B:704:ILE:CG2	2.47	0.61
1:B:2:LYS:N	1:B:173:ASP:HB3	2.15	0.61
1:A:597:ALA:HB1	1:A:631:ILE:HG23	1.83	0.61
1:B:734:ILE:HD11	1:B:745:THR:HG23	1.82	0.60
1:A:271:LYS:HE3	1:A:271:LYS:H	1.66	0.60
1:A:456:ASP:O	1:A:457:GLN:HB2	2.01	0.60
1:B:493:THR:HG23	1:B:694:MSE:SE	2.51	0.60
1:A:270:ALA:HB2	1:A:276:PHE:CZ	2.37	0.60
1:A:32:ALA:HB2	1:A:96:TYR:CE2	2.36	0.60
1:B:28:GLN:O	1:B:30:VAL:HG13	2.02	0.60
1:B:292:ASN:C	1:B:292:ASN:OD1	2.44	0.60
1:B:249:TRP:CE3	1:B:249:TRP:HA	2.36	0.59
1:A:239:VAL:O	1:A:243:VAL:HG23	2.03	0.59
1:A:190:LEU:HD11	1:A:218:SER:HB3	1.84	0.59
1:B:520:TYR:HB2	1:B:554:PHE:CE2	2.37	0.59
1:B:431:MSE:HE1	1:B:451:ILE:HG12	1.85	0.59
1:B:30:VAL:CG1	1:B:98:PHE:HB2	2.32	0.59
1:B:182:PHE:O	1:B:186:GLN:HB3	2.02	0.59
1:B:412:GLN:O	1:B:416:ALA:CB	2.51	0.59
1:B:77:PHE:CE2	1:B:301:LEU:HA	2.37	0.59
1:A:51:HIS:CD2	1:A:54:ILE:H	2.20	0.58
1:B:617:HIS:CE1	1:B:619:LEU:HD12	2.38	0.58
1:B:195:ALA:C	1:B:197:PRO:HD3	2.29	0.58
1:B:637:GLU:CD	1:B:661:ARG:HH11	2.11	0.58
1:B:146:ASN:N	1:B:146:ASN:ND2	2.50	0.58
1:B:310:PHE:CE2	1:B:314:MSE:HE3	2.38	0.58
1:B:365:ILE:O	1:B:365:ILE:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:LEU:HD12	1:B:698:VAL:HG13	1.84	0.58
1:B:661:ARG:HG3	1:B:663:ASN:H	1.67	0.58
1:B:682:SER:HB3	1:B:712:ALA:CB	2.33	0.58
1:A:39:THR:HB	1:A:40:PRO:HD2	1.85	0.58
1:A:679:MSE:HE3	1:A:708:LEU:CD2	2.29	0.58
1:A:683:TYR:HA	1:A:686:LEU:HD12	1.84	0.58
1:A:241:LYS:HD3	1:A:241:LYS:N	2.18	0.58
1:A:683:TYR:CE1	1:A:712:ALA:HB2	2.39	0.57
1:B:41:HIS:HD2	1:B:42:PRO:HD2	1.69	0.57
1:A:433:LEU:HD12	1:A:433:LEU:N	2.18	0.57
1:A:487:MSE:HE2	1:A:694:MSE:HG3	1.86	0.57
1:A:729:MSE:HG2	1:A:732:MSE:HG3	1.86	0.57
1:B:611:VAL:CG1	1:B:612:ALA:N	2.67	0.57
1:A:73:LEU:HD12	1:A:73:LEU:N	2.20	0.57
1:A:466:HIS:CD2	1:A:753:PHE:CE2	2.89	0.57
1:A:606:SER:O	1:A:610:LEU:HB2	2.04	0.57
1:B:30:VAL:HG23	1:B:31:THR:O	2.04	0.57
1:B:458:PHE:CD2	1:B:471:LYS:HD2	2.39	0.57
1:B:582:PHE:CE1	1:B:728:PRO:HB2	2.39	0.57
1:A:289:PHE:CZ	1:A:307:ILE:HD13	2.40	0.57
1:A:686:LEU:HD22	1:A:719:TRP:CZ2	2.40	0.57
1:B:99:PRO:HG2	1:B:410:LEU:HB2	1.87	0.57
1:A:30:VAL:HG13	1:A:35:ALA:O	2.04	0.56
1:A:183:LEU:HD23	1:A:186:GLN:HE22	1.70	0.56
1:A:194:ALA:HB1	1:A:217:ARG:O	2.06	0.56
1:A:452:LEU:HD13	1:B:492:VAL:HG13	1.88	0.56
1:B:729:MSE:O	1:B:730:MSE:HB2	2.05	0.56
1:A:39:THR:HB	1:A:40:PRO:CD	2.36	0.56
1:B:357:GLU:O	1:B:360:SER:HB2	2.06	0.56
1:A:56:THR:HA	1:A:63:LEU:HA	1.86	0.56
1:A:513:LEU:HD23	1:A:513:LEU:C	2.31	0.56
1:B:137:LYS:O	1:B:140:VAL:HG22	2.05	0.56
1:B:51:HIS:CE1	1:B:54:ILE:H	2.23	0.56
1:A:447:ILE:HG21	1:A:461:LEU:HB3	1.87	0.56
1:B:682:SER:CB	1:B:712:ALA:HB2	2.36	0.56
1:A:647:THR:H	1:A:650:SER:CB	2.13	0.55
1:A:29:ARG:HH21	1:A:61:SER:HA	1.70	0.55
1:A:647:THR:HG22	1:A:648:ILE:N	2.21	0.55
1:B:564:GLU:HA	1:B:564:GLU:OE2	2.06	0.55
1:B:755:GLU:O	1:B:756:LEU:C	2.50	0.55
1:B:682:SER:HB3	1:B:712:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:GLU:HG2	1:B:724:ALA:N	2.20	0.55
1:A:487:MSE:SE	1:A:726:PHE:HB3	2.56	0.55
1:A:581:PHE:CD1	1:A:591:VAL:HG22	2.42	0.55
1:B:30:VAL:O	1:B:96:TYR:N	2.39	0.55
1:A:104:ALA:HB1	1:A:404:GLN:HG3	1.89	0.55
1:B:385:PRO:O	1:B:388:THR:HB	2.07	0.55
1:A:503:ASN:H	1:A:719:TRP:HZ3	1.55	0.55
1:B:456:ASP:C	1:B:457:GLN:HG2	2.30	0.55
1:B:682:SER:HB2	1:B:712:ALA:HB2	1.89	0.55
1:B:581:PHE:CD2	1:B:581:PHE:N	2.74	0.55
1:B:433:LEU:HD12	1:B:433:LEU:H	1.72	0.55
1:A:607:VAL:HG23	1:A:652:PRO:HD3	1.88	0.55
1:A:461:LEU:N	1:A:461:LEU:CD1	2.69	0.54
1:A:596:PRO:O	1:A:597:ALA:C	2.50	0.54
1:B:5:HIS:O	1:B:5:HIS:ND1	2.40	0.54
1:B:30:VAL:HB	1:B:35:ALA:O	2.07	0.54
1:A:192:LEU:HB2	1:A:193:LEU:HD12	1.90	0.54
1:B:96:TYR:CE1	1:B:415:LYS:HD2	2.43	0.54
1:B:514:GLU:HG2	1:B:515:LYS:N	2.22	0.54
1:B:273:ALA:HA	1:B:276:PHE:CD2	2.42	0.54
1:A:70:THR:OG1	1:A:76:THR:HG23	2.07	0.54
1:A:153:LEU:C	1:A:153:LEU:HD12	2.33	0.54
1:A:263:SER:O	1:A:287:ARG:HD3	2.08	0.54
1:A:466:HIS:CD2	1:A:753:PHE:CD2	2.94	0.54
1:B:620:ARG:NH2	1:B:628:LEU:HD22	2.23	0.54
1:A:621:GLY:O	1:A:629:LYS:HA	2.08	0.53
1:B:481:TYR:O	1:B:484:PRO:HD2	2.08	0.53
1:A:680:HIS:HB2	1:A:708:LEU:O	2.09	0.53
1:B:104:ALA:HB1	1:B:404:GLN:HA	1.90	0.53
1:B:531:LYS:HB3	1:B:541:ILE:HG12	1.90	0.53
1:A:190:LEU:HD21	1:A:337:ALA:HA	1.91	0.53
1:B:198:THR:CG2	1:B:199:VAL:N	2.71	0.53
1:B:283:TYR:O	1:B:284:LEU:HD23	2.09	0.53
1:A:51:HIS:CD2	1:A:52:PRO:HD2	2.45	0.52
1:A:716:LEU:HA	1:A:719:TRP:O	2.09	0.52
1:B:611:VAL:HG12	1:B:612:ALA:N	2.24	0.52
1:A:617:HIS:CE1	1:A:618:PRO:HD2	2.44	0.52
1:A:584:LEU:HD12	1:A:698:VAL:HG22	1.91	0.52
1:B:77:PHE:CZ	1:B:301:LEU:HA	2.44	0.52
1:B:664:SER:O	1:B:665:ASN:C	2.50	0.52
1:B:102:MSE:HE3	1:B:102:MSE:CA	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LYS:HE3	1:B:419:PHE:HE2	1.75	0.52
1:A:679:MSE:HG3	1:A:680:HIS:H	1.73	0.52
1:B:244:GLU:HA	1:B:247:GLU:HG2	1.91	0.52
1:B:423:TYR:HA	1:B:735:PHE:CZ	2.45	0.52
1:A:65:LEU:HD12	1:A:65:LEU:N	2.24	0.52
1:A:184:ARG:HA	1:A:329:GLY:HA3	1.92	0.52
1:A:438:LEU:HD23	1:A:459:LEU:HD22	1.92	0.52
1:A:85:GLU:O	1:A:89:ARG:HG3	2.10	0.52
1:A:392:ARG:HG2	1:A:395:ARG:CZ	2.39	0.52
1:A:97:ILE:O	1:A:411:ALA:CB	2.58	0.51
1:A:427:ALA:HB3	1:A:428:PHE:CD1	2.45	0.51
1:B:247:GLU:OE1	1:B:274:ARG:NH2	2.43	0.51
1:A:489:ASN:HB3	1:A:492:VAL:H	1.74	0.51
1:A:755:GLU:HG2	1:A:756:LEU:N	2.26	0.51
1:B:29:ARG:NH1	1:B:95:GLU:OE2	2.44	0.51
1:B:175:TYR:HD1	1:B:284:LEU:HG	1.74	0.51
1:B:520:TYR:HB2	1:B:554:PHE:HE2	1.75	0.51
1:B:471:LYS:O	1:B:475:MSE:HB2	2.11	0.51
1:B:637:GLU:CD	1:B:661:ARG:NH1	2.69	0.51
1:A:428:PHE:HB3	1:A:431:MSE:HE2	1.92	0.51
1:B:394:VAL:O	1:B:397:ILE:HG22	2.09	0.51
1:A:46:GLY:HA3	1:A:445:LYS:O	2.10	0.51
1:A:300:SER:OG	1:A:303:ASP:HB2	2.10	0.51
1:B:680:HIS:HB2	1:B:708:LEU:O	2.10	0.51
1:B:48:ARG:NE	1:B:56:THR:CG2	2.74	0.50
1:A:492:VAL:O	1:A:493:THR:C	2.54	0.50
1:B:182:PHE:HE1	1:B:189:LEU:HD12	1.76	0.50
1:B:447:ILE:HD11	1:B:756:LEU:HD11	1.92	0.50
1:B:458:PHE:CE2	1:B:471:LYS:HD2	2.46	0.50
1:B:513:LEU:HB2	1:B:562:PHE:CD1	2.47	0.50
1:A:97:ILE:O	1:A:411:ALA:HB1	2.12	0.50
1:B:415:LYS:HE3	1:B:419:PHE:CE2	2.46	0.50
1:A:686:LEU:HD22	1:A:719:TRP:CH2	2.47	0.50
1:B:234:VAL:CG1	1:B:235:SER:N	2.74	0.50
1:B:274:ARG:CD	1:B:274:ARG:N	2.74	0.50
1:B:405:GLN:O	1:B:409:GLN:HB2	2.11	0.50
1:A:183:LEU:HA	1:A:186:GLN:NE2	2.27	0.50
1:A:392:ARG:O	1:A:395:ARG:HD2	2.12	0.50
1:B:41:HIS:CE1	1:B:63:LEU:HD11	2.46	0.50
1:A:309:VAL:HG12	1:A:358:LEU:HD23	1.93	0.50
1:B:683:TYR:HA	1:B:686:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:PHE:CG	1:A:431:MSE:HE2	2.47	0.50
1:B:436:GLN:O	1:B:439:LEU:HB2	2.11	0.50
1:A:448:HIS:HB3	1:A:462:LYS:O	2.12	0.49
1:A:489:ASN:HB3	1:A:492:VAL:HB	1.93	0.49
1:B:388:THR:HG22	1:B:390:ALA:N	2.27	0.49
1:A:17:GLN:NE2	1:A:17:GLN:N	2.59	0.49
1:A:187:TRP:HB3	1:A:333:LEU:HB2	1.93	0.49
1:A:309:VAL:CG1	1:A:362:LEU:HD21	2.41	0.49
1:A:470:VAL:HG12	1:A:476:THR:HG22	1.94	0.49
1:B:388:THR:HG22	1:B:390:ALA:H	1.77	0.49
1:A:471:LYS:O	1:A:472:ASN:HB2	2.11	0.49
1:B:349:VAL:CG2	1:B:350:GLU:N	2.75	0.49
1:B:397:ILE:CG2	1:B:398:GLU:N	2.75	0.49
1:B:600:VAL:HG12	1:B:601:GLY:N	2.27	0.49
1:B:606:SER:O	1:B:610:LEU:N	2.40	0.49
1:B:698:VAL:O	1:B:728:PRO:HG2	2.12	0.49
1:A:73:LEU:H	1:A:73:LEU:CD1	2.17	0.49
1:A:595:VAL:O	1:A:670:GLY:HA3	2.12	0.49
1:B:85:GLU:O	1:B:89:ARG:HG3	2.13	0.49
1:B:102:MSE:HA	1:B:102:MSE:CE	2.36	0.49
1:B:52:PRO:HG2	1:B:53:TYR:CD2	2.47	0.49
1:A:30:VAL:CG1	1:A:31:THR:N	2.75	0.49
1:B:726:PHE:CD2	1:B:726:PHE:N	2.81	0.49
1:A:6:ILE:O	1:A:6:ILE:HG12	2.11	0.49
1:A:88:GLN:OE1	1:A:97:ILE:HB	2.13	0.49
1:A:582:PHE:HE1	1:A:728:PRO:HB2	1.77	0.49
1:A:601:GLY:HA2	1:A:610:LEU:HD21	1.94	0.49
1:B:513:LEU:O	1:B:513:LEU:HG	2.10	0.49
1:A:86:VAL:HG22	1:A:440:PHE:CD1	2.47	0.49
1:A:428:PHE:CD2	1:A:431:MSE:HE2	2.48	0.49
1:B:41:HIS:CD2	1:B:42:PRO:HD2	2.47	0.49
1:B:582:PHE:HE1	1:B:728:PRO:HB2	1.78	0.49
1:A:241:LYS:HD3	1:A:241:LYS:H	1.77	0.49
1:B:60:GLU:H	1:B:114:VAL:HA	1.77	0.49
1:A:601:GLY:HA2	1:A:652:PRO:HB2	1.92	0.49
1:A:734:ILE:HD11	1:A:745:THR:HG23	1.94	0.49
1:B:584:LEU:HD12	1:B:698:VAL:HG22	1.94	0.48
1:B:621:GLY:O	1:B:629:LYS:HA	2.13	0.48
1:A:164:TYR:O	1:A:165:GLN:CB	2.60	0.48
1:B:264:ASN:ND2	1:B:288:LEU:HD13	2.28	0.48
1:B:205:LYS:C	1:B:207:GLY:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:TRP:HA	1:B:249:TRP:HE3	1.76	0.48
1:B:683:TYR:O	1:B:686:LEU:N	2.47	0.48
1:A:58:PHE:CG	1:A:59:ALA:N	2.78	0.48
1:A:58:PHE:O	1:A:115:ALA:HA	2.13	0.48
1:A:690:ILE:O	1:A:694:MSE:HG2	2.13	0.48
1:A:734:ILE:HA	1:A:742:ARG:O	2.13	0.48
1:B:683:TYR:HA	1:B:686:LEU:HB2	1.95	0.48
1:B:51:HIS:HE1	1:B:53:TYR:HB2	1.77	0.48
1:B:679:MSE:HE1	1:B:705:ILE:HD12	1.95	0.48
1:A:460:CYS:C	1:A:461:LEU:HD12	2.37	0.48
1:A:485:LEU:HD13	1:B:471:LYS:HD3	1.95	0.48
1:B:310:PHE:CZ	1:B:314:MSE:HE3	2.48	0.48
1:A:524:GLU:C	1:A:526:ARG:H	2.22	0.48
1:A:528:VAL:O	1:A:544:PHE:HB2	2.14	0.48
1:A:408:ALA:O	1:A:412:GLN:HG3	2.13	0.48
1:A:489:ASN:C	1:A:491:VAL:H	2.21	0.48
1:B:91:LEU:HD23	1:B:91:LEU:HA	1.71	0.48
1:B:148:GLN:HB2	1:B:283:TYR:HB3	1.95	0.48
1:B:412:GLN:O	1:B:416:ALA:HB2	2.13	0.47
1:B:679:MSE:CE	1:B:705:ILE:HD12	2.43	0.47
1:A:481:TYR:HD1	1:B:481:TYR:HA	1.77	0.47
1:A:527:ALA:HA	1:A:547:GLY:HA2	1.97	0.47
1:A:682:SER:O	1:A:686:LEU:HD12	2.13	0.47
1:A:51:HIS:HD2	1:A:53:TYR:H	1.61	0.47
1:A:471:LYS:HD3	1:B:485:LEU:HD22	1.95	0.47
1:A:733:HIS:CB	1:A:744:LEU:HD11	2.44	0.47
1:B:482:ILE:O	1:B:482:ILE:HG22	2.14	0.47
1:B:703:LEU:CD2	1:B:719:TRP:CE3	2.98	0.47
1:A:309:VAL:HG12	1:A:358:LEU:CD2	2.45	0.47
1:A:376:LYS:HA	1:A:379:LEU:HD12	1.95	0.47
1:A:229:ASP:CB	1:A:230:PRO:HD2	2.44	0.47
1:B:164:TYR:OH	1:B:173:ASP:OD2	2.28	0.47
1:B:532:PRO:O	1:B:533:LYS:C	2.58	0.47
1:A:581:PHE:CD2	1:A:703:LEU:HD13	2.50	0.47
1:A:632:ALA:O	1:A:637:GLU:CG	2.60	0.47
1:B:15:LEU:HB3	1:B:153:LEU:HB2	1.97	0.47
1:B:345:THR:HG23	1:B:348:ALA:HB2	1.97	0.47
1:B:704:ILE:O	1:B:704:ILE:HG22	2.14	0.47
1:A:736:PRO:HB2	1:A:739:GLY:N	2.28	0.47
1:B:15:LEU:C	1:B:153:LEU:HD13	2.40	0.47
1:B:97:ILE:HG22	1:B:98:PHE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:VAL:HG22	1:B:671:ASP:O	2.15	0.47
1:B:601:GLY:CA	1:B:652:PRO:HB2	2.44	0.47
1:A:481:TYR:O	1:A:484:PRO:HD2	2.15	0.47
1:A:370:GLU:O	1:A:373:GLU:HB2	2.15	0.47
1:A:651:ILE:HG23	1:A:652:PRO:O	2.15	0.47
1:A:704:ILE:CG1	1:A:722:ILE:CG1	2.92	0.47
1:B:602:ASP:HA	1:B:655:ASP:H	1.80	0.47
1:B:755:GLU:HG2	1:B:756:LEU:N	2.30	0.47
1:A:540:GLY:HA2	1:A:560:ILE:CG2	2.46	0.46
1:B:25:LYS:HE2	1:B:291:LEU:CD2	2.44	0.46
1:A:309:VAL:HG11	1:A:362:LEU:HD21	1.96	0.46
1:A:471:LYS:O	1:A:475:MSE:HB2	2.14	0.46
1:A:509:GLU:HG3	1:A:569:MSE:CB	2.44	0.46
1:A:503:ASN:CB	1:A:719:TRP:HE3	2.28	0.46
1:B:560:ILE:CG1	1:B:561:ALA:N	2.78	0.46
1:B:651:ILE:CG1	1:B:651:ILE:O	2.63	0.46
1:A:190:LEU:HD11	1:A:218:SER:CB	2.45	0.46
1:A:433:LEU:N	1:A:433:LEU:CD1	2.78	0.46
1:B:28:GLN:O	1:B:30:VAL:CG1	2.63	0.46
1:B:433:LEU:HD12	1:B:433:LEU:N	2.29	0.46
1:B:96:TYR:HE1	1:B:415:LYS:HD2	1.79	0.46
1:B:243:VAL:CG1	1:B:274:ARG:HD2	2.46	0.46
1:B:312:LEU:N	1:B:312:LEU:HD23	2.30	0.46
1:B:349:VAL:HG23	1:B:350:GLU:H	1.81	0.46
1:B:557:ALA:O	1:B:560:ILE:HG12	2.15	0.46
1:A:271:LYS:HD2	1:A:275:GLU:CB	2.45	0.46
1:A:731:MSE:HE3	1:A:732:MSE:HG2	1.96	0.46
1:A:36:ILE:HG13	1:A:105:GLY:O	2.16	0.46
1:A:282:GLN:OE1	1:A:282:GLN:HA	2.15	0.46
1:A:433:LEU:CD1	1:A:433:LEU:H	2.29	0.46
1:B:350:GLU:O	1:B:354:VAL:HG23	2.15	0.46
1:A:98:PHE:CZ	1:A:104:ALA:HB2	2.51	0.46
1:A:145:TYR:HB3	1:A:289:PHE:HE1	1.80	0.46
1:A:607:VAL:HG22	1:A:652:PRO:CG	2.46	0.46
1:B:148:GLN:HB2	1:B:283:TYR:CB	2.46	0.46
1:B:176:LEU:O	1:B:177:LYS:C	2.59	0.46
1:B:205:LYS:C	1:B:207:GLY:H	2.23	0.46
1:B:377:GLU:O	1:B:381:GLN:HG3	2.16	0.46
1:A:168:VAL:HG23	1:A:169:ASP:N	2.31	0.45
1:A:268:ARG:NE	1:A:283:TYR:OH	2.49	0.45
1:A:493:THR:HA	1:A:694:MSE:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:O	1:A:588:THR:CG2	2.63	0.45
1:B:489:ASN:O	1:B:490:LYS:HB2	2.17	0.45
1:B:497:LEU:O	1:B:500:ALA:HB3	2.16	0.45
1:B:604:VAL:HG23	1:B:604:VAL:O	2.16	0.45
1:A:187:TRP:CB	1:A:333:LEU:HA	2.46	0.45
1:B:16:PHE:N	1:B:153:LEU:HD13	2.31	0.45
1:B:127:GLU:O	1:B:131:LYS:N	2.45	0.45
1:B:146:ASN:HD22	1:B:146:ASN:H	1.61	0.45
1:A:81:SER:HA	1:A:297:TYR:CZ	2.50	0.45
1:A:146:ASN:OD1	1:A:285:GLU:HG3	2.16	0.45
1:A:184:ARG:HH12	1:A:350:GLU:CD	2.23	0.45
1:A:313:PHE:CD2	1:A:314:MSE:HE2	2.51	0.45
1:A:420:GLU:O	1:A:421:ARG:HB2	2.16	0.45
1:A:647:THR:O	1:A:650:SER:HB3	2.16	0.45
1:B:483:SER:CB	1:B:484:PRO:CD	2.94	0.45
1:B:658:VAL:O	1:B:658:VAL:HG23	2.16	0.45
1:A:20:SER:HB2	1:A:148:GLN:HB3	1.98	0.45
1:B:104:ALA:HB1	1:B:404:GLN:CB	2.46	0.45
1:B:538:GLY:HA2	1:B:541:ILE:HD12	1.97	0.45
1:A:330:LYS:O	1:A:330:LYS:HG3	2.17	0.45
1:B:218:SER:O	1:B:337:ALA:HB1	2.16	0.45
1:B:362:LEU:HD22	1:B:367:ALA:CB	2.47	0.45
1:B:412:GLN:O	1:B:416:ALA:HB3	2.17	0.45
1:B:606:SER:O	1:B:607:VAL:C	2.58	0.45
1:B:683:TYR:O	1:B:686:LEU:HB2	2.16	0.45
1:B:312:LEU:O	1:B:316:TRP:HB2	2.16	0.45
1:B:427:ALA:HB3	1:B:428:PHE:CD2	2.51	0.45
1:B:468:GLU:OE2	1:B:477:SER:OG	2.28	0.45
1:A:15:LEU:HB3	1:A:153:LEU:HB2	1.97	0.45
1:A:75:ASP:O	1:A:76:THR:C	2.57	0.45
1:A:265:VAL:O	1:A:265:VAL:HG13	2.17	0.45
1:A:637:GLU:OE1	1:A:661:ARG:NH1	2.50	0.45
1:B:729:MSE:O	1:B:730:MSE:CB	2.65	0.45
1:A:634:GLY:O	1:A:638:GLN:N	2.48	0.45
1:B:217:ARG:CG	1:B:341:PRO:HA	2.47	0.45
1:A:192:LEU:CB	1:A:193:LEU:HD12	2.47	0.44
1:A:456:ASP:O	1:A:457:GLN:CB	2.62	0.44
1:A:651:ILE:CG2	1:A:652:PRO:O	2.65	0.44
1:B:554:PHE:CZ	1:B:558:LEU:HD11	2.53	0.44
1:A:267:LEU:O	1:A:268:ARG:HG2	2.17	0.44
1:A:57:ASP:OD1	1:A:57:ASP:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:HB	1:A:245:SER:HB2	1.99	0.44
1:A:691:THR:OG1	1:A:699:CYS:HB3	2.17	0.44
1:B:26:GLU:O	1:B:141:SER:HB3	2.18	0.44
1:B:365:ILE:O	1:B:365:ILE:CG2	2.65	0.44
1:A:51:HIS:O	1:A:55:GLN:NE2	2.51	0.44
1:A:489:ASN:CB	1:A:492:VAL:HB	2.46	0.44
1:A:607:VAL:CG2	1:A:652:PRO:HD3	2.47	0.44
1:B:104:ALA:HB1	1:B:404:GLN:CA	2.47	0.44
1:A:730:MSE:O	1:A:733:HIS:HB2	2.18	0.44
1:B:187:TRP:HA	1:B:333:LEU:HD23	1.99	0.44
1:B:482:ILE:HA	1:B:485:LEU:HB2	2.00	0.44
1:B:130:VAL:O	1:B:134:GLY:N	2.50	0.44
1:B:168:VAL:O	1:B:172:ASN:ND2	2.51	0.44
1:B:545:GLN:O	1:B:546:GLN:CB	2.63	0.44
1:A:130:VAL:HA	1:A:138:GLN:HE22	1.83	0.44
1:A:178:MSE:CE	1:A:315:ILE:HD11	2.48	0.44
1:A:292:ASN:HA	1:A:293:PRO:HD3	1.71	0.44
1:B:471:LYS:O	1:B:472:ASN:HB2	2.17	0.44
1:A:737:TYR:CD2	1:A:738:ALA:HB2	2.52	0.44
1:B:102:MSE:CE	1:B:103:PRO:HD2	2.41	0.44
1:B:217:ARG:HG2	1:B:341:PRO:HA	2.00	0.44
1:B:484:PRO:HA	1:B:487:MSE:HE3	2.00	0.44
1:A:190:LEU:CD2	1:A:337:ALA:HB2	2.48	0.44
1:A:249:TRP:O	1:A:254:LYS:HA	2.17	0.44
1:B:335:GLU:HG3	1:B:336:VAL:N	2.32	0.44
1:A:190:LEU:HD21	1:A:337:ALA:CB	2.47	0.43
1:A:688:VAL:O	1:A:691:THR:HG22	2.18	0.43
1:A:700:GLY:N	1:A:728:PRO:HG3	2.33	0.43
1:B:641:LEU:HG	1:B:660:LEU:HD23	2.01	0.43
1:B:682:SER:CB	1:B:712:ALA:CB	2.94	0.43
1:A:78:ARG:HB3	1:A:427:ALA:HB1	1.99	0.43
1:A:271:LYS:HG2	1:A:272:LYS:N	2.32	0.43
1:A:428:PHE:CB	1:A:431:MSE:HE2	2.47	0.43
1:A:603:SER:O	1:A:604:VAL:CB	2.62	0.43
1:B:314:MSE:O	1:B:317:MSE:HG2	2.19	0.43
1:B:647:THR:O	1:B:648:ILE:C	2.62	0.43
1:A:31:THR:C	1:A:33:ASP:N	2.73	0.43
1:A:481:TYR:CD1	1:B:484:PRO:HG2	2.52	0.43
1:A:755:GLU:O	1:A:756:LEU:C	2.59	0.43
1:B:15:LEU:HD13	1:B:153:LEU:HA	2.00	0.43
1:A:240:GLU:CD	1:A:240:GLU:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LYS:N	1:A:241:LYS:CD	2.82	0.43
1:A:265:VAL:O	1:A:265:VAL:CG1	2.65	0.43
1:A:463:TYR:CD2	1:A:463:TYR:C	2.95	0.43
1:A:502:PHE:CZ	1:A:689:GLY:C	2.96	0.43
1:A:671:ASP:HB3	1:A:737:TYR:CD2	2.54	0.43
1:B:266:ARG:CG	1:B:268:ARG:HH11	2.31	0.43
1:A:378:LYS:O	1:A:381:GLN:HB2	2.17	0.43
1:A:493:THR:HG23	1:A:694:MSE:CE	2.49	0.43
1:B:48:ARG:NE	1:B:56:THR:HG22	2.33	0.43
1:B:52:PRO:HG2	1:B:53:TYR:CE2	2.53	0.43
1:B:238:SER:HB3	1:B:241:LYS:HE3	1.99	0.43
1:B:476:THR:CG2	1:B:752:LEU:HD21	2.48	0.43
1:A:17:GLN:N	1:A:17:GLN:HE21	2.17	0.43
1:A:115:ALA:O	1:A:116:GLN:HB2	2.17	0.43
1:A:607:VAL:HG22	1:A:652:PRO:HG3	2.01	0.43
1:A:660:LEU:N	1:A:660:LEU:HD12	2.34	0.43
1:A:663:ASN:O	1:A:664:SER:C	2.60	0.43
1:B:292:ASN:OD1	1:B:294:PHE:N	2.52	0.43
1:B:427:ALA:HB3	1:B:428:PHE:CE2	2.53	0.43
1:B:584:LEU:HA	1:B:697:ALA:O	2.17	0.43
1:A:28:GLN:HE21	1:A:62:GLN:HE21	1.64	0.43
1:A:602:ASP:CA	1:A:655:ASP:H	2.27	0.43
1:B:737:TYR:CD2	1:B:737:TYR:C	2.97	0.43
1:A:629:LYS:O	1:A:669:GLY:HA2	2.19	0.43
1:B:59:ALA:O	1:B:60:GLU:C	2.61	0.43
1:B:192:LEU:HD13	1:B:378:LYS:HD2	2.01	0.43
1:A:29:ARG:NH1	1:A:95:GLU:OE1	2.52	0.43
1:A:30:VAL:CG2	1:A:36:ILE:HA	2.41	0.43
1:A:178:MSE:HE2	1:A:315:ILE:HD11	2.01	0.43
1:A:582:PHE:CD2	1:A:582:PHE:C	2.97	0.43
1:A:249:TRP:HA	1:A:249:TRP:CE3	2.54	0.42
1:B:601:GLY:O	1:B:602:ASP:C	2.62	0.42
1:B:661:ARG:HD2	1:B:663:ASN:OD1	2.19	0.42
1:A:190:LEU:HD21	1:A:337:ALA:HB2	2.01	0.42
1:B:158:PHE:CD2	1:B:158:PHE:C	2.97	0.42
1:B:463:TYR:CD2	1:B:463:TYR:O	2.72	0.42
1:B:619:LEU:CD2	1:B:627:PRO:HG2	2.49	0.42
1:A:24:GLU:HB2	1:A:144:HIS:HB2	2.00	0.42
1:A:442:VAL:HG11	1:A:449:THR:CB	2.45	0.42
1:A:328:LEU:C	1:A:328:LEU:HD23	2.44	0.42
1:A:481:TYR:HE2	1:B:475:MSE:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LEU:CD2	1:A:652:PRO:HG2	2.50	0.42
1:B:266:ARG:CG	1:B:268:ARG:NH1	2.82	0.42
1:B:310:PHE:CD2	1:B:314:MSE:HE3	2.54	0.42
1:B:475:MSE:HE3	1:B:727:ASN:HB2	2.00	0.42
1:B:635:GLU:O	1:B:639:LEU:HB2	2.20	0.42
1:B:704:ILE:O	1:B:704:ILE:HG23	2.19	0.42
1:A:190:LEU:HD21	1:A:337:ALA:CA	2.50	0.42
1:A:734:ILE:HG12	1:A:743:ARG:HA	2.01	0.42
1:B:603:SER:CB	1:B:605:HIS:HD2	2.32	0.42
1:A:691:THR:CG2	1:A:692:LYS:HD3	2.49	0.42
1:B:263:SER:CB	1:B:265:VAL:O	2.68	0.42
1:B:292:ASN:HA	1:B:293:PRO:HD3	1.75	0.42
1:B:683:TYR:O	1:B:684:LYS:C	2.62	0.42
1:A:15:LEU:HD13	1:A:15:LEU:HA	1.84	0.42
1:B:175:TYR:CD1	1:B:284:LEU:HG	2.53	0.42
1:A:273:ALA:O	1:A:276:PHE:HB2	2.20	0.42
1:B:265:VAL:HB	1:B:286:PHE:CD1	2.54	0.42
1:B:265:VAL:HB	1:B:286:PHE:CE1	2.55	0.42
1:A:67:THR:O	1:A:67:THR:HG23	2.19	0.42
1:A:136:ASN:O	1:A:139:MSE:HB2	2.20	0.42
1:A:376:LYS:O	1:A:377:GLU:C	2.63	0.42
1:B:104:ALA:CB	1:B:404:GLN:HA	2.50	0.42
1:B:447:ILE:HD11	1:B:756:LEU:CD1	2.50	0.42
1:B:596:PRO:O	1:B:597:ALA:C	2.61	0.42
1:A:182:PHE:HE1	1:A:189:LEU:HD12	1.84	0.41
1:A:351:GLY:HA3	1:A:382:PHE:CZ	2.55	0.41
1:B:238:SER:CB	1:B:241:LYS:HE3	2.50	0.41
1:B:474:ASN:HD21	1:B:730:MSE:HG3	1.85	0.41
1:B:730:MSE:O	1:B:734:ILE:HG13	2.19	0.41
1:A:481:TYR:CE2	1:B:475:MSE:HE2	2.55	0.41
1:A:6:ILE:O	1:A:6:ILE:CG1	2.69	0.41
1:A:357:GLU:O	1:A:358:LEU:C	2.62	0.41
1:A:469:TYR:HB2	1:B:482:ILE:HG21	2.01	0.41
1:B:25:LYS:HE2	1:B:291:LEU:HD22	2.01	0.41
1:A:691:THR:HG22	1:A:692:LYS:HD3	2.01	0.41
1:B:273:ALA:O	1:B:276:PHE:HB2	2.20	0.41
1:B:474:ASN:ND2	1:B:728:PRO:O	2.54	0.41
1:B:530:ILE:O	1:B:541:ILE:HA	2.20	0.41
1:A:92:PRO:O	1:A:93:GLU:C	2.61	0.41
1:A:532:PRO:HB2	1:A:565:ASP:HB2	2.03	0.41
1:B:381:GLN:OE1	1:B:388:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:GLN:HE21	1:B:457:GLN:HA	1.86	0.41
1:B:483:SER:O	1:B:486:ILE:HB	2.20	0.41
1:A:187:TRP:HB2	1:A:333:LEU:HA	2.01	0.41
1:A:39:THR:CB	1:A:40:PRO:CD	2.98	0.41
1:A:150:SER:HA	1:A:151:PRO:HD3	1.95	0.41
1:A:267:LEU:N	1:A:267:LEU:HD12	2.36	0.41
1:A:375:VAL:O	1:A:378:LYS:HB2	2.19	0.41
1:A:432:GLU:O	1:A:436:GLN:HG3	2.20	0.41
1:A:674:ASP:H	1:A:739:GLY:HA3	1.86	0.41
1:B:26:GLU:HA	1:B:63:LEU:O	2.21	0.41
1:B:529:VAL:HG23	1:B:573:TYR:HB2	2.02	0.41
1:A:470:VAL:O	1:A:470:VAL:HG23	2.20	0.41
1:A:634:GLY:O	1:A:637:GLU:HB2	2.20	0.41
1:B:323:GLN:O	1:B:326:VAL:HB	2.21	0.41
1:B:550:ASN:ND2	1:B:553:ASP:HB2	2.36	0.41
1:A:59:ALA:O	1:A:60:GLU:C	2.64	0.41
1:A:62:GLN:NE2	1:A:139:MSE:O	2.54	0.41
1:A:143:ILE:HD11	1:A:298:GLY:O	2.21	0.41
1:A:447:ILE:HD11	1:A:756:LEU:CD2	2.51	0.41
1:A:503:ASN:CB	1:A:719:TRP:CE3	3.04	0.41
1:A:733:HIS:HB3	1:A:744:LEU:HD11	2.03	0.41
1:B:196:THR:O	1:B:219:LEU:N	2.45	0.41
1:B:234:VAL:CG1	1:B:235:SER:H	2.28	0.41
1:B:266:ARG:HB2	1:B:287:ARG:HD2	2.03	0.41
1:B:322:ASP:C	1:B:322:ASP:OD1	2.63	0.41
1:B:449:THR:HB	1:B:461:LEU:HD23	2.03	0.41
1:B:703:LEU:HD21	1:B:719:TRP:CE3	2.55	0.41
1:A:47:ASN:HB3	1:A:50:TYR:CE2	2.56	0.41
1:A:439:LEU:HD12	1:A:439:LEU:HA	1.75	0.41
1:B:149:LEU:H	1:B:149:LEU:HD12	1.86	0.41
1:B:349:VAL:CG2	1:B:350:GLU:H	2.34	0.41
1:B:532:PRO:HG2	1:B:539:LEU:O	2.20	0.41
1:A:583:VAL:HG21	1:A:687:ALA:C	2.46	0.40
1:A:674:ASP:HB3	1:A:739:GLY:HA3	2.03	0.40
1:B:690:ILE:O	1:B:694:MSE:HG2	2.21	0.40
1:A:513:LEU:HA	1:A:562:PHE:CE2	2.56	0.40
1:B:155:THR:O	1:B:156:ARG:C	2.63	0.40
1:B:189:LEU:HD23	1:B:189:LEU:HA	1.81	0.40
1:A:106:LEU:HA	1:A:107:PRO:HD2	1.96	0.40
1:B:154:ILE:O	1:B:157:LEU:HB2	2.22	0.40
1:A:137:LYS:CB	1:A:226:TYR:HB3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:CD1	1:A:178:MSE:HE3	2.56	0.40
1:B:187:TRP:CZ2	1:B:350:GLU:HB3	2.55	0.40
1:B:187:TRP:HB3	1:B:333:LEU:HA	2.03	0.40
1:B:242:TYR:CD2	1:B:242:TYR:C	2.98	0.40
1:A:26:GLU:O	1:A:141:SER:CB	2.70	0.40
1:A:428:PHE:HB3	1:A:431:MSE:CE	2.50	0.40
1:B:482:ILE:HA	1:B:485:LEU:HD12	2.04	0.40
1:B:595:VAL:HA	1:B:596:PRO:HD3	1.86	0.40
1:B:737:TYR:CD2	1:B:738:ALA:HB2	2.57	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	740/757 (98%)	713 (96%)	23 (3%)	4 (0%)	24	59
1	B	713/757 (94%)	690 (97%)	22 (3%)	1 (0%)	48	79
All	All	1453/1514 (96%)	1403 (97%)	45 (3%)	5 (0%)	36	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	604	VAL
1	B	548	VAL
1	A	457	GLN
1	A	52	PRO
1	A	597	ALA

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	462/637 (72%)	403 (87%)	59 (13%)	4	20
1	B	435/637 (68%)	373 (86%)	62 (14%)	3	16
All	All	897/1274 (70%)	776 (86%)	121 (14%)	4	19

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PHE
1	A	17	GLN
1	A	30	VAL
1	A	33	ASP
1	A	48	ARG
1	A	55	GLN
1	A	63	LEU
1	A	73	LEU
1	A	75	ASP
1	A	91	LEU
1	A	97	ILE
1	A	140	VAL
1	A	153	LEU
1	A	178	MSE
1	A	190	LEU
1	A	228	ASN
1	A	234	VAL
1	A	271	LYS
1	A	287	ARG
1	A	333	LEU
1	A	350	GLU
1	A	358	LEU
1	A	394	VAL
1	A	395	ARG
1	A	403	ASP
1	A	421	ARG
1	A	447	ILE

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Mol	Chain	Res	Type
1	A	458	PHE
1	A	459	LEU
1	A	477	SER
1	A	479	ASP
1	A	488	GLU
1	A	494	LYS
1	A	504	VAL
1	A	508	VAL
1	A	523	PHE
1	A	530	ILE
1	A	539	LEU
1	A	572	ASP
1	A	580	ARG
1	A	587	GLU
1	A	592	LEU
1	A	593	LEU
1	A	609	GLU
1	A	635	GLU
1	A	651	ILE
1	A	665	ASN
1	A	671	ASP
1	A	674	ASP
1	A	679	MSE
1	A	682	SER
1	A	691	THR
1	A	692	LYS
1	A	705	ILE
1	A	715	ASN
1	A	731	MSE
1	A	751	MSE
1	A	752	LEU
1	A	756	LEU
1	B	4	GLN
1	B	12	LEU
1	B	27	SER
1	B	30	VAL
1	B	60	GLU
1	B	75	ASP
1	B	94	GLU
1	B	139	MSE
1	B	146	ASN
1	B	148	GLN

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Mol	Chain	Res	Type
1	B	153	LEU
1	B	168	VAL
1	B	196	THR
1	B	244	GLU
1	B	265	VAL
1	B	274	ARG
1	B	305	LYS
1	B	333	LEU
1	B	345	THR
1	B	360	SER
1	B	372	PHE
1	B	373	GLU
1	B	383	THR
1	B	415	LYS
1	B	431	MSE
1	B	435	THR
1	B	450	GLU
1	B	451	ILE
1	B	453	ASP
1	B	457	GLN
1	B	458	PHE
1	B	470	VAL
1	B	475	MSE
1	B	486	ILE
1	B	489	ASN
1	B	494	LYS
1	B	504	VAL
1	B	513	LEU
1	B	523	PHE
1	B	539	LEU
1	B	542	THR
1	B	545	GLN
1	B	550	ASN
1	B	580	ARG
1	B	581	PHE
1	B	584	LEU
1	B	587	GLU
1	B	594	ARG
1	B	599	VAL
1	B	610	LEU
1	B	611	VAL
1	B	616	ASP

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Mol	Chain	Res	Type
1	B	642	LYS
1	B	644	GLN
1	B	657	LEU
1	B	673	ILE
1	B	699	CYS
1	B	703	LEU
1	B	726	PHE
1	B	729	MSE
1	B	730	MSE
1	B	731	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	51	HIS
1	A	55	GLN
1	A	62	GLN
1	A	88	GLN
1	A	136	ASN
1	A	138	GLN
1	A	412	GLN
1	A	466	HIS
1	A	472	ASN
1	A	506	GLN
1	A	644	GLN
1	A	663	ASN
1	A	665	ASN
1	A	733	HIS
1	B	4	GLN
1	B	41	HIS
1	B	138	GLN
1	B	144	HIS
1	B	146	ASN
1	B	404	GLN
1	B	412	GLN
1	B	430	ASN
1	B	474	ASN
1	B	478	HIS
1	B	503	ASN
1	B	605	HIS
1	B	656	GLN

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Mol	Chain	Res	Type
1	B	733	HIS
1	B	747	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	728/757 (96%)	0.41	21 (2%)	53 35	17, 39, 66, 88	1 (0%)
1	B	710/757 (93%)	0.46	32 (4%)	38 24	20, 41, 71, 102	0
All	All	1438/1514 (94%)	0.43	53 (3%)	45 28	17, 40, 68, 102	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	TYR	4.6
1	B	104	ALA	4.4
1	A	725[A]	ASN	3.9
1	B	602	ASP	3.8
1	A	228	ASN	3.8
1	B	215	PHE	3.6
1	B	663	ASN	3.2
1	B	403	ASP	3.1
1	A	208	SER	3.0
1	A	38	THR	2.9
1	A	196	THR	2.9
1	B	47	ASN	2.8
1	B	668	THR	2.7
1	A	601	GLY	2.6
1	B	221	SER	2.6
1	A	604	VAL	2.6
1	B	339	GLU	2.5
1	B	164	TYR	2.5
1	A	262	TYR	2.5
1	B	280	GLY	2.5
1	A	719	TRP	2.4
1	B	115	ALA	2.4
1	A	138	GLN	2.4
1	A	227	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	247	GLU	2.4
1	B	390	ALA	2.3
1	A	61	SER	2.3
1	B	208	SER	2.3
1	B	77	PHE	2.3
1	A	322	ASP	2.3
1	B	275	GLU	2.3
1	B	227	VAL	2.2
1	B	604	VAL	2.2
1	B	12	LEU	2.2
1	B	105	GLY	2.2
1	B	547	GLY	2.2
1	A	205	LYS	2.2
1	B	61	SER	2.2
1	B	664	SER	2.2
1	A	353	LEU	2.2
1	B	270	ALA	2.2
1	A	647	THR	2.1
1	B	133	TYR	2.1
1	A	652	PRO	2.1
1	B	218	SER	2.1
1	A	118	ASP	2.1
1	A	363	GLU	2.1
1	B	523	PHE	2.1
1	B	228	ASN	2.1
1	B	214	GLN	2.1
1	A	162	ASN	2.1
1	A	481	TYR	2.0
1	B	548	VAL	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.