



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 09:50 AM BST

PDB ID : 1B70
Title : PHENYLALANYL TRNA SYNTHETASE COMPLEXED WITH PHENYLALANINE
Authors : Reshetnikova, L.; Moor, N.; Lavrik, O.; Vassilyev, D.G.
Deposited on : 1999-01-26
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

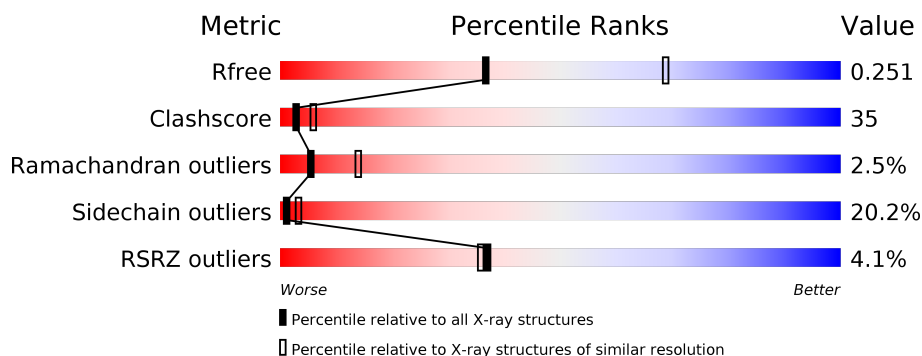
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	350	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>33%</div> <div>8%</div> <div>24%</div> </div> </div>
2	B	785	<div> <div>5%</div> <div> <div></div> <div>44%</div> <div>42%</div> <div>12%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8313 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 PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2112	1382	359	364	7			

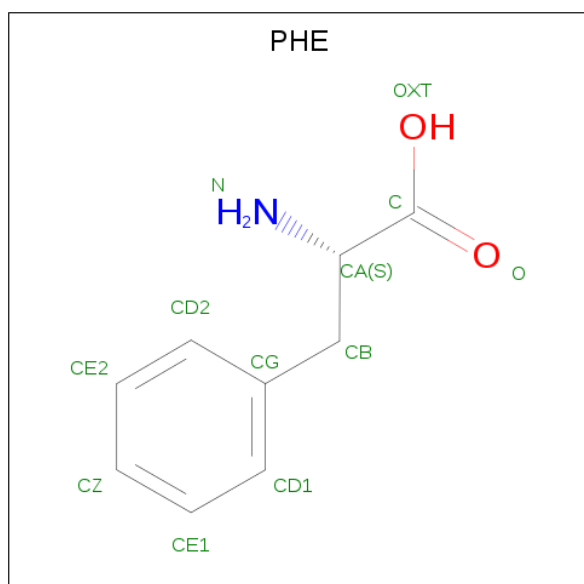
- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	775	Total	C	N	O	S	0	0	0
			6054	3879	1078	1087	10			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		

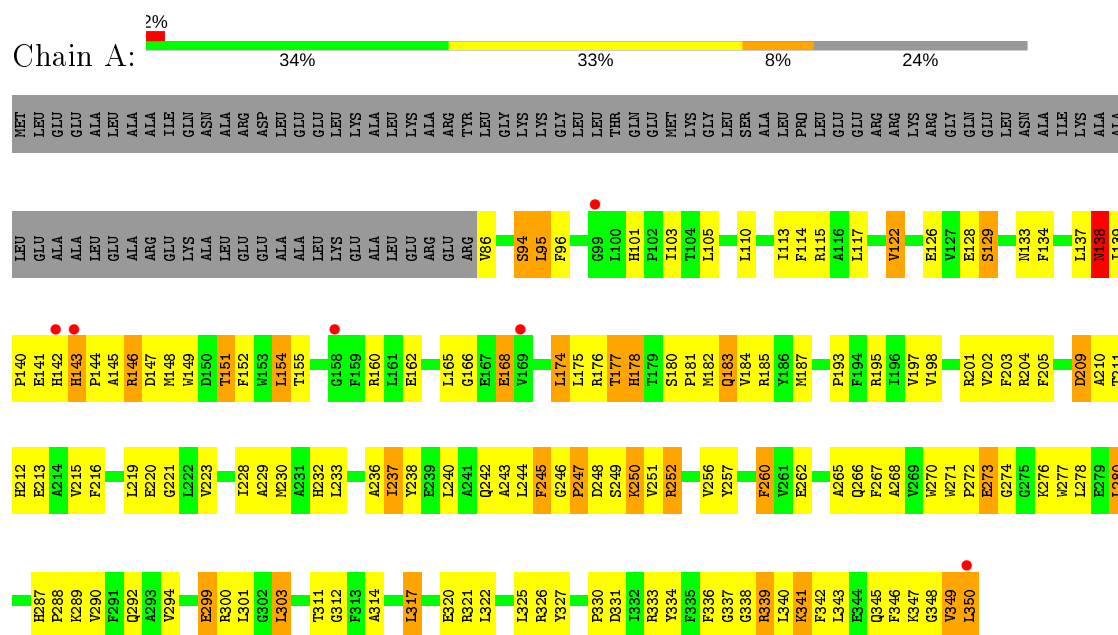
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	106	Total	O	0	0
			106	106		

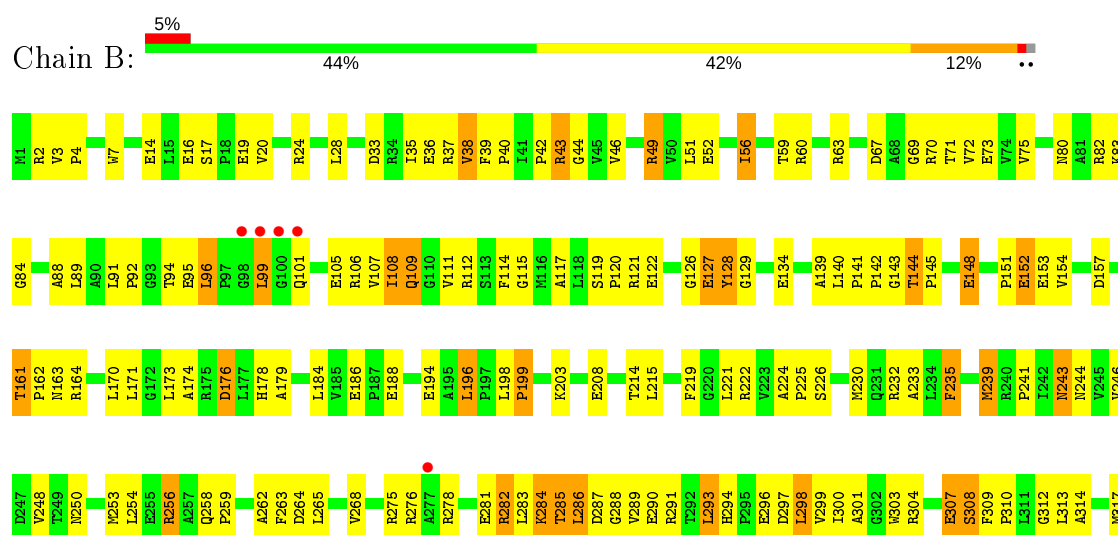
3 Residue-property plots

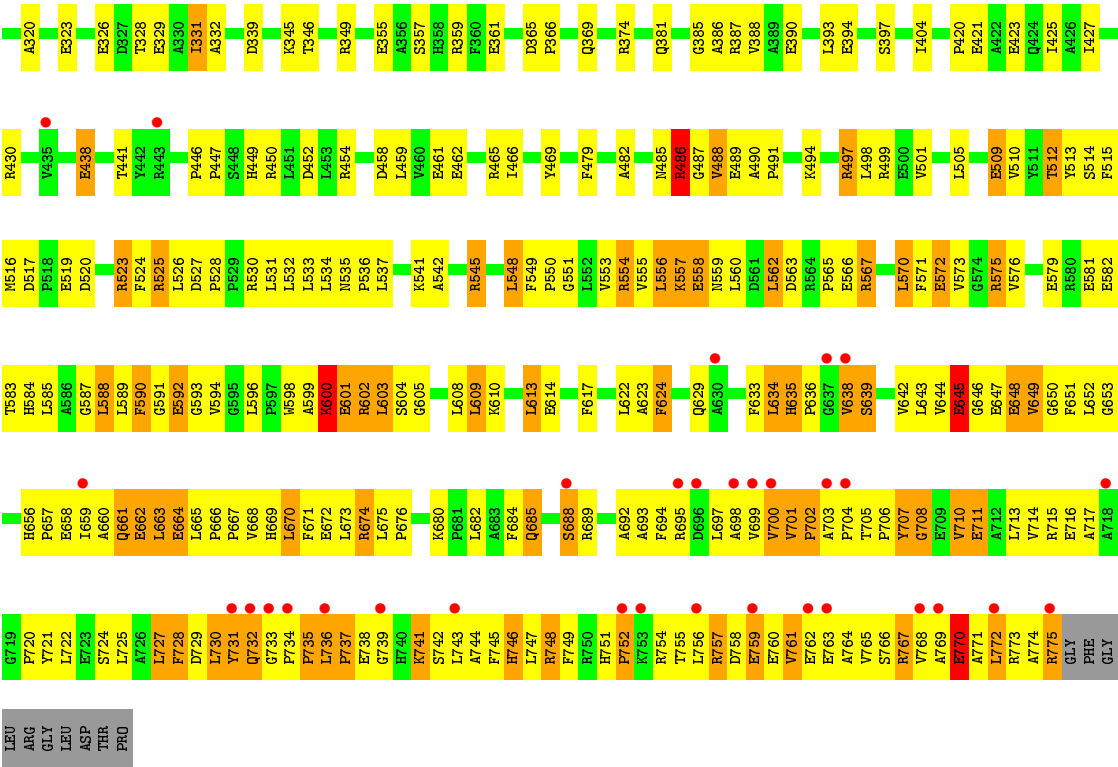
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: PHENYLALANYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.00Å 174.00Å 140.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 47.29 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.70) 88.8 (47.29-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3001.55 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.224 , 0.256 0.223 , 0.251	Depositor DCC
R_{free} test set	3018 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8313	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/2180	0.71	0/2957
2	B	0.50	0/6205	0.73	3/8436 (0.0%)
All	All	0.50	0/8385	0.73	3/11393 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	GLY	N-CA-C	-5.72	98.80	113.10
2	B	69	GLY	N-CA-C	-5.39	99.64	113.10
2	B	38	VAL	N-CA-C	5.37	125.50	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2112	0	2062	143	0
2	B	6054	0	6109	455	0
3	A	1	0	0	0	0
4	A	12	0	8	0	0
5	A	28	0	0	0	0
5	B	106	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8313	0	8179	576	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 35.

All (576) 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:165:LEU:HD12	1:A:301:LEU:HD13	1.35	1.08
2:B:285:THR:HG21	2:B:291:ARG:HE	1.25	0.99
2:B:614:GLU:HG2	2:B:624:PHE:HE1	1.24	0.97
2:B:75:VAL:HG11	2:B:108:ILE:HG21	1.45	0.97
2:B:707:TYR:HE1	2:B:711:GLU:HB2	1.30	0.93
2:B:600:LYS:HG2	2:B:601:GLU:H	1.30	0.93
2:B:294:HIS:CD2	2:B:296:GLU:H	1.86	0.93
2:B:294:HIS:HD2	2:B:296:GLU:H	0.95	0.92
2:B:121:ARG:HD3	2:B:127:GLU:O	1.71	0.89
1:A:101:HIS:HB2	2:B:509:GLU:HG2	1.55	0.88
2:B:516:MET:HE3	2:B:545:ARG:HA	1.56	0.88
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.55	0.87
2:B:701:VAL:HG22	2:B:702:PRO:HD2	1.57	0.87
1:A:143:HIS:ND1	1:A:144:PRO:HD2	1.89	0.86
2:B:707:TYR:CE1	2:B:711:GLU:HB2	2.10	0.86
2:B:764:ALA:HA	2:B:767:ARG:HG2	1.55	0.86
1:A:246:GLY:HA2	1:A:248:ASP:N	1.91	0.85
2:B:286:LEU:HD11	2:B:323:GLU:CD	1.98	0.84
2:B:710:VAL:O	2:B:714:VAL:HG23	1.77	0.84
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.59	0.84
2:B:761:VAL:HG23	2:B:762:GLU:H	1.44	0.83
1:A:331:ASP:HB3	1:A:334:TYR:CD2	2.14	0.83
1:A:113:ILE:HD13	1:A:243:ALA:HB1	1.61	0.82
2:B:512:THR:HG22	2:B:545:ARG:HH21	1.44	0.81
2:B:194:GLU:OE2	2:B:387:ARG:HG2	1.80	0.81
1:A:229:ALA:H	1:A:232:HIS:HD2	1.24	0.81
2:B:219:PHE:HE2	2:B:387:ARG:HE	1.26	0.81
2:B:563:ASP:O	2:B:565:PRO:HD3	1.80	0.81
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.61	0.81
2:B:589:LEU:HB3	2:B:609:LEU:HD12	1.64	0.79
1:A:287:HIS:HD2	1:A:289:LYS:H	1.26	0.79
1:A:257:TYR:HB3	2:B:161:THR:HG21	1.65	0.79
1:A:250:LYS:H	1:A:270:TRP:HB3	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:HIS:HD2	1:A:103:ILE:H	1.31	0.78
1:A:311:THR:HG22	1:A:312:GLY:H	1.50	0.77
1:A:311:THR:HG22	1:A:312:GLY:N	1.97	0.77
2:B:757:ARG:HG3	2:B:759:GLU:HB2	1.66	0.77
2:B:729:ASP:N	2:B:744:ALA:HB3	2.00	0.77
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.68	0.76
2:B:673:LEU:HD22	2:B:673:LEU:N	2.00	0.76
1:A:299:GLU:HG3	1:A:300:ARG:N	2.01	0.76
1:A:246:GLY:HA2	1:A:248:ASP:H	1.47	0.75
1:A:278:LEU:HD13	1:A:325:LEU:HD13	1.68	0.75
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.69	0.74
2:B:730:LEU:HB2	2:B:742:SER:O	1.87	0.74
2:B:761:VAL:HG23	2:B:762:GLU:N	2.02	0.74
2:B:549:PHE:O	2:B:553:VAL:HG23	1.85	0.74
2:B:722:LEU:HD11	2:B:724:SER:O	1.87	0.74
1:A:113:ILE:HD13	1:A:243:ALA:CB	2.18	0.74
2:B:614:GLU:HG2	2:B:624:PHE:CE1	2.16	0.73
2:B:757:ARG:HD3	2:B:759:GLU:H	1.52	0.73
2:B:497:ARG:O	2:B:501:VAL:HG23	1.88	0.73
2:B:702:PRO:C	2:B:704:PRO:HD2	2.09	0.73
2:B:287:ASP:N	2:B:317:MET:HE2	2.04	0.73
1:A:249:SER:HB2	1:A:270:TRP:O	1.89	0.72
2:B:243:ASN:HD21	2:B:246:VAL:HG23	1.54	0.72
2:B:770:GLU:CG	2:B:771:ALA:N	2.50	0.72
2:B:99:LEU:HD22	2:B:101:GLN:NE2	2.05	0.72
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.23	0.72
2:B:600:LYS:HG2	2:B:601:GLU:N	2.02	0.72
2:B:697:LEU:HD23	2:B:698:ALA:N	2.04	0.72
2:B:610:LYS:O	2:B:614:GLU:HG3	1.90	0.72
1:A:331:ASP:O	1:A:334:TYR:HB2	1.89	0.71
1:A:134:PHE:HZ	1:A:151:THR:HG21	1.56	0.71
1:A:211:THR:C	1:A:212:HIS:HD1	1.93	0.71
2:B:99:LEU:HD13	2:B:101:GLN:HB2	1.72	0.71
2:B:730:LEU:HD12	2:B:730:LEU:C	2.11	0.71
2:B:770:GLU:O	2:B:774:ALA:HB2	1.91	0.71
1:A:149:TRP:CD1	1:A:177:THR:HG23	2.26	0.70
2:B:702:PRO:CB	2:B:704:PRO:HD2	2.21	0.70
2:B:762:GLU:O	2:B:765:VAL:HG12	1.89	0.70
2:B:519:GLU:HB3	2:B:523:ARG:HH12	1.56	0.70
2:B:656:HIS:NE2	2:B:658:GLU:HB2	2.06	0.70
1:A:137:LEU:O	1:A:139:ILE:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:HD12	1:A:301:LEU:CD1	2.18	0.70
2:B:734:PRO:HB2	2:B:735:PRO:HD3	1.74	0.70
1:A:155:THR:CG2	2:B:534:LEU:HD21	2.22	0.69
2:B:666:PRO:HB2	2:B:667:PRO:CD	2.22	0.69
2:B:258:GLN:HE22	2:B:369:GLN:NE2	1.90	0.69
2:B:751:HIS:HD2	2:B:752:PRO:HD2	1.57	0.69
2:B:278:ARG:NH2	2:B:308:SER:HB3	2.06	0.69
1:A:134:PHE:CZ	1:A:151:THR:HG21	2.28	0.69
2:B:153:GLU:HG3	2:B:154:VAL:N	2.07	0.69
2:B:287:ASP:H	2:B:317:MET:HE2	1.57	0.68
2:B:51:LEU:HD21	2:B:67:ASP:HB2	1.73	0.68
2:B:602:ARG:HG2	2:B:602:ARG:HH11	1.57	0.68
2:B:604:SER:HA	2:B:608:LEU:HD22	1.75	0.68
2:B:724:SER:HB2	2:B:748:ARG:HB2	1.76	0.68
2:B:643:LEU:HA	2:B:647:GLU:O	1.93	0.68
2:B:656:HIS:CD2	2:B:658:GLU:H	2.12	0.67
2:B:663:LEU:O	2:B:665:LEU:N	2.27	0.67
2:B:700:VAL:HA	2:B:741:LYS:O	1.93	0.67
2:B:736:LEU:HB2	2:B:737:PRO:HD2	1.77	0.67
2:B:698:ALA:HA	2:B:743:LEU:O	1.95	0.67
2:B:243:ASN:ND2	2:B:246:VAL:H	1.94	0.66
2:B:728:PHE:HE1	2:B:745:PHE:C	1.99	0.66
2:B:693:ALA:HB3	2:B:749:PHE:HB2	1.77	0.66
2:B:688:SER:HB3	2:B:752:PRO:HA	1.76	0.66
2:B:656:HIS:HB3	2:B:659:ILE:HD12	1.77	0.66
1:A:101:HIS:CD2	1:A:103:ILE:H	2.13	0.66
2:B:243:ASN:ND2	2:B:246:VAL:HG23	2.11	0.66
2:B:663:LEU:C	2:B:665:LEU:H	1.99	0.66
2:B:178:HIS:O	2:B:430:ARG:NH1	2.29	0.66
2:B:278:ARG:HH21	2:B:308:SER:HB3	1.61	0.66
2:B:767:ARG:N	2:B:767:ARG:HE	1.95	0.65
1:A:180:SER:O	1:A:183:GLN:HB2	1.95	0.65
2:B:215:LEU:HB2	2:B:393:LEU:HB2	1.78	0.65
2:B:751:HIS:HB3	2:B:754:ARG:O	1.95	0.65
2:B:438:GLU:HA	2:B:438:GLU:OE1	1.97	0.65
2:B:650:GLY:HA3	2:B:673:LEU:HD13	1.77	0.65
2:B:770:GLU:HG2	2:B:771:ALA:H	1.62	0.65
2:B:551:GLY:O	2:B:555:VAL:HG23	1.96	0.64
1:A:160:ARG:HG2	1:A:168:GLU:OE2	1.97	0.64
2:B:600:LYS:N	2:B:600:LYS:HD2	2.12	0.64
1:A:145:ALA:O	1:A:148:MET:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:CA	1:A:248:ASP:H	2.09	0.64
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.78	0.64
2:B:285:THR:CG2	2:B:291:ARG:HE	2.06	0.64
2:B:567:ARG:HA	2:B:591:GLY:HA3	1.79	0.64
1:A:138:ASN:HD21	1:A:289:LYS:HE2	1.62	0.64
1:A:336:PHE:HB3	2:B:513:TYR:CE1	2.32	0.64
2:B:656:HIS:HD2	2:B:658:GLU:H	1.45	0.64
2:B:707:TYR:HE1	2:B:711:GLU:CB	2.07	0.64
2:B:517:ASP:HB3	2:B:520:ASP:OD1	1.96	0.64
1:A:341:LYS:H	1:A:341:LYS:HE2	1.63	0.64
2:B:758:ASP:O	2:B:761:VAL:HG22	1.98	0.64
1:A:349:VAL:O	1:A:350:LEU:HD13	1.98	0.64
2:B:600:LYS:HG2	2:B:601:GLU:HG2	1.78	0.63
2:B:644:VAL:HG22	2:B:645:GLU:H	1.63	0.63
1:A:287:HIS:CD2	1:A:289:LYS:H	2.14	0.63
2:B:294:HIS:HD2	2:B:296:GLU:N	1.81	0.63
2:B:609:LEU:HD23	2:B:613:LEU:CD2	2.28	0.63
2:B:635:HIS:ND1	2:B:636:PRO:O	2.30	0.63
1:A:246:GLY:CA	1:A:248:ASP:N	2.60	0.63
2:B:767:ARG:CA	2:B:767:ARG:HE	2.11	0.63
2:B:602:ARG:CG	2:B:602:ARG:HH11	2.11	0.63
2:B:509:GLU:HG3	2:B:510:VAL:N	2.14	0.63
1:A:155:THR:HG21	2:B:534:LEU:HD21	1.81	0.63
2:B:170:LEU:HA	2:B:173:LEU:HD12	1.81	0.63
1:A:341:LYS:HE3	2:B:563:ASP:OD2	1.99	0.63
2:B:194:GLU:O	2:B:390:GLU:HG2	1.98	0.62
2:B:609:LEU:HD22	2:B:652:LEU:CD1	2.29	0.62
2:B:548:LEU:HD13	2:B:576:VAL:CG1	2.29	0.62
1:A:349:VAL:HG12	1:A:350:LEU:HD22	1.80	0.62
2:B:108:ILE:O	2:B:109:GLN:HG2	1.98	0.62
2:B:285:THR:HG21	2:B:291:ARG:NE	2.08	0.62
2:B:265:LEU:HD23	2:B:268:VAL:HG21	1.81	0.61
2:B:355:GLU:O	2:B:359:ARG:HG3	1.99	0.61
1:A:96:PHE:CZ	2:B:567:ARG:HG3	2.34	0.61
2:B:331:ILE:HG12	2:B:332:ALA:N	2.16	0.61
2:B:645:GLU:OE2	2:B:680:LYS:HB2	2.00	0.61
2:B:773:ARG:HB2	2:B:773:ARG:NH1	2.15	0.61
2:B:286:LEU:HB3	2:B:317:MET:CE	2.30	0.61
2:B:553:VAL:O	2:B:556:LEU:HB3	2.01	0.61
2:B:662:GLU:HG3	2:B:662:GLU:O	1.98	0.61
2:B:707:TYR:HE2	2:B:727:LEU:HD22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:757:ARG:CG	2:B:759:GLU:HB2	2.30	0.61
2:B:761:VAL:CG2	2:B:762:GLU:H	2.12	0.61
1:A:134:PHE:O	1:A:137:LEU:O	2.18	0.61
2:B:767:ARG:NE	2:B:767:ARG:HA	2.14	0.61
2:B:707:TYR:HD1	2:B:707:TYR:C	2.03	0.61
2:B:762:GLU:C	2:B:765:VAL:HG12	2.21	0.61
1:A:242:GLN:OE1	1:A:247:PRO:HA	2.01	0.61
2:B:707:TYR:CD1	2:B:707:TYR:C	2.73	0.61
2:B:108:ILE:HG22	2:B:109:GLN:N	2.17	0.60
2:B:764:ALA:HA	2:B:767:ARG:CG	2.29	0.60
1:A:290:VAL:O	1:A:294:VAL:HG23	2.00	0.60
2:B:613:LEU:O	2:B:617:PHE:HD1	1.82	0.60
2:B:643:LEU:HD13	2:B:648:GLU:HA	1.84	0.60
2:B:688:SER:CB	2:B:752:PRO:HA	2.30	0.60
1:A:162:GLU:CG	1:A:166:GLY:HA2	2.31	0.60
2:B:303:TRP:HA	2:B:307:GLU:O	2.02	0.60
2:B:671:PHE:HD1	2:B:673:LEU:HD21	1.66	0.59
1:A:209:ASP:OD1	1:A:210:ALA:N	2.35	0.59
2:B:697:LEU:C	2:B:697:LEU:HD23	2.22	0.59
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.31	0.59
2:B:732:GLN:OE1	2:B:732:GLN:HA	2.00	0.59
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.38	0.59
1:A:219:LEU:HB3	1:A:317:LEU:CD2	2.33	0.59
1:A:148:MET:HE2	2:B:162:PRO:HG2	1.84	0.59
2:B:482:ALA:HB3	2:B:485:ASN:ND2	2.18	0.59
2:B:730:LEU:HD12	2:B:731:TYR:N	2.18	0.58
2:B:275:ARG:O	2:B:299:VAL:HG12	2.03	0.58
2:B:588:LEU:HD23	2:B:588:LEU:C	2.24	0.58
2:B:703:ALA:N	2:B:704:PRO:CD	2.66	0.58
1:A:143:HIS:CG	1:A:144:PRO:HD2	2.39	0.58
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.39	0.58
2:B:652:LEU:HD12	2:B:670:LEU:O	2.04	0.58
1:A:311:THR:CG2	1:A:312:GLY:H	2.16	0.58
2:B:706:PRO:O	2:B:710:VAL:HG23	2.03	0.58
2:B:751:HIS:CD2	2:B:752:PRO:HD2	2.39	0.58
2:B:161:THR:HG22	2:B:162:PRO:HD2	1.85	0.58
1:A:210:ALA:HA	1:A:331:ASP:OD1	2.04	0.58
2:B:671:PHE:CD1	2:B:673:LEU:HD21	2.39	0.58
1:A:114:PHE:HA	1:A:117:LEU:HD13	1.84	0.58
1:A:265:ALA:HB2	2:B:469:TYR:HE2	1.69	0.58
2:B:575:ARG:HG2	2:B:581:GLU:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:757:ARG:HD2	2:B:759:GLU:HG2	1.86	0.57
2:B:770:GLU:CG	2:B:771:ALA:H	2.16	0.57
1:A:96:PHE:CE1	2:B:567:ARG:HG3	2.40	0.57
2:B:570:LEU:N	2:B:570:LEU:HD22	2.19	0.57
2:B:7:TRP:CE3	2:B:233:ALA:HB1	2.39	0.57
2:B:657:PRO:HA	2:B:660:ALA:HB3	1.86	0.57
2:B:462:GLU:OE1	2:B:465:ARG:NH1	2.38	0.57
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.87	0.57
2:B:758:ASP:HA	2:B:761:VAL:HG22	1.87	0.57
1:A:311:THR:CG2	1:A:312:GLY:N	2.66	0.57
2:B:286:LEU:HB3	2:B:317:MET:HE2	1.86	0.56
2:B:728:PHE:O	2:B:729:ASP:HB2	2.05	0.56
2:B:770:GLU:HG3	2:B:771:ALA:N	2.18	0.56
2:B:20:VAL:O	2:B:24:ARG:HG2	2.06	0.56
2:B:359:ARG:HH11	2:B:359:ARG:HG3	1.69	0.56
1:A:210:ALA:HA	1:A:333:ARG:HD2	1.87	0.56
2:B:239:MET:HE3	2:B:355:GLU:HG3	1.88	0.56
2:B:601:GLU:O	2:B:602:ARG:HD2	2.05	0.56
1:A:349:VAL:O	1:A:350:LEU:HD22	2.06	0.56
2:B:557:LYS:HZ2	2:B:664:GLU:HG2	1.71	0.56
2:B:767:ARG:NE	2:B:767:ARG:CA	2.67	0.56
2:B:555:VAL:HA	2:B:558:GLU:CD	2.26	0.56
2:B:235:PHE:CZ	2:B:241:PRO:HD2	2.40	0.56
2:B:570:LEU:HD21	2:B:588:LEU:HD22	1.88	0.56
2:B:39:PHE:HB2	2:B:152:GLU:HA	1.88	0.55
2:B:600:LYS:H	2:B:600:LYS:HD2	1.71	0.55
2:B:644:VAL:O	2:B:646:GLY:N	2.40	0.55
1:A:343:LEU:HD13	2:B:509:GLU:O	2.06	0.55
2:B:516:MET:CE	2:B:545:ARG:HA	2.34	0.55
2:B:381:GLN:HE21	2:B:388:VAL:HG23	1.72	0.55
1:A:228:ILE:O	1:A:311:THR:HG21	2.06	0.55
2:B:71:THR:HG22	2:B:72:VAL:N	2.20	0.55
1:A:278:LEU:HD13	1:A:325:LEU:CD1	2.35	0.55
1:A:337:GLY:O	1:A:339:ARG:N	2.33	0.55
2:B:80:ASN:O	2:B:82:ARG:HD3	2.06	0.55
2:B:557:LYS:HA	2:B:560:LEU:HD12	1.88	0.55
1:A:195:ARG:HG2	1:A:223:VAL:HG13	1.90	0.54
2:B:520:ASP:OD2	2:B:524:PHE:HE1	1.91	0.54
1:A:162:GLU:HG2	1:A:166:GLY:HA2	1.89	0.54
2:B:589:LEU:CB	2:B:609:LEU:HD12	2.35	0.54
2:B:734:PRO:CB	2:B:735:PRO:HD3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:771:ALA:HA	2:B:774:ALA:HB3	1.89	0.54
1:A:138:ASN:ND2	1:A:289:LYS:HE2	2.23	0.54
2:B:587:GLY:HA3	2:B:671:PHE:CE2	2.42	0.54
2:B:703:ALA:N	2:B:704:PRO:HD2	2.23	0.54
2:B:705:THR:HG23	2:B:706:PRO:HD2	1.90	0.54
1:A:113:ILE:O	1:A:117:LEU:HD12	2.08	0.54
2:B:635:HIS:HB2	2:B:656:HIS:HA	1.89	0.54
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.07	0.54
2:B:661:GLN:C	2:B:663:LEU:N	2.60	0.54
2:B:609:LEU:HD21	2:B:671:PHE:HD2	1.73	0.54
1:A:229:ALA:N	1:A:232:HIS:HD2	2.00	0.54
2:B:570:LEU:N	2:B:570:LEU:CD2	2.71	0.54
1:A:252:ARG:NH2	1:A:277:TRP:HB3	2.23	0.53
2:B:520:ASP:HA	2:B:523:ARG:HB2	1.90	0.53
2:B:359:ARG:HH11	2:B:359:ARG:CG	2.21	0.53
2:B:589:LEU:HD21	2:B:608:LEU:HD23	1.90	0.53
1:A:122:VAL:O	1:A:198:VAL:HG13	2.09	0.53
1:A:342:PHE:O	1:A:345:GLN:HB2	2.09	0.53
2:B:224:ALA:HB1	2:B:225:PRO:HD2	1.89	0.53
2:B:286:LEU:HD11	2:B:323:GLU:OE1	2.08	0.53
2:B:519:GLU:HB3	2:B:523:ARG:NH1	2.21	0.53
2:B:695:ARG:HB2	2:B:747:LEU:HB2	1.91	0.53
1:A:201:ARG:HD2	1:A:215:VAL:CG1	2.39	0.53
1:A:339:ARG:NH1	2:B:562:LEU:HD22	2.24	0.53
1:A:140:PRO:O	1:A:146:ARG:HB2	2.08	0.52
2:B:671:PHE:HD1	2:B:673:LEU:CD2	2.22	0.52
2:B:523:ARG:NH1	2:B:523:ARG:HG3	2.24	0.52
2:B:589:LEU:HD12	2:B:590:PHE:H	1.74	0.52
2:B:623:ALA:O	2:B:645:GLU:N	2.43	0.52
2:B:636:PRO:C	2:B:638:VAL:H	2.12	0.52
2:B:285:THR:HG23	2:B:287:ASP:OD1	2.09	0.52
2:B:684:PHE:C	2:B:685:GLN:HG2	2.28	0.52
2:B:702:PRO:HB2	2:B:704:PRO:HD2	1.90	0.52
1:A:165:LEU:HD11	1:A:303:LEU:HD21	1.92	0.52
1:A:155:THR:HG23	2:B:534:LEU:HD11	1.92	0.52
1:A:126:GLU:HG3	2:B:575:ARG:HD2	1.91	0.52
2:B:174:ALA:HB1	2:B:184:LEU:CD1	2.39	0.52
2:B:557:LYS:NZ	2:B:664:GLU:HG2	2.25	0.52
2:B:602:ARG:NH1	2:B:602:ARG:CG	2.70	0.52
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.92	0.51
1:A:180:SER:N	1:A:181:PRO:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:PRO:HA	2:B:660:ALA:CB	2.41	0.51
1:A:348:GLY:O	1:A:350:LEU:N	2.43	0.51
2:B:282:ARG:NH2	2:B:290:GLU:HG3	2.24	0.51
2:B:284:LYS:HD3	2:B:288:GLY:HA2	1.93	0.51
2:B:299:VAL:HG22	2:B:300:ILE:N	2.26	0.51
2:B:262:ALA:HB1	2:B:331:ILE:HG13	1.92	0.51
2:B:369:GLN:CD	2:B:369:GLN:H	2.14	0.51
2:B:694:PHE:O	2:B:695:ARG:NE	2.43	0.51
2:B:644:VAL:O	2:B:645:GLU:C	2.50	0.51
2:B:728:PHE:HE1	2:B:746:HIS:N	2.09	0.51
2:B:751:HIS:HD2	2:B:752:PRO:CD	2.24	0.51
2:B:161:THR:HB	2:B:163:ASN:OD1	2.11	0.51
2:B:381:GLN:O	2:B:385:GLY:HA2	2.10	0.51
2:B:702:PRO:HA	2:B:739:GLY:O	2.12	0.50
2:B:751:HIS:HB2	2:B:756:LEU:HD21	1.92	0.50
2:B:219:PHE:CZ	2:B:387:ARG:HB3	2.47	0.50
2:B:563:ASP:C	2:B:565:PRO:HD3	2.31	0.50
2:B:294:HIS:NE2	2:B:296:GLU:HB2	2.27	0.50
2:B:509:GLU:HA	2:B:571:PHE:CE1	2.46	0.50
2:B:596:LEU:CB	2:B:599:ALA:HB3	2.39	0.50
2:B:661:GLN:HG2	2:B:662:GLU:N	2.25	0.50
2:B:548:LEU:HD22	2:B:584:HIS:HB3	1.93	0.50
2:B:707:TYR:O	2:B:707:TYR:HD1	1.95	0.50
1:A:101:HIS:CB	2:B:509:GLU:HG2	2.36	0.50
2:B:52:GLU:HA	2:B:52:GLU:OE1	2.11	0.50
2:B:198:LEU:HD12	2:B:393:LEU:CD1	2.34	0.50
1:A:211:THR:C	1:A:212:HIS:ND1	2.64	0.50
2:B:164:ARG:HH12	2:B:465:ARG:NH2	2.09	0.50
2:B:554:ARG:O	2:B:558:GLU:HG3	2.11	0.50
1:A:134:PHE:HZ	1:A:151:THR:CG2	2.24	0.49
2:B:108:ILE:CG2	2:B:109:GLN:N	2.75	0.49
2:B:49:ARG:HG3	2:B:67:ASP:HB3	1.94	0.49
1:A:287:HIS:CD2	1:A:288:PRO:HD2	2.46	0.49
2:B:520:ASP:OD2	2:B:554:ARG:NH1	2.42	0.49
2:B:609:LEU:CD2	2:B:652:LEU:HD13	2.42	0.49
2:B:299:VAL:HG23	2:B:312:GLY:O	2.13	0.49
2:B:19:GLU:CD	2:B:19:GLU:H	2.16	0.49
2:B:582:GLU:OE2	2:B:674:ARG:HD3	2.13	0.49
2:B:38:VAL:HG22	2:B:153:GLU:O	2.13	0.49
2:B:729:ASP:H	2:B:744:ALA:HB3	1.73	0.49
2:B:725:LEU:HD23	2:B:725:LEU:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:O	1:A:245:PHE:O	2.30	0.49
2:B:140:LEU:HB3	2:B:141:PRO:HD2	1.94	0.49
2:B:300:ILE:HD13	2:B:314:ALA:HA	1.93	0.49
1:A:271:TRP:CH2	1:A:274:GLY:HA3	2.48	0.49
2:B:603:LEU:C	2:B:603:LEU:HD12	2.33	0.49
2:B:663:LEU:C	2:B:665:LEU:N	2.65	0.49
1:A:209:ASP:O	1:A:333:ARG:HD2	2.13	0.48
1:A:268:ALA:HA	1:A:278:LEU:O	2.13	0.48
2:B:120:PRO:HD2	2:B:129:GLY:H	1.77	0.48
1:A:246:GLY:C	1:A:248:ASP:H	2.16	0.48
1:A:339:ARG:HH12	2:B:562:LEU:HD22	1.78	0.48
2:B:293:LEU:HD13	2:B:293:LEU:N	2.28	0.48
2:B:742:SER:O	2:B:743:LEU:HD23	2.14	0.48
1:A:128:GLU:HG3	1:A:129:SER:H	1.78	0.48
1:A:341:LYS:HE2	1:A:341:LYS:N	2.28	0.48
2:B:139:ALA:O	2:B:140:LEU:HD12	2.12	0.48
2:B:644:VAL:HG13	2:B:645:GLU:N	2.28	0.48
2:B:661:GLN:C	2:B:663:LEU:H	2.16	0.48
2:B:720:PRO:C	2:B:721:TYR:HD1	2.16	0.48
2:B:404:ILE:HD12	2:B:446:PRO:HD3	1.95	0.48
2:B:757:ARG:HB3	2:B:760:GLU:OE2	2.14	0.48
2:B:773:ARG:C	2:B:775:ARG:N	2.66	0.48
2:B:549:PHE:CD2	2:B:550:PRO:HD3	2.49	0.48
2:B:671:PHE:CD1	2:B:673:LEU:CD2	2.97	0.48
2:B:119:SER:OG	2:B:122:GLU:HG3	2.13	0.48
2:B:281:GLU:HG2	2:B:310:PRO:HG3	1.96	0.48
2:B:527:ASP:HB3	2:B:528:PRO:HD2	1.95	0.48
2:B:635:HIS:CE1	2:B:636:PRO:O	2.67	0.48
2:B:35:ILE:O	2:B:36:GLU:HG2	2.13	0.48
2:B:42:PRO:HA	2:B:43:ARG:NH1	2.29	0.48
2:B:705:THR:CG2	2:B:706:PRO:HD2	2.44	0.48
2:B:721:TYR:N	2:B:721:TYR:CD1	2.81	0.48
1:A:277:TRP:C	1:A:278:LEU:HD23	2.34	0.47
2:B:294:HIS:CD2	2:B:296:GLU:HB2	2.49	0.47
2:B:765:VAL:HG13	2:B:766:SER:N	2.29	0.47
1:A:229:ALA:H	1:A:232:HIS:CD2	2.17	0.47
2:B:600:LYS:CG	2:B:601:GLU:H	2.11	0.47
2:B:585:LEU:HB2	2:B:675:LEU:HD11	1.96	0.47
2:B:728:PHE:CD1	2:B:728:PHE:N	2.82	0.47
2:B:120:PRO:HG2	2:B:128:TYR:HB3	1.96	0.47
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:GLY:O	2:B:608:LEU:HB3	2.14	0.47
2:B:688:SER:OG	2:B:752:PRO:HA	2.13	0.47
1:A:233:LEU:O	1:A:236:ALA:HB3	2.14	0.47
2:B:92:PRO:HD3	2:B:114:PHE:O	2.15	0.47
1:A:219:LEU:HB3	1:A:317:LEU:HD21	1.97	0.47
2:B:509:GLU:HB2	2:B:571:PHE:CZ	2.49	0.47
2:B:757:ARG:CD	2:B:759:GLU:H	2.24	0.47
1:A:271:TRP:NE1	1:A:273:GLU:HB2	2.29	0.47
2:B:498:LEU:O	2:B:498:LEU:HD12	2.14	0.47
2:B:759:GLU:O	2:B:763:GLU:HB2	2.15	0.47
2:B:770:GLU:O	2:B:774:ALA:CB	2.61	0.47
2:B:221:LEU:CD2	2:B:386:ALA:HB2	2.44	0.47
1:A:143:HIS:CB	1:A:144:PRO:HD2	2.44	0.47
2:B:63:ARG:HD2	2:B:73:GLU:OE2	2.14	0.47
2:B:91:LEU:HB3	2:B:92:PRO:HD2	1.96	0.47
1:A:178:HIS:HA	1:A:202:VAL:HG11	1.95	0.47
2:B:198:LEU:N	2:B:198:LEU:HD23	2.29	0.47
2:B:482:ALA:HB3	2:B:485:ASN:HD21	1.78	0.47
1:A:252:ARG:O	1:A:267:PHE:HA	2.14	0.47
2:B:265:LEU:HA	2:B:268:VAL:HG23	1.96	0.47
2:B:56:ILE:HG12	2:B:56:ILE:H	1.60	0.47
2:B:16:GLU:O	2:B:17:SER:HB3	2.15	0.46
2:B:374:ARG:HA	2:B:374:ARG:HD3	1.76	0.46
2:B:635:HIS:HB2	2:B:657:PRO:HD3	1.97	0.46
2:B:286:LEU:HB3	2:B:317:MET:HE3	1.97	0.46
2:B:761:VAL:CG2	2:B:762:GLU:N	2.70	0.46
1:A:267:PHE:CE1	1:A:280:LEU:HB3	2.51	0.46
2:B:244:ASN:O	2:B:248:VAL:HG23	2.16	0.46
2:B:629:GLN:O	2:B:639:SER:HB3	2.15	0.46
1:A:216:PHE:HB2	1:A:320:GLU:OE1	2.16	0.46
2:B:660:ALA:O	2:B:665:LEU:O	2.33	0.46
2:B:727:LEU:HA	2:B:744:ALA:O	2.16	0.46
1:A:260:PHE:CD1	1:A:260:PHE:N	2.84	0.46
2:B:303:TRP:HB2	2:B:307:GLU:O	2.15	0.46
2:B:559:ASN:O	2:B:563:ASP:O	2.33	0.46
2:B:651:PHE:CE2	2:B:672:GLU:HB3	2.51	0.46
2:B:730:LEU:CD1	2:B:730:LEU:C	2.79	0.46
1:A:187:MET:HB3	1:A:294:VAL:HG11	1.97	0.46
2:B:107:VAL:HA	2:B:112:ARG:HA	1.97	0.46
2:B:243:ASN:HD21	2:B:246:VAL:H	1.60	0.46
1:A:110:LEU:HD11	1:A:322:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:MET:HG3	2:B:259:PRO:HA	1.97	0.46
2:B:276:ARG:NH1	2:B:296:GLU:O	2.38	0.46
2:B:623:ALA:O	2:B:645:GLU:HA	2.15	0.46
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.98	0.46
2:B:573:VAL:HG22	2:B:585:LEU:HD13	1.97	0.46
1:A:175:LEU:HB3	1:A:203:PHE:CD1	2.50	0.45
1:A:197:VAL:HG22	1:A:219:LEU:HD11	1.98	0.45
1:A:95:LEU:HA	1:A:95:LEU:HD12	1.73	0.45
2:B:531:LEU:O	2:B:532:LEU:HD13	2.16	0.45
2:B:600:LYS:HG2	2:B:601:GLU:CG	2.44	0.45
2:B:617:PHE:HB3	2:B:622:LEU:O	2.16	0.45
2:B:769:ALA:O	2:B:772:LEU:HB3	2.16	0.45
1:A:349:VAL:CG1	1:A:349:VAL:O	2.65	0.45
2:B:219:PHE:HE2	2:B:387:ARG:NE	2.04	0.45
2:B:523:ARG:HH11	2:B:523:ARG:CG	2.29	0.45
2:B:535:ASN:N	2:B:536:PRO:HD3	2.31	0.45
2:B:635:HIS:HB2	2:B:657:PRO:CD	2.46	0.45
2:B:692:ALA:HA	2:B:749:PHE:O	2.16	0.45
2:B:94:THR:HG22	2:B:96:LEU:HD13	1.99	0.45
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.74	0.45
2:B:672:GLU:C	2:B:673:LEU:HD22	2.36	0.45
1:A:154:LEU:HD22	1:A:174:LEU:CA	2.47	0.45
2:B:105:GLU:HG3	2:B:114:PHE:CD1	2.52	0.45
2:B:642:VAL:HG23	2:B:651:PHE:HA	1.99	0.45
2:B:649:VAL:CG2	2:B:674:ARG:H	2.30	0.45
2:B:381:GLN:HG3	2:B:386:ALA:O	2.17	0.45
2:B:669:HIS:O	2:B:670:LEU:HD12	2.17	0.45
1:A:113:ILE:O	1:A:117:LEU:CD1	2.65	0.45
1:A:174:LEU:HD23	1:A:174:LEU:C	2.38	0.45
1:A:94:SER:HB2	2:B:567:ARG:NH2	2.32	0.45
1:A:221:GLY:O	1:A:314:ALA:HA	2.16	0.44
1:A:256:VAL:HG22	1:A:257:TYR:H	1.82	0.44
2:B:264:ASP:CG	2:B:328:THR:HG23	2.37	0.44
1:A:193:PRO:HB2	2:B:479:PHE:CE1	2.52	0.44
1:A:252:ARG:HE	1:A:268:ALA:HB3	1.82	0.44
2:B:427:ILE:HG12	2:B:466:ILE:HG21	1.99	0.44
2:B:549:PHE:CD1	2:B:550:PRO:N	2.85	0.44
2:B:121:ARG:HA	2:B:126:GLY:O	2.17	0.44
2:B:707:TYR:CE2	2:B:727:LEU:HD22	2.49	0.44
2:B:731:TYR:CE2	2:B:733:GLY:HA2	2.52	0.44
2:B:458:ASP:O	2:B:462:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:CG1	2:B:488:VAL:HG13	2.47	0.44
1:A:141:GLU:HG3	1:A:142:HIS:N	2.32	0.44
1:A:149:TRP:CD1	1:A:177:THR:CG2	2.98	0.44
2:B:717:ALA:C	2:B:768:VAL:HG22	2.38	0.44
2:B:420:PRO:HG2	2:B:423:GLU:HB2	1.99	0.44
2:B:775:ARG:HE	2:B:775:ARG:HB3	1.49	0.44
1:A:146:ARG:HB2	1:A:146:ARG:HE	1.66	0.44
2:B:650:GLY:HA3	2:B:673:LEU:CD1	2.45	0.44
2:B:592:GLU:OE1	2:B:592:GLU:N	2.50	0.44
2:B:609:LEU:HD21	2:B:671:PHE:CD2	2.52	0.44
1:A:133:ASN:OD1	1:A:176:ARG:HA	2.17	0.44
2:B:275:ARG:O	2:B:298:LEU:HD23	2.18	0.44
2:B:163:ASN:O	2:B:452:ASP:HB3	2.18	0.44
2:B:728:PHE:CE1	2:B:746:HIS:N	2.86	0.44
2:B:72:VAL:HG22	2:B:73:GLU:N	2.33	0.43
2:B:661:GLN:O	2:B:663:LEU:N	2.51	0.43
2:B:666:PRO:HB2	2:B:667:PRO:HD2	1.97	0.43
2:B:765:VAL:CG1	2:B:766:SER:N	2.81	0.43
2:B:699:VAL:HG12	2:B:773:ARG:NH2	2.33	0.43
1:A:300:ARG:HG3	1:A:300:ARG:O	2.19	0.43
2:B:289:VAL:HG12	2:B:291:ARG:HG2	2.00	0.43
2:B:523:ARG:HH11	2:B:523:ARG:HG3	1.81	0.43
2:B:515:PHE:CE1	2:B:533:LEU:HD21	2.54	0.43
2:B:548:LEU:HD12	2:B:548:LEU:HA	1.88	0.43
2:B:647:GLU:HA	2:B:647:GLU:OE1	2.18	0.43
2:B:680:LYS:O	2:B:680:LYS:HG2	2.18	0.43
2:B:710:VAL:HG11	2:B:743:LEU:CD1	2.49	0.43
1:A:238:TYR:C	1:A:238:TYR:CD1	2.91	0.43
2:B:652:LEU:HD12	2:B:653:GLY:N	2.33	0.43
1:A:270:TRP:O	1:A:272:PRO:HD3	2.18	0.43
1:A:317:LEU:O	1:A:317:LEU:HD23	2.17	0.43
2:B:75:VAL:CG1	2:B:108:ILE:HG21	2.33	0.43
2:B:161:THR:HG22	2:B:162:PRO:CD	2.47	0.43
1:A:262:GLU:OE1	2:B:458:ASP:HA	2.18	0.43
2:B:548:LEU:HD13	2:B:576:VAL:HG12	1.99	0.43
2:B:88:ALA:O	2:B:117:ALA:HA	2.19	0.43
2:B:141:PRO:HG2	2:B:144:THR:CG2	2.49	0.43
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.75	0.43
2:B:486:ARG:HA	2:B:486:ARG:HD3	1.66	0.43
2:B:609:LEU:CD2	2:B:652:LEU:CD1	2.97	0.43
2:B:600:LYS:CD	2:B:600:LYS:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:675:LEU:HB3	2:B:676:PRO:HA	2.01	0.43
2:B:40:PRO:HA	2:B:152:GLU:OE2	2.19	0.43
2:B:447:PRO:HB2	2:B:449:HIS:CE1	2.54	0.43
2:B:514:SER:O	2:B:545:ARG:HG2	2.19	0.43
2:B:548:LEU:HD22	2:B:584:HIS:CB	2.49	0.42
2:B:768:VAL:O	2:B:772:LEU:N	2.51	0.42
1:A:101:HIS:CD2	1:A:103:ILE:HB	2.55	0.42
2:B:600:LYS:N	2:B:600:LYS:CD	2.82	0.42
2:B:668:VAL:HG12	2:B:669:HIS:N	2.34	0.42
2:B:761:VAL:C	2:B:763:GLU:H	2.21	0.42
2:B:766:SER:O	2:B:770:GLU:HB3	2.19	0.42
1:A:105:LEU:HD22	1:A:349:VAL:CG1	2.49	0.42
2:B:258:GLN:NE2	5:B:854:HOH:O	2.48	0.42
2:B:572:GLU:HG3	2:B:573:VAL:N	2.35	0.42
2:B:365:ASP:HA	2:B:366:PRO:HD2	1.76	0.42
2:B:421:GLU:O	2:B:425:ILE:HG12	2.19	0.42
2:B:642:VAL:HG23	2:B:651:PHE:CA	2.49	0.42
2:B:44:GLY:O	2:B:91:LEU:HD12	2.20	0.42
1:A:117:LEU:N	1:A:117:LEU:HD12	2.35	0.42
2:B:285:THR:OG1	2:B:286:LEU:N	2.52	0.42
2:B:725:LEU:CD2	2:B:725:LEU:C	2.88	0.42
1:A:327:TYR:HB3	1:A:346:PHE:HE2	1.85	0.42
2:B:707:TYR:O	2:B:707:TYR:CD1	2.72	0.42
2:B:731:TYR:HD1	2:B:742:SER:HG	1.59	0.42
2:B:754:ARG:HD2	2:B:755:THR:O	2.19	0.42
2:B:46:VAL:HB	2:B:143:GLY:O	2.19	0.42
2:B:145:PRO:O	2:B:148:GLU:HB2	2.20	0.42
2:B:300:ILE:HD12	2:B:314:ALA:HB2	2.02	0.42
2:B:707:TYR:O	2:B:708:GLY:C	2.58	0.42
1:A:237:ILE:O	1:A:240:LEU:HB3	2.20	0.42
2:B:286:LEU:HD13	2:B:320:ALA:HA	2.01	0.42
2:B:297:ASP:OD1	2:B:346:THR:HG23	2.20	0.42
1:A:265:ALA:HB2	2:B:469:TYR:CE2	2.52	0.42
2:B:263:PHE:O	2:B:331:ILE:HB	2.20	0.42
2:B:265:LEU:HD23	2:B:268:VAL:CG2	2.48	0.42
2:B:533:LEU:HB2	2:B:536:PRO:HG3	2.02	0.42
2:B:557:LYS:HE3	2:B:664:GLU:OE2	2.20	0.42
2:B:490:ALA:HB3	2:B:491:PRO:CD	2.41	0.42
1:A:175:LEU:O	1:A:176:ARG:C	2.58	0.41
1:A:238:TYR:HA	1:A:251:VAL:HG11	2.01	0.41
2:B:35:ILE:C	2:B:36:GLU:HG2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:548:LEU:C	2:B:550:PRO:HD2	2.41	0.41
2:B:634:LEU:HB3	2:B:639:SER:OG	2.20	0.41
2:B:141:PRO:HA	2:B:142:PRO:HD2	1.94	0.41
2:B:250:ASN:O	2:B:254:LEU:HG	2.20	0.41
2:B:450:ARG:HA	2:B:450:ARG:HD2	1.64	0.41
2:B:702:PRO:O	2:B:741:LYS:HE2	2.20	0.41
2:B:773:ARG:HB2	2:B:773:ARG:HH11	1.85	0.41
1:A:183:GLN:NE2	1:A:220:GLU:OE2	2.52	0.41
2:B:532:LEU:N	2:B:532:LEU:HD22	2.35	0.41
2:B:253:MET:O	2:B:256:ARG:O	2.39	0.41
2:B:537:LEU:HA	2:B:537:LEU:HD23	1.69	0.41
2:B:688:SER:HB3	2:B:752:PRO:O	2.20	0.41
2:B:700:VAL:CG1	2:B:736:LEU:HD13	2.50	0.41
2:B:83:LYS:HG2	2:B:84:GLY:N	2.35	0.41
1:A:152:PHE:CE1	1:A:205:PHE:HD2	2.39	0.41
1:A:348:GLY:C	1:A:350:LEU:N	2.74	0.41
2:B:151:PRO:HD2	2:B:232:ARG:NE	2.36	0.41
2:B:617:PHE:CE2	2:B:644:VAL:HG23	2.55	0.41
2:B:219:PHE:N	2:B:219:PHE:CD1	2.88	0.41
2:B:505:LEU:HD12	2:B:505:LEU:HA	1.67	0.41
2:B:530:ARG:NH1	2:B:530:ARG:HB2	2.36	0.41
2:B:566:GLU:CG	2:B:592:GLU:HG2	2.51	0.41
2:B:598:TRP:CZ3	2:B:599:ALA:HB2	2.56	0.41
2:B:755:THR:CG2	2:B:756:LEU:N	2.84	0.41
1:A:184:VAL:O	1:A:185:ARG:C	2.59	0.41
2:B:523:ARG:NH1	2:B:523:ARG:CG	2.84	0.41
2:B:733:GLY:HA3	2:B:736:LEU:HD21	2.02	0.41
2:B:304:ARG:O	2:B:307:GLU:HB2	2.21	0.41
2:B:3:VAL:HA	2:B:4:PRO:HD3	1.83	0.41
2:B:119:SER:HB2	2:B:129:GLY:HA2	2.03	0.41
1:A:242:GLN:OE1	1:A:247:PRO:HB3	2.20	0.41
2:B:176:ASP:O	2:B:179:ALA:HB3	2.21	0.41
2:B:557:LYS:HG3	2:B:557:LYS:HZ2	1.82	0.41
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.56	0.41
2:B:751:HIS:HE1	5:B:811:HOH:O	2.04	0.41
1:A:128:GLU:HG3	1:A:129:SER:N	2.36	0.40
1:A:94:SER:O	2:B:594:VAL:HG12	2.22	0.40
2:B:404:ILE:HG12	2:B:454:ARG:O	2.21	0.40
2:B:556:LEU:C	2:B:556:LEU:HD12	2.41	0.40
2:B:535:ASN:OD1	2:B:535:ASN:N	2.54	0.40
2:B:487:GLY:O	2:B:489:GLU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:758:ASP:CA	2:B:761:VAL:HG22	2.51	0.40
2:B:82:ARG:HH12	2:B:134:GLU:CD	2.24	0.40
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.84	0.40
2:B:198:LEU:HA	2:B:199:PRO:HD2	1.74	0.40
2:B:509:GLU:CA	2:B:571:PHE:CE1	3.04	0.40
2:B:14:GLU:HG3	2:B:14:GLU:H	1.73	0.40
2:B:294:HIS:CD2	2:B:296:GLU:N	2.70	0.40
2:B:301:ALA:HB1	2:B:309:PHE:O	2.21	0.40
2:B:346:THR:O	2:B:349:ARG:HB3	2.22	0.40
2:B:761:VAL:C	2:B:763:GLU:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/350 (75%)	243 (92%)	13 (5%)	7 (3%)	5	12
2	B	773/785 (98%)	684 (88%)	70 (9%)	19 (2%)	5	14
All	All	1036/1135 (91%)	927 (90%)	83 (8%)	26 (2%)	5	14

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	488	VAL
2	B	664	GLU
1	A	94	SER
1	A	338	GLY
2	B	128	TYR
2	B	645	GLU
2	B	708	GLY

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Mol	Chain	Res	Type
2	B	772	LEU
2	B	486	ARG
2	B	525	ARG
2	B	600	LYS
2	B	735	PRO
2	B	199	PRO
2	B	557	LYS
1	A	330	PRO
1	A	349	VAL
2	B	196	LEU
2	B	737	PRO
2	B	752	PRO
2	B	770	GLU
1	A	273	GLU
2	B	761	VAL
2	B	702	PRO
2	B	710	VAL
1	A	247	PRO

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	213/277 (77%)	173 (81%)	40 (19%)	1	4
2	B	623/630 (99%)	494 (79%)	129 (21%)	1	3
All	All	836/907 (92%)	667 (80%)	169 (20%)	1	3

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	95	LEU
1	A	115	ARG
1	A	122	VAL
1	A	129	SER

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Mol	Chain	Res	Type
1	A	138	ASN
1	A	143	HIS
1	A	146	ARG
1	A	147	ASP
1	A	151	THR
1	A	154	LEU
1	A	168	GLU
1	A	174	LEU
1	A	177	THR
1	A	178	HIS
1	A	182	MET
1	A	183	GLN
1	A	204	ARG
1	A	209	ASP
1	A	213	GLU
1	A	230	MET
1	A	237	ILE
1	A	245	PHE
1	A	250	LYS
1	A	252	ARG
1	A	260	PHE
1	A	266	GLN
1	A	276	LYS
1	A	280	LEU
1	A	292	GLN
1	A	299	GLU
1	A	303	LEU
1	A	317	LEU
1	A	321	ARG
1	A	326	ARG
1	A	339	ARG
1	A	340	LEU
1	A	341	LYS
1	A	347	LYS
1	A	350	LEU
2	B	2	ARG
2	B	33	ASP
2	B	37	ARG
2	B	43	ARG
2	B	49	ARG
2	B	56	ILE
2	B	59	THR

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Mol	Chain	Res	Type
2	B	60	ARG
2	B	70	ARG
2	B	89	LEU
2	B	95	GLU
2	B	96	LEU
2	B	99	LEU
2	B	106	ARG
2	B	108	ILE
2	B	109	GLN
2	B	111	VAL
2	B	127	GLU
2	B	144	THR
2	B	148	GLU
2	B	152	GLU
2	B	157	ASP
2	B	161	THR
2	B	171	LEU
2	B	176	ASP
2	B	186	GLU
2	B	188	GLU
2	B	196	LEU
2	B	203	LYS
2	B	208	GLU
2	B	222	ARG
2	B	226	SER
2	B	230	MET
2	B	235	PHE
2	B	239	MET
2	B	243	ASN
2	B	256	ARG
2	B	282	ARG
2	B	283	LEU
2	B	284	LYS
2	B	285	THR
2	B	286	LEU
2	B	293	LEU
2	B	298	LEU
2	B	307	GLU
2	B	308	SER
2	B	313	LEU
2	B	326	GLU
2	B	329	GLU

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Mol	Chain	Res	Type
2	B	331	ILE
2	B	339	ASP
2	B	345	LYS
2	B	357	SER
2	B	361	GLU
2	B	397	SER
2	B	438	GLU
2	B	441	THR
2	B	459	LEU
2	B	461	GLU
2	B	486	ARG
2	B	494	LYS
2	B	497	ARG
2	B	499	ARG
2	B	509	GLU
2	B	512	THR
2	B	523	ARG
2	B	525	ARG
2	B	526	LEU
2	B	541	LYS
2	B	545	ARG
2	B	548	LEU
2	B	554	ARG
2	B	556	LEU
2	B	558	GLU
2	B	562	LEU
2	B	567	ARG
2	B	570	LEU
2	B	572	GLU
2	B	575	ARG
2	B	579	GLU
2	B	588	LEU
2	B	590	PHE
2	B	592	GLU
2	B	600	LYS
2	B	601	GLU
2	B	602	ARG
2	B	603	LEU
2	B	609	LEU
2	B	613	LEU
2	B	624	PHE
2	B	633	PHE

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Mol	Chain	Res	Type
2	B	634	LEU
2	B	635	HIS
2	B	638	VAL
2	B	639	SER
2	B	645	GLU
2	B	648	GLU
2	B	649	VAL
2	B	661	GLN
2	B	662	GLU
2	B	663	LEU
2	B	670	LEU
2	B	674	ARG
2	B	682	LEU
2	B	685	GLN
2	B	688	SER
2	B	689	ARG
2	B	700	VAL
2	B	701	VAL
2	B	707	TYR
2	B	711	GLU
2	B	713	LEU
2	B	715	ARG
2	B	716	GLU
2	B	727	LEU
2	B	728	PHE
2	B	730	LEU
2	B	731	TYR
2	B	732	GLN
2	B	736	LEU
2	B	738	GLU
2	B	741	LYS
2	B	746	HIS
2	B	748	ARG
2	B	757	ARG
2	B	759	GLU
2	B	767	ARG
2	B	770	GLU
2	B	775	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	120	GLN
1	A	138	ASN
1	A	142	HIS
1	A	178	HIS
1	A	183	GLN
1	A	232	HIS
1	A	287	HIS
2	B	101	GLN
2	B	109	GLN
2	B	178	HIS
2	B	231	GLN
2	B	243	ASN
2	B	258	GLN
2	B	294	HIS
2	B	656	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
4	PHE	A	352	-	9,12,12	0.90	0	10,15,15	0.49	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
4	PHE	A	352	-	-	2/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	352	PHE	C-CA-CB-CG
4	A	352	PHE	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/350 (75%)	0.00	6 (2%) 60 62	30, 62, 101, 121	0
2	B	775/785 (98%)	0.11	37 (4%) 30 28	28, 66, 115, 130	0
All	All	1040/1135 (91%)	0.08	43 (4%) 37 36	28, 65, 114, 130	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	99	LEU	5.6
2	B	768	VAL	4.4
2	B	718	ALA	4.3
2	B	769	ALA	4.1
2	B	696	ASP	3.9
2	B	743	LEU	3.7
2	B	731	TYR	3.6
2	B	753	LYS	3.6
2	B	762	GLU	3.5
2	B	659	ILE	3.5
2	B	637	GLY	3.3
2	B	736	LEU	3.2
2	B	688	SER	3.1
2	B	98	GLY	3.1
2	B	699	VAL	3.0
2	B	704	PRO	3.0
2	B	101	GLN	2.9
2	B	700	VAL	2.8
2	B	752	PRO	2.8
1	A	158	GLY	2.8
2	B	734	PRO	2.8
2	B	100	GLY	2.8
2	B	638	VAL	2.8
2	B	739	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	772	LEU	2.6
2	B	703	ALA	2.6
2	B	695	ARG	2.5
2	B	759	GLU	2.5
1	A	99	GLY	2.3
2	B	630	ALA	2.3
2	B	443	ARG	2.3
2	B	732	GLN	2.3
2	B	763	GLU	2.2
2	B	733	GLY	2.2
1	A	143	HIS	2.1
2	B	698	ALA	2.1
1	A	142	HIS	2.1
2	B	756	LEU	2.1
1	A	169	VAL	2.1
1	A	350	LEU	2.1
2	B	277	ALA	2.1
2	B	435	VAL	2.0
2	B	775	ARG	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 monosaccharides 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(\AA^2)	Q<0.9
3	MG	A	351	1/1	0.94	0.18	36,36,36,36	0
4	PHE	A	352	12/12	0.95	0.22	58,64,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.