



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:02 PM UTC

PDB ID : 3TEH / pdb_00003teh
Title : Crystal structure of Thermus thermophilus Phenylalanyl-tRNA synthetase complexed with L-dopa
Authors : Safro, M.; Klipcan, L.; Moor, N.
Deposited on : 2011-08-14
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

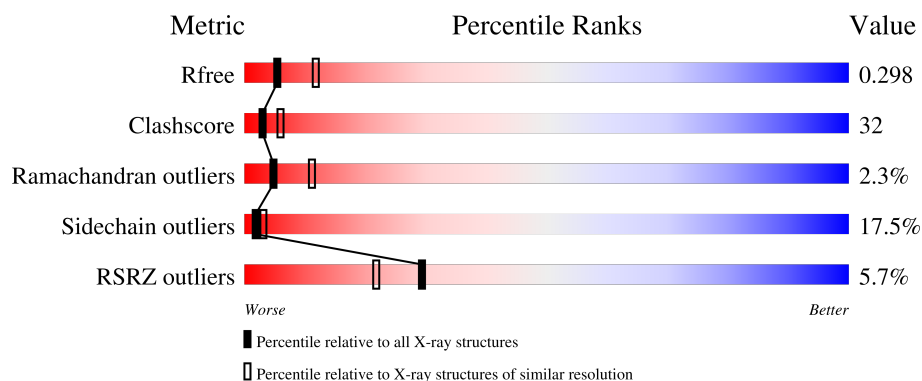
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	350	
2	B	785	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DAH	A	351	-	-	X	-
3	DAH	B	786	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8670 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	11	0	0
			2123	1388	363	365	7			

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	785	Total	C	N	O	S	46	0	0
			6127	3925	1091	1101	10			

- Molecule 3 is a ligand with the chemical component id DAH but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for DAH. ERROR THIS SHOULD NOT HAPPEN FOLLOWING ANNOTATION.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	9	1	4		
3	B	1	Total	C	N	O	0	0
			14	9	1	4		

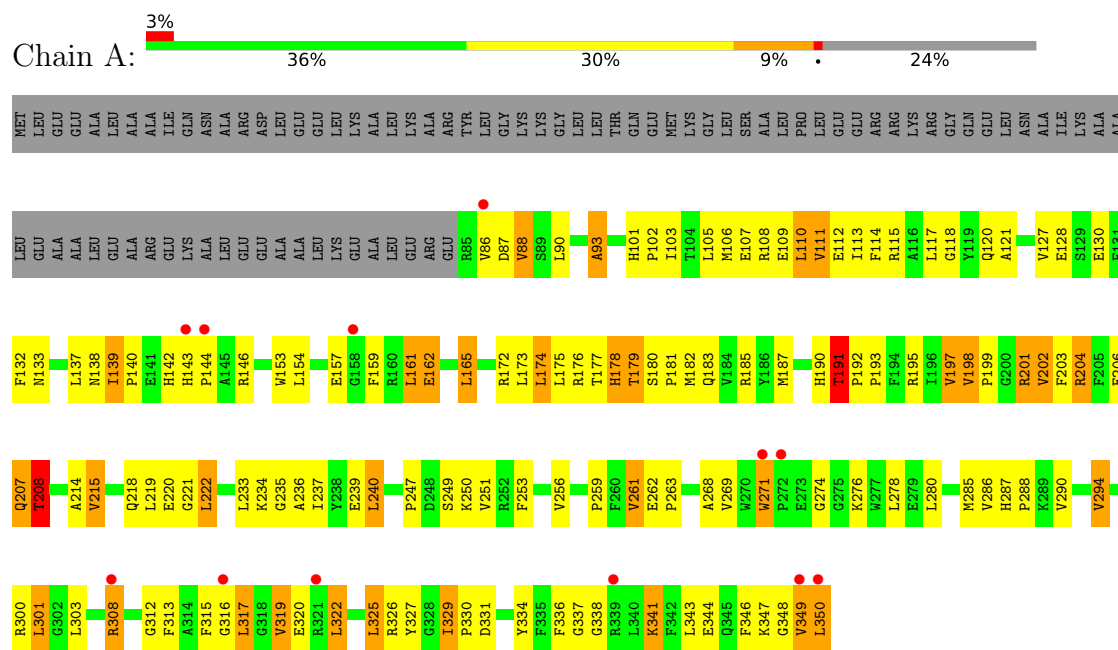
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	289	Total	O	0	0
			289	289		

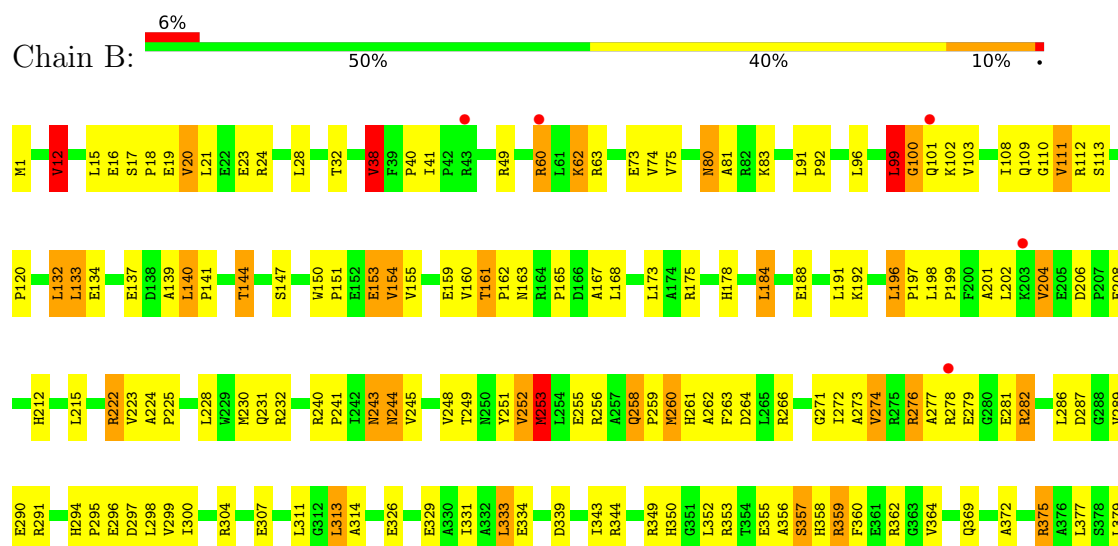
3 Residue-property plots

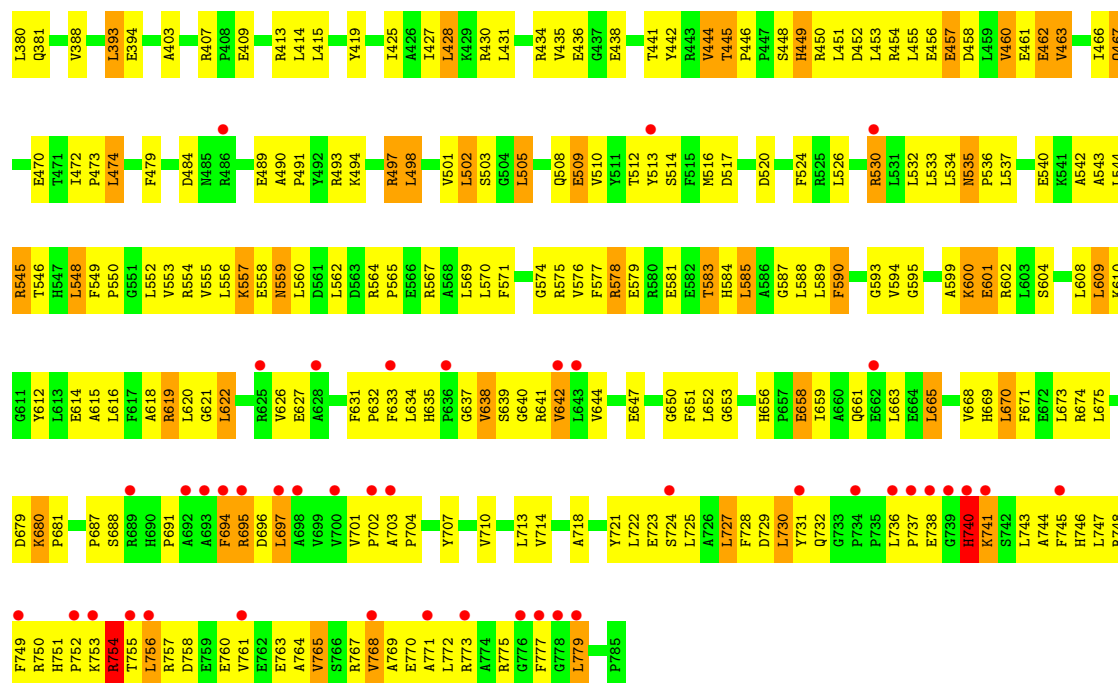
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Phenylalanyl-tRNA synthetase beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.32Å 173.32Å 139.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.88 – 2.85 31.88 – 2.85	Depositor EDS
% Data completeness (in resolution range)	90.5 (31.88-2.85) 90.5 (31.88-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.235 , 0.297 0.241 , 0.298	Depositor DCC
R_{free} test set	2592 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8670	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/2191	0.94	6/2971 (0.2%)
2	B	0.51	0/6280	0.98	19/8536 (0.2%)
All	All	0.51	0/8471	0.97	25/11507 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	VAL	N-CA-C	15.10	124.81	112.12
2	B	252	VAL	N-CA-C	-8.43	98.59	109.80
1	A	271	TRP	CA-C-N	7.84	127.39	119.24
1	A	271	TRP	C-N-CA	7.84	127.39	119.24
1	A	191	THR	CA-C-N	7.42	125.00	119.66
1	A	191	THR	C-N-CA	7.42	125.00	119.66
2	B	161	THR	CA-C-N	6.74	127.29	119.47
2	B	161	THR	C-N-CA	6.74	127.29	119.47
2	B	12	VAL	CA-C-N	5.96	125.66	119.05
2	B	12	VAL	C-N-CA	5.96	125.66	119.05
2	B	41	ILE	CA-C-N	5.69	125.66	120.03
2	B	41	ILE	C-N-CA	5.69	125.66	120.03
2	B	153	GLU	CA-C-N	-5.58	116.27	123.19
2	B	153	GLU	C-N-CA	-5.58	116.27	123.19
2	B	680	LYS	CA-C-N	5.43	125.90	120.14
2	B	680	LYS	C-N-CA	5.43	125.90	120.14
2	B	665	LEU	CA-C-N	5.28	125.82	120.38
2	B	665	LEU	C-N-CA	5.28	125.82	120.38
1	A	214	ALA	N-CA-C	-5.20	106.78	113.23
2	B	258	GLN	CA-C-N	5.15	125.08	119.78
2	B	258	GLN	C-N-CA	5.15	125.08	119.78
1	A	319	VAL	N-CA-C	5.13	117.01	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	150	TRP	CA-C-N	5.12	125.10	120.03
2	B	150	TRP	C-N-CA	5.12	125.10	120.03
2	B	779	LEU	N-CA-C	5.00	116.89	108.73

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	2123	0	2075	142	2
2	B	6127	0	6180	395	0
3	A	14	0	8	9	0
3	B	14	0	8	14	0
4	A	103	0	0	38	0
4	B	289	0	0	97	3
All	All	8670	0	8271	526	3

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 32.

All (526) 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)
2:B:261:HIS:CD2	3:B:786:DAH:N	1.80	1.47
2:B:261:HIS:HD2	3:B:786:DAH:N	0.90	1.38
2:B:261:HIS:CD2	3:B:786:DAH:H	1.45	1.26
3:A:351:DAH:N	4:A:352:HOH:O	1.74	1.16
2:B:619:ARG:HG2	2:B:619:ARG:HH11	1.02	1.13
1:A:130:GLU:HB2	4:A:436:HOH:O	1.61	0.99
2:B:261:HIS:CD2	3:B:786:DAH:H2	1.71	0.99
2:B:553:VAL:HA	4:B:876:HOH:O	1.62	0.99
1:A:191:THR:HG23	2:B:484:ASP:OD2	1.64	0.98
1:A:278:LEU:HD11	1:A:325:LEU:HD22	1.43	0.95
1:A:88:VAL:HA	4:A:396:HOH:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:786:DAH:OE2	4:B:932:HOH:O	1.85	0.93
1:A:172:ARG:HB3	4:A:436:HOH:O	1.68	0.91
2:B:252:VAL:O	2:B:253:MET:HB2	1.68	0.91
2:B:619:ARG:HG2	2:B:619:ARG:NH1	1.78	0.90
2:B:192:LYS:H	2:B:381:GLN:HE22	1.20	0.89
2:B:313:LEU:HA	4:B:966:HOH:O	1.72	0.88
2:B:80:ASN:HD21	2:B:132:LEU:H	1.17	0.88
2:B:587:GLY:HA3	2:B:671:PHE:CE1	2.09	0.88
1:A:308:ARG:HE	1:A:308:ARG:HA	1.36	0.88
2:B:279:GLU:HG2	2:B:295:PRO:HG3	1.53	0.88
2:B:290:GLU:HG3	4:B:837:HOH:O	1.74	0.87
1:A:331:ASP:HB3	1:A:334:TYR:CE2	2.10	0.86
2:B:223:VAL:HA	2:B:244:ASN:HD22	1.41	0.86
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.57	0.85
2:B:272:ILE:HB	4:B:969:HOH:O	1.76	0.84
1:A:117:LEU:HD21	1:A:239:GLU:HG2	1.57	0.84
2:B:610:LYS:O	2:B:614:GLU:HG2	1.79	0.83
2:B:299:VAL:HA	4:B:966:HOH:O	1.77	0.83
2:B:409:GLU:OE1	2:B:413:ARG:HD3	1.79	0.83
2:B:460:VAL:HB	4:B:923:HOH:O	1.78	0.83
1:A:120:GLN:HG2	2:B:489:GLU:HB3	1.59	0.83
2:B:589:LEU:HD21	2:B:608:LEU:HD23	1.62	0.80
2:B:258:GLN:HE22	2:B:369:GLN:NE2	1.79	0.80
2:B:419:TYR:CE1	2:B:467:GLN:HG2	2.17	0.79
2:B:297:ASP:OD2	2:B:350:HIS:HE1	1.65	0.79
2:B:722:LEU:HB2	4:B:978:HOH:O	1.83	0.79
2:B:255:GLU:OE2	2:B:375:ARG:HD3	1.83	0.78
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.64	0.78
2:B:727:LEU:HG	4:B:866:HOH:O	1.83	0.78
1:A:235:GLY:HA2	4:A:443:HOH:O	1.84	0.78
1:A:331:ASP:HB3	1:A:334:TYR:CD2	2.19	0.77
1:A:139:ILE:HD13	1:A:259:PRO:HG2	1.67	0.77
1:A:202:VAL:HG23	4:A:446:HOH:O	1.84	0.76
2:B:204:VAL:HB	2:B:274:VAL:HG13	1.68	0.76
2:B:564:ARG:HD3	4:B:938:HOH:O	1.86	0.75
2:B:271:GLY:HA3	4:B:1049:HOH:O	1.85	0.75
2:B:445:THR:HG22	4:B:835:HOH:O	1.86	0.75
2:B:461:GLU:HG3	4:B:1017:HOH:O	1.85	0.75
1:A:326:ARG:HB2	4:A:427:HOH:O	1.87	0.75
2:B:448:SER:O	2:B:449:HIS:HB3	1.86	0.74
2:B:151:PRO:HD2	2:B:232:ARG:NE	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:ALA:HB2	3:B:786:DAH:HD1	1.68	0.74
2:B:680:LYS:HG3	4:B:955:HOH:O	1.87	0.74
2:B:431:LEU:HD13	2:B:462:GLU:HG3	1.69	0.73
1:A:278:LEU:HD11	1:A:325:LEU:CD2	2.19	0.73
2:B:615:ALA:HB1	4:B:817:HOH:O	1.89	0.72
1:A:233:LEU:HD12	4:A:429:HOH:O	1.88	0.72
1:A:178:HIS:HA	1:A:202:VAL:HG21	1.71	0.72
2:B:414:LEU:HD23	2:B:460:VAL:HG21	1.71	0.72
1:A:143:HIS:HB3	4:A:400:HOH:O	1.89	0.72
2:B:110:GLY:HA2	4:B:884:HOH:O	1.90	0.71
2:B:514:SER:O	2:B:545:ARG:HB2	1.90	0.71
1:A:161:LEU:C	1:A:161:LEU:HD22	2.16	0.71
1:A:300:ARG:HD2	4:A:423:HOH:O	1.91	0.71
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.55	0.71
1:A:175:LEU:HB3	1:A:203:PHE:CD1	2.25	0.70
2:B:286:LEU:CD1	3:B:786:DAH:OXT	2.40	0.70
2:B:604:SER:HA	2:B:608:LEU:HD22	1.74	0.70
1:A:176:ARG:HD2	4:A:446:HOH:O	1.91	0.70
2:B:372:ALA:HA	4:B:1063:HOH:O	1.91	0.70
2:B:730:LEU:HA	4:B:933:HOH:O	1.92	0.70
2:B:575:ARG:HG3	4:B:1018:HOH:O	1.90	0.69
2:B:588:LEU:HD11	4:B:876:HOH:O	1.92	0.69
2:B:258:GLN:HE22	2:B:369:GLN:HE21	1.39	0.69
2:B:294:HIS:CE1	2:B:296:GLU:HB2	2.27	0.69
2:B:681:PRO:HD2	4:B:955:HOH:O	1.92	0.69
1:A:153:TRP:HZ3	4:A:436:HOH:O	1.75	0.69
2:B:252:VAL:O	2:B:253:MET:CB	2.41	0.69
1:A:173:LEU:HB3	4:A:449:HOH:O	1.93	0.69
1:A:179:THR:OG1	1:A:220:GLU:HG2	1.93	0.69
2:B:286:LEU:HD11	3:B:786:DAH:OXT	1.93	0.68
2:B:362:ARG:HG3	4:B:891:HOH:O	1.92	0.68
2:B:297:ASP:OD2	2:B:350:HIS:CE1	2.46	0.68
2:B:12:VAL:HG22	2:B:15:LEU:HG	1.75	0.68
2:B:393:LEU:HB2	4:B:959:HOH:O	1.94	0.68
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.75	0.68
2:B:141:PRO:HG2	2:B:144:THR:HG21	1.76	0.67
1:A:133:ASN:HA	1:A:181:PRO:HG3	1.76	0.67
2:B:313:LEU:HD23	4:B:966:HOH:O	1.94	0.67
2:B:713:LEU:CD2	2:B:775:ARG:HD3	2.24	0.67
3:A:351:DAH:CA	4:A:352:HOH:O	2.30	0.67
1:A:240:LEU:HB2	4:A:392:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:HIS:HB2	2:B:756:LEU:HD13	1.77	0.67
1:A:327:TYR:HB3	1:A:346:PHE:HE2	1.61	0.66
2:B:192:LYS:H	2:B:381:GLN:NE2	1.93	0.66
2:B:256:ARG:HD3	4:B:1063:HOH:O	1.95	0.66
2:B:261:HIS:HB3	4:B:932:HOH:O	1.96	0.66
2:B:253:MET:CG	2:B:259:PRO:HA	2.25	0.66
2:B:294:HIS:CD2	4:B:1054:HOH:O	2.48	0.66
2:B:505:LEU:HD13	2:B:612:TYR:HD1	1.60	0.65
1:A:263:PRO:O	4:A:411:HOH:O	2.15	0.65
1:A:220:GLU:HB3	4:A:437:HOH:O	1.97	0.65
2:B:18:PRO:CG	2:B:154:VAL:HG21	2.26	0.65
1:A:236:ALA:HB3	4:A:429:HOH:O	1.96	0.64
2:B:509:GLU:HB3	2:B:571:PHE:CE1	2.32	0.64
2:B:141:PRO:O	2:B:144:THR:HG22	1.98	0.64
2:B:721:TYR:CE1	2:B:751:HIS:CD2	2.85	0.64
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.80	0.64
2:B:294:HIS:HD2	4:B:1054:HOH:O	1.80	0.64
2:B:502:LEU:HD23	2:B:571:PHE:CD2	2.33	0.64
2:B:261:HIS:HD2	3:B:786:DAH:H	0.64	0.64
1:A:344:GLU:HG2	1:A:347:LYS:HE3	1.80	0.63
1:A:349:VAL:HG12	1:A:350:LEU:HG	1.80	0.63
1:A:138:ASN:O	1:A:140:PRO:HD3	1.99	0.63
2:B:516:MET:CE	2:B:546:THR:H	2.10	0.63
2:B:188:GLU:HB3	4:B:1041:HOH:O	1.96	0.63
2:B:743:LEU:HD23	4:B:933:HOH:O	1.98	0.63
2:B:517:ASP:O	2:B:520:ASP:HB2	1.99	0.63
2:B:502:LEU:HD23	2:B:571:PHE:CE2	2.34	0.62
2:B:567:ARG:NH1	2:B:594:VAL:HG12	2.14	0.62
2:B:230:MET:HG2	4:B:962:HOH:O	1.99	0.62
2:B:357:SER:O	2:B:358:HIS:HB3	1.98	0.62
2:B:96:LEU:HB2	2:B:99:LEU:HD12	1.81	0.62
2:B:178:HIS:CD2	2:B:184:LEU:HB2	2.34	0.62
1:A:261:VAL:HG13	4:A:411:HOH:O	1.99	0.62
1:A:234:LYS:HE2	2:B:474:LEU:HD11	1.81	0.61
3:A:351:DAH:HA	4:A:352:HOH:O	1.97	0.61
1:A:208:THR:HG22	1:A:208:THR:O	2.00	0.61
1:A:316:GLY:HA3	3:A:351:DAH:HB3	1.82	0.61
2:B:298:LEU:HD21	4:B:975:HOH:O	2.00	0.61
2:B:635:HIS:HB3	2:B:638:VAL:H	1.66	0.61
2:B:635:HIS:O	2:B:639:SER:HB2	2.00	0.61
2:B:141:PRO:O	2:B:144:THR:CG2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:VAL:O	2:B:40:PRO:HD3	2.01	0.60
2:B:552:LEU:O	2:B:555:VAL:HG12	2.01	0.60
2:B:356:ALA:C	2:B:357:SER:O	2.42	0.60
2:B:407:ARG:HG3	2:B:456:GLU:OE2	2.02	0.60
2:B:530:ARG:HG3	4:B:952:HOH:O	2.03	0.59
2:B:753:LYS:HE3	4:B:860:HOH:O	2.01	0.59
2:B:725:LEU:HD11	2:B:745:PHE:CD1	2.38	0.59
2:B:631:PHE:HB2	2:B:634:LEU:HD12	1.84	0.59
2:B:261:HIS:CG	3:B:786:DAH:H2	2.20	0.58
2:B:714:VAL:O	2:B:718:ALA:HB2	2.03	0.58
2:B:769:ALA:HA	4:B:874:HOH:O	2.02	0.58
2:B:356:ALA:CB	3:B:786:DAH:HD1	2.33	0.58
2:B:588:LEU:C	2:B:588:LEU:HD23	2.29	0.58
1:A:101:HIS:CG	1:A:102:PRO:HD2	2.39	0.58
1:A:251:VAL:HG12	1:A:269:VAL:HG12	1.85	0.58
2:B:151:PRO:HD2	2:B:232:ARG:HE	1.69	0.58
2:B:509:GLU:HA	2:B:571:PHE:O	2.03	0.58
2:B:669:HIS:HD2	4:B:814:HOH:O	1.86	0.58
2:B:688:SER:HB3	2:B:750:ARG:HD3	1.84	0.58
2:B:201:ALA:HB3	4:B:1049:HOH:O	2.04	0.58
2:B:589:LEU:HB2	2:B:609:LEU:CD2	2.33	0.58
2:B:589:LEU:HB2	2:B:609:LEU:HD22	1.85	0.58
2:B:619:ARG:NH1	2:B:619:ARG:CG	2.60	0.58
2:B:713:LEU:HD21	2:B:775:ARG:HD3	1.85	0.58
2:B:224:ALA:N	2:B:244:ASN:ND2	2.52	0.58
2:B:609:LEU:HG	4:B:913:HOH:O	2.02	0.58
1:A:162:GLU:O	1:A:185:ARG:NH2	2.36	0.58
2:B:494:LYS:HE3	2:B:679:ASP:OD1	2.04	0.58
2:B:554:ARG:O	2:B:558:GLU:HG3	2.04	0.58
2:B:620:LEU:CB	2:B:622:LEU:HD22	2.34	0.57
2:B:710:VAL:HA	4:B:974:HOH:O	2.03	0.57
1:A:176:ARG:HD3	4:A:368:HOH:O	2.04	0.57
2:B:192:LYS:N	2:B:381:GLN:HE22	1.97	0.57
2:B:431:LEU:CD1	2:B:462:GLU:HG3	2.35	0.57
2:B:516:MET:HE3	2:B:545:ARG:HA	1.86	0.57
2:B:721:TYR:HE1	2:B:751:HIS:CD2	2.22	0.57
2:B:642:VAL:HG23	2:B:650:GLY:C	2.29	0.57
2:B:585:LEU:O	2:B:673:LEU:HD23	2.04	0.57
2:B:516:MET:HE1	2:B:546:THR:H	1.70	0.57
2:B:730:LEU:HD23	4:B:933:HOH:O	2.05	0.57
2:B:141:PRO:HG2	2:B:144:THR:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:O	2:B:281:GLU:HB2	2.04	0.57
2:B:497:ARG:HB3	4:B:1025:HOH:O	2.03	0.56
2:B:583:THR:HG23	4:B:1018:HOH:O	2.05	0.56
2:B:695:ARG:HD3	2:B:761:VAL:HG11	1.85	0.56
2:B:740:HIS:O	2:B:741:LYS:HB3	2.06	0.56
2:B:763:GLU:O	2:B:767:ARG:HG2	2.06	0.56
2:B:755:THR:HG23	4:B:1034:HOH:O	2.06	0.56
2:B:356:ALA:CB	3:B:786:DAH:CD1	2.83	0.56
1:A:336:PHE:HB3	2:B:513:TYR:CE2	2.39	0.56
2:B:20:VAL:O	2:B:24:ARG:HB2	2.05	0.56
2:B:224:ALA:H	2:B:244:ASN:ND2	2.03	0.56
2:B:356:ALA:HB1	3:B:786:DAH:CE1	2.36	0.56
2:B:751:HIS:HB2	2:B:756:LEU:CD1	2.35	0.56
1:A:331:ASP:O	1:A:334:TYR:HD2	1.89	0.56
2:B:581:GLU:HG2	4:B:937:HOH:O	2.05	0.56
2:B:1:MET:HE2	4:B:893:HOH:O	2.05	0.55
2:B:255:GLU:OE1	2:B:375:ARG:NH1	2.39	0.55
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.88	0.55
2:B:616:LEU:N	4:B:920:HOH:O	2.38	0.55
1:A:261:VAL:HG22	4:A:411:HOH:O	2.05	0.55
2:B:673:LEU:HD23	2:B:673:LEU:N	2.22	0.55
2:B:20:VAL:HA	2:B:23:GLU:HG2	1.88	0.55
2:B:415:LEU:HG	4:B:923:HOH:O	2.05	0.55
1:A:317:LEU:C	1:A:317:LEU:HD23	2.32	0.55
2:B:710:VAL:HG23	4:B:1019:HOH:O	2.07	0.55
2:B:243:ASN:HA	4:B:819:HOH:O	2.06	0.54
1:A:178:HIS:CA	1:A:202:VAL:HG21	2.37	0.54
2:B:350:HIS:HD2	4:B:904:HOH:O	1.90	0.54
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.89	0.54
2:B:178:HIS:CD2	2:B:430:ARG:HH12	2.25	0.54
2:B:253:MET:HG3	2:B:259:PRO:HA	1.88	0.54
2:B:516:MET:HB3	4:B:843:HOH:O	2.06	0.54
1:A:154:LEU:HD12	4:A:449:HOH:O	2.05	0.54
2:B:694:PHE:CD1	2:B:694:PHE:N	2.76	0.54
2:B:670:LEU:HB3	4:B:1053:HOH:O	2.08	0.54
2:B:80:ASN:ND2	2:B:132:LEU:H	1.98	0.54
2:B:548:LEU:HD22	2:B:584:HIS:HB3	1.89	0.54
2:B:579:GLU:N	4:B:952:HOH:O	2.38	0.54
2:B:691:PRO:HG3	4:B:916:HOH:O	2.08	0.53
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.88	0.53
1:A:179:THR:C	1:A:181:PRO:HD2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:LEU:HA	4:B:969:HOH:O	2.07	0.53
2:B:524:PHE:CZ	2:B:663:LEU:HD11	2.44	0.53
2:B:691:PRO:HB3	4:B:994:HOH:O	2.09	0.53
2:B:12:VAL:HG22	2:B:12:VAL:O	2.09	0.53
1:A:93:ALA:HA	2:B:595:GLY:O	2.08	0.53
2:B:501:VAL:HB	4:B:1046:HOH:O	2.08	0.53
4:A:447:HOH:O	2:B:594:VAL:HA	2.07	0.53
2:B:633:PHE:CD1	2:B:634:LEU:HG	2.43	0.53
1:A:117:LEU:HD21	1:A:239:GLU:CG	2.33	0.52
2:B:696:ASP:OD2	2:B:746:HIS:CD2	2.62	0.52
2:B:419:TYR:CZ	2:B:467:GLN:HG2	2.45	0.52
2:B:761:VAL:O	2:B:765:VAL:HG13	2.09	0.52
1:A:142:HIS:HA	2:B:344:ARG:NH2	2.23	0.52
2:B:357:SER:O	2:B:358:HIS:CB	2.58	0.52
2:B:621:GLY:C	2:B:622:LEU:HD13	2.35	0.52
2:B:428:LEU:HD13	4:B:889:HOH:O	2.09	0.52
2:B:509:GLU:CB	2:B:571:PHE:CE1	2.92	0.52
1:A:338:GLY:HA3	2:B:555:VAL:CG2	2.40	0.52
1:A:237:ILE:HA	4:A:392:HOH:O	2.09	0.52
1:A:237:ILE:HD13	4:A:392:HOH:O	2.10	0.52
2:B:62:LYS:HB2	2:B:62:LYS:NZ	2.25	0.52
2:B:533:LEU:C	2:B:535:ASN:H	2.18	0.52
1:A:262:GLU:HA	1:A:263:PRO:C	2.34	0.52
2:B:102:LYS:HG3	2:B:103:VAL:H	1.75	0.51
2:B:253:MET:HG2	2:B:259:PRO:HA	1.91	0.51
1:A:144:PRO:HB2	4:B:891:HOH:O	2.09	0.51
1:A:341:LYS:HB3	4:A:453:HOH:O	2.09	0.51
2:B:620:LEU:HB2	2:B:622:LEU:HD22	1.93	0.51
1:A:271:TRP:CZ3	1:A:276:LYS:HE2	2.41	0.51
1:A:316:GLY:HA3	3:A:351:DAH:CD2	2.40	0.51
1:A:262:GLU:OE2	2:B:461:GLU:OE1	2.29	0.51
1:A:278:LEU:HA	4:A:431:HOH:O	2.10	0.51
2:B:163:ASN:O	2:B:452:ASP:HB3	2.11	0.51
2:B:599:ALA:HB1	4:B:879:HOH:O	2.10	0.51
2:B:713:LEU:HB3	4:B:974:HOH:O	2.10	0.51
1:A:322:LEU:HB2	4:A:445:HOH:O	2.10	0.51
2:B:175:ARG:HD2	4:B:822:HOH:O	2.10	0.51
2:B:212:HIS:HE1	2:B:394:GLU:OE2	1.92	0.51
2:B:427:ILE:HG23	2:B:466:ILE:HG21	1.92	0.51
2:B:722:LEU:HD12	2:B:748:ARG:O	2.11	0.51
2:B:273:ALA:HB1	4:B:970:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:LEU:HD13	2:B:612:TYR:CD1	2.43	0.51
2:B:627:GLU:OE1	2:B:641:ARG:NH2	2.44	0.51
1:A:178:HIS:HB2	3:A:351:DAH:H	1.76	0.51
1:A:338:GLY:HA3	2:B:555:VAL:HG21	1.93	0.51
1:A:165:LEU:HD21	1:A:303:LEU:HD11	1.93	0.50
2:B:696:ASP:C	2:B:697:LEU:HD13	2.36	0.50
2:B:99:LEU:HD13	2:B:100:GLY:N	2.26	0.50
2:B:549:PHE:CD1	2:B:549:PHE:C	2.89	0.50
1:A:343:LEU:HD13	2:B:509:GLU:O	2.12	0.50
2:B:339:ASP:O	2:B:343:ILE:HG12	2.10	0.50
2:B:703:ALA:HB3	2:B:704:PRO:HD3	1.94	0.50
1:A:180:SER:O	1:A:183:GLN:HG2	2.10	0.50
1:A:193:PRO:HB2	2:B:479:PHE:CD1	2.46	0.50
2:B:575:ARG:NE	4:B:1018:HOH:O	2.44	0.50
2:B:749:PHE:O	2:B:750:ARG:HB2	2.12	0.50
2:B:533:LEU:HB2	2:B:536:PRO:HG3	1.93	0.50
2:B:153:GLU:HG3	2:B:154:VAL:N	2.27	0.50
2:B:710:VAL:O	2:B:714:VAL:HG23	2.12	0.50
1:A:308:ARG:HE	1:A:308:ARG:CA	2.18	0.49
2:B:656:HIS:CE1	2:B:658:GLU:HB2	2.47	0.49
2:B:725:LEU:HD11	2:B:745:PHE:HD1	1.75	0.49
1:A:215:VAL:HG22	1:A:336:PHE:CE2	2.47	0.49
2:B:674:ARG:NH1	4:B:864:HOH:O	2.44	0.49
2:B:771:ALA:O	2:B:775:ARG:HG3	2.12	0.49
2:B:724:SER:HB2	2:B:748:ARG:HD3	1.95	0.49
2:B:223:VAL:CA	2:B:244:ASN:HD22	2.18	0.49
2:B:615:ALA:C	4:B:920:HOH:O	2.55	0.49
2:B:779:LEU:N	2:B:779:LEU:HD12	2.28	0.49
2:B:736:LEU:HD23	4:B:896:HOH:O	2.11	0.49
2:B:601:GLU:O	2:B:602:ARG:HG2	2.13	0.49
2:B:768:VAL:O	2:B:772:LEU:HB2	2.13	0.49
1:A:288:PRO:CG	2:B:457:GLU:HG3	2.43	0.49
2:B:80:ASN:N	2:B:80:ASN:HD22	2.09	0.49
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.21	0.49
2:B:282:ARG:HG2	4:B:980:HOH:O	2.13	0.49
1:A:103:ILE:HD11	1:A:320:GLU:HG3	1.94	0.48
2:B:556:LEU:HB3	4:B:876:HOH:O	2.13	0.48
2:B:764:ALA:O	2:B:768:VAL:HG23	2.13	0.48
2:B:160:VAL:CG1	2:B:167:ALA:HB3	2.44	0.48
2:B:727:LEU:O	2:B:727:LEU:HD23	2.12	0.48
2:B:516:MET:HE3	2:B:546:THR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:PHE:N	2:B:524:PHE:CD2	2.82	0.48
1:A:108:ARG:O	1:A:112:GLU:HG2	2.13	0.48
2:B:425:ILE:HD11	2:B:442:TYR:CZ	2.47	0.48
2:B:428:LEU:N	4:B:889:HOH:O	2.46	0.48
2:B:467:GLN:HE21	2:B:467:GLN:HA	1.78	0.48
2:B:544:LEU:O	2:B:545:ARG:C	2.56	0.48
2:B:757:ARG:HD2	2:B:758:ASP:H	1.78	0.48
1:A:280:LEU:HD21	1:A:322:LEU:HD23	1.95	0.48
2:B:75:VAL:HG23	2:B:111:VAL:HG22	1.95	0.48
2:B:230:MET:HE2	2:B:251:TYR:CG	2.49	0.48
2:B:627:GLU:O	2:B:640:GLY:HA2	2.14	0.48
2:B:710:VAL:CG2	4:B:1019:HOH:O	2.61	0.48
1:A:182:MET:HG2	1:A:198:VAL:HG21	1.95	0.48
1:A:331:ASP:HB3	1:A:334:TYR:HE2	1.71	0.48
2:B:191:LEU:HD23	2:B:381:GLN:NE2	2.28	0.48
2:B:355:GLU:HB3	2:B:359:ARG:NH1	2.29	0.47
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.49	0.47
1:A:139:ILE:HG22	1:A:146:ARG:HG2	1.95	0.47
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.48	0.47
2:B:99:LEU:O	2:B:101:GLN:N	2.44	0.47
2:B:775:ARG:HG2	4:B:821:HOH:O	2.13	0.47
1:A:268:ALA:HA	1:A:278:LEU:O	2.14	0.47
1:A:280:LEU:HD22	4:A:445:HOH:O	2.14	0.47
2:B:578:ARG:O	2:B:579:GLU:HB2	2.15	0.47
1:A:183:GLN:NE2	4:A:444:HOH:O	2.48	0.47
2:B:670:LEU:C	4:B:913:HOH:O	2.57	0.47
2:B:671:PHE:HB3	4:B:913:HOH:O	2.14	0.47
2:B:764:ALA:HA	2:B:767:ARG:CG	2.44	0.47
2:B:620:LEU:HB3	2:B:622:LEU:HD22	1.95	0.47
1:A:308:ARG:HA	1:A:308:ARG:NE	2.16	0.47
2:B:450:ARG:HB3	2:B:453:LEU:HG	1.96	0.47
2:B:722:LEU:HD12	2:B:723:GLU:H	1.80	0.47
2:B:713:LEU:HD22	2:B:775:ARG:HD3	1.97	0.47
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.49	0.47
1:A:130:GLU:HB3	4:A:438:HOH:O	2.14	0.47
2:B:457:GLU:O	2:B:460:VAL:HG22	2.15	0.47
2:B:291:ARG:NH2	2:B:352:LEU:HD21	2.31	0.46
2:B:353:ARG:C	2:B:353:ARG:HD3	2.40	0.46
2:B:407:ARG:NH1	2:B:456:GLU:OE1	2.48	0.46
2:B:731:TYR:HD2	4:B:1023:HOH:O	1.98	0.46
1:A:117:LEU:CD2	1:A:239:GLU:HG2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:C	1:A:161:LEU:CD2	2.87	0.46
2:B:264:ASP:OD2	2:B:266:ARG:HD3	2.16	0.46
2:B:178:HIS:NE2	2:B:430:ARG:NH1	2.63	0.46
2:B:326:GLU:CD	2:B:326:GLU:H	2.24	0.46
2:B:642:VAL:HG23	2:B:650:GLY:O	2.14	0.46
1:A:316:GLY:HA3	3:A:351:DAH:HD2	1.97	0.46
2:B:355:GLU:HB3	2:B:359:ARG:HH11	1.80	0.46
2:B:501:VAL:HG13	2:B:619:ARG:HD3	1.97	0.46
2:B:615:ALA:O	2:B:618:ALA:HB3	2.15	0.46
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.46	0.46
1:A:206:GLU:HG3	1:A:207:GLN:H	1.81	0.46
1:A:162:GLU:H	1:A:162:GLU:HG2	1.59	0.46
1:A:285:MET:N	4:A:411:HOH:O	2.48	0.46
2:B:548:LEU:HD21	2:B:574:GLY:H	1.80	0.46
2:B:569:LEU:HD13	2:B:589:LEU:HD13	1.97	0.46
2:B:718:ALA:HA	2:B:768:VAL:HG22	1.96	0.46
2:B:635:HIS:ND1	2:B:637:GLY:N	2.60	0.45
2:B:765:VAL:HA	2:B:768:VAL:HG23	1.98	0.45
1:A:201:ARG:HD2	1:A:336:PHE:HZ	1.81	0.45
2:B:49:ARG:HD2	2:B:137:GLU:HG3	1.97	0.45
2:B:139:ALA:O	2:B:140:LEU:HD13	2.16	0.45
2:B:356:ALA:HB1	3:B:786:DAH:CD1	2.46	0.45
2:B:549:PHE:CD2	2:B:651:PHE:HZ	2.35	0.45
1:A:127:VAL:HG13	4:A:449:HOH:O	2.15	0.45
1:A:348:GLY:O	1:A:349:VAL:C	2.58	0.45
2:B:549:PHE:CD1	2:B:550:PRO:N	2.85	0.45
2:B:206:ASP:OD1	2:B:208:GLU:HB2	2.16	0.45
2:B:455:LEU:O	2:B:458:ASP:HB2	2.17	0.45
2:B:634:LEU:O	2:B:656:HIS:CD2	2.69	0.45
1:A:109:GLU:O	1:A:113:ILE:HG13	2.17	0.45
1:A:313:PHE:CD1	1:A:313:PHE:C	2.94	0.45
2:B:188:GLU:HG3	2:B:188:GLU:O	2.16	0.45
2:B:311:LEU:HA	2:B:311:LEU:HD23	1.70	0.45
2:B:570:LEU:HG	2:B:588:LEU:HD22	1.97	0.45
2:B:1:MET:HE1	2:B:168:LEU:C	2.42	0.45
2:B:243:ASN:O	2:B:244:ASN:C	2.59	0.45
2:B:569:LEU:HD12	2:B:588:LEU:O	2.17	0.45
2:B:773:ARG:HG3	4:B:874:HOH:O	2.16	0.45
1:A:179:THR:OG1	1:A:220:GLU:CG	2.64	0.45
2:B:99:LEU:HD13	2:B:99:LEU:C	2.42	0.45
2:B:223:VAL:CG1	2:B:326:GLU:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ARG:HA	2:B:241:PRO:HD3	1.82	0.45
2:B:651:PHE:C	2:B:651:PHE:CD1	2.95	0.45
1:A:179:THR:C	1:A:181:PRO:CD	2.90	0.45
1:A:343:LEU:HB2	4:A:419:HOH:O	2.17	0.45
2:B:457:GLU:HA	2:B:460:VAL:HG13	1.99	0.45
2:B:489:GLU:O	2:B:490:ALA:C	2.60	0.45
2:B:549:PHE:HB2	2:B:670:LEU:HD22	1.99	0.45
1:A:247:PRO:C	1:A:249:SER:H	2.25	0.44
2:B:196:LEU:HB2	2:B:197:PRO:CD	2.48	0.44
2:B:656:HIS:HB3	2:B:659:ILE:HG13	1.99	0.44
2:B:74:VAL:HA	2:B:113:SER:HA	1.97	0.44
2:B:261:HIS:CB	4:B:932:HOH:O	2.61	0.44
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.84	0.44
1:A:101:HIS:O	1:A:102:PRO:C	2.60	0.44
1:A:240:LEU:HD11	1:A:317:LEU:HD11	1.98	0.44
2:B:588:LEU:HG	4:B:1053:HOH:O	2.18	0.44
2:B:590:PHE:HA	4:B:814:HOH:O	2.17	0.44
1:A:107:GLU:O	1:A:111:VAL:HG13	2.17	0.44
2:B:63:ARG:NH1	2:B:73:GLU:OE2	2.44	0.44
2:B:668:VAL:HG12	4:B:1053:HOH:O	2.16	0.44
2:B:707:TYR:CE1	2:B:727:LEU:HD13	2.53	0.44
2:B:773:ARG:C	2:B:775:ARG:H	2.26	0.44
2:B:512:THR:HG22	2:B:513:TYR:O	2.18	0.44
2:B:761:VAL:O	2:B:765:VAL:CG1	2.66	0.44
1:A:114:PHE:CZ	1:A:240:LEU:HG	2.53	0.44
1:A:190:HIS:HB3	2:B:484:ASP:OD1	2.18	0.44
2:B:543:ALA:HB3	4:B:843:HOH:O	2.17	0.44
2:B:722:LEU:HD21	2:B:725:LEU:HB2	2.00	0.44
1:A:165:LEU:HD22	1:A:301:LEU:HD23	2.00	0.43
2:B:434:ARG:HH12	2:B:436:GLU:CD	2.26	0.43
2:B:445:THR:HA	2:B:446:PRO:HD3	1.83	0.43
1:A:174:LEU:HD13	1:A:174:LEU:N	2.34	0.43
2:B:505:LEU:CD1	2:B:612:TYR:HD1	2.29	0.43
1:A:177:THR:O	1:A:204:ARG:NH2	2.51	0.43
2:B:204:VAL:CB	2:B:274:VAL:HG13	2.45	0.43
2:B:215:LEU:HA	2:B:333:LEU:O	2.19	0.43
2:B:294:HIS:CG	2:B:295:PRO:HD2	2.53	0.43
2:B:178:HIS:CD2	2:B:430:ARG:NH1	2.86	0.43
2:B:259:PRO:HB2	2:B:360:PHE:CE2	2.53	0.43
2:B:262:ALA:HB1	2:B:331:ILE:HD12	2.00	0.43
2:B:548:LEU:HD22	2:B:584:HIS:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:HIS:HB2	1:A:218:GLN:HE22	1.84	0.43
2:B:160:VAL:HA	4:B:793:HOH:O	2.19	0.43
2:B:740:HIS:HB3	2:B:741:LYS:H	1.54	0.43
1:A:344:GLU:HG2	1:A:347:LYS:CE	2.48	0.43
2:B:314:ALA:C	4:B:1016:HOH:O	2.61	0.43
2:B:743:LEU:HA	4:B:933:HOH:O	2.19	0.43
1:A:87:ASP:HB3	1:A:90:LEU:HD22	2.01	0.43
2:B:91:LEU:HB3	2:B:92:PRO:HD2	2.00	0.43
1:A:198:VAL:HA	1:A:199:PRO:HD3	1.76	0.43
1:A:233:LEU:HA	4:A:429:HOH:O	2.18	0.43
1:A:287:HIS:ND1	1:A:288:PRO:HD2	2.33	0.43
4:A:419:HOH:O	2:B:508:GLN:HG2	2.18	0.43
1:A:197:VAL:HG13	1:A:219:LEU:HD21	2.00	0.42
2:B:304:ARG:O	2:B:307:GLU:HB2	2.18	0.42
2:B:524:PHE:O	2:B:633:PHE:HB3	2.19	0.42
2:B:559:ASN:O	2:B:565:PRO:HD2	2.19	0.42
2:B:589:LEU:O	2:B:590:PHE:CB	2.67	0.42
2:B:80:ASN:HD22	2:B:80:ASN:H	1.65	0.42
2:B:168:LEU:HD13	2:B:359:ARG:HG3	2.01	0.42
2:B:224:ALA:HB1	2:B:225:PRO:HD2	2.00	0.42
1:A:187:MET:HE2	1:A:222:LEU:HD11	2.01	0.42
2:B:718:ALA:HA	2:B:768:VAL:CG2	2.50	0.42
2:B:222:ARG:HH21	2:B:222:ARG:CG	2.32	0.42
2:B:380:LEU:HD23	2:B:380:LEU:HA	1.84	0.42
2:B:556:LEU:O	2:B:557:LYS:C	2.63	0.42
2:B:763:GLU:HG3	4:B:928:HOH:O	2.20	0.42
1:A:329:ILE:HA	1:A:330:PRO:HD3	1.86	0.42
2:B:198:LEU:HA	2:B:199:PRO:HD3	1.89	0.42
2:B:279:GLU:CG	2:B:295:PRO:HG3	2.37	0.42
2:B:463:VAL:O	2:B:467:GLN:HB2	2.19	0.42
2:B:707:TYR:HA	4:B:1019:HOH:O	2.19	0.42
2:B:754:ARG:H	2:B:754:ARG:HG2	1.61	0.42
1:A:113:ILE:HG21	1:A:240:LEU:HD23	2.02	0.42
1:A:201:ARG:HG2	4:B:946:HOH:O	2.20	0.42
2:B:349:ARG:HG2	2:B:350:HIS:ND1	2.34	0.42
2:B:355:GLU:OE1	2:B:359:ARG:NH1	2.52	0.42
2:B:764:ALA:HA	2:B:767:ARG:HG3	2.02	0.42
2:B:81:ALA:HB2	2:B:132:LEU:HD22	2.02	0.42
2:B:249:THR:HB	2:B:260:MET:HG2	2.02	0.42
2:B:461:GLU:CG	4:B:1017:HOH:O	2.56	0.42
1:A:206:GLU:CG	1:A:207:GLN:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:GLU:CD	2:B:326:GLU:N	2.78	0.41
2:B:472:ILE:HA	2:B:473:PRO:HD3	1.90	0.41
1:A:137:LEU:HA	1:A:137:LEU:HD23	1.86	0.41
2:B:600:LYS:HG2	4:B:879:HOH:O	2.21	0.41
1:A:128:GLU:OE1	1:A:132:PHE:HB2	2.20	0.41
1:A:285:MET:HA	1:A:312:GLY:O	2.21	0.41
2:B:255:GLU:CD	2:B:375:ARG:HH11	2.28	0.41
2:B:264:ASP:OD1	2:B:264:ASP:C	2.63	0.41
1:A:159:PHE:HD1	4:B:952:HOH:O	2.01	0.41
1:A:287:HIS:CG	1:A:288:PRO:HD2	2.56	0.41
2:B:60:ARG:H	2:B:60:ARG:HG3	1.74	0.41
2:B:263:PHE:CZ	2:B:300:ILE:HG21	2.55	0.41
2:B:701:VAL:CG1	2:B:702:PRO:HD2	2.49	0.41
2:B:725:LEU:CD1	2:B:745:PHE:HD1	2.32	0.41
2:B:773:ARG:HD2	4:B:951:HOH:O	2.19	0.41
1:A:121:ALA:HA	1:A:197:VAL:O	2.19	0.41
1:A:316:GLY:CA	3:A:351:DAH:CD2	2.98	0.41
2:B:231:GLN:HG2	2:B:241:PRO:CG	2.50	0.41
2:B:445:THR:HG21	4:B:965:HOH:O	2.18	0.41
2:B:723:GLU:HB3	2:B:724:SER:H	1.59	0.41
2:B:286:LEU:HD23	2:B:286:LEU:HA	1.80	0.41
2:B:498:LEU:HD22	4:B:1075:HOH:O	2.20	0.41
2:B:249:THR:O	2:B:252:VAL:O	2.37	0.41
2:B:652:LEU:HD12	2:B:653:GLY:H	1.85	0.41
1:A:106:MET:HE3	1:A:106:MET:HA	2.03	0.41
1:A:118:GLY:O	1:A:195:ARG:HB2	2.21	0.41
1:A:127:VAL:HG23	2:B:577:PHE:CE2	2.55	0.41
2:B:159:GLU:O	2:B:159:GLU:HG3	2.20	0.41
2:B:161:THR:HA	2:B:162:PRO:HD3	1.89	0.41
1:A:142:HIS:N	4:A:439:HOH:O	2.53	0.41
1:A:290:VAL:O	1:A:294:VAL:CG1	2.69	0.41
2:B:16:GLU:O	2:B:17:SER:HB3	2.20	0.41
2:B:175:ARG:O	2:B:178:HIS:HB3	2.21	0.41
2:B:231:GLN:HG2	2:B:241:PRO:CB	2.51	0.41
2:B:604:SER:HA	2:B:608:LEU:CD2	2.48	0.41
2:B:747:LEU:O	2:B:748:ARG:HG3	2.21	0.41
1:A:221:GLY:HA3	1:A:315:PHE:CZ	2.57	0.40
1:A:237:ILE:HG22	1:A:251:VAL:HG11	2.02	0.40
2:B:224:ALA:N	2:B:244:ASN:HD22	2.18	0.40
2:B:287:ASP:OD2	2:B:291:ARG:NH2	2.53	0.40
2:B:710:VAL:HB	4:B:1019:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ILE:HG22	2:B:109:GLN:HG2	2.04	0.40
2:B:294:HIS:ND1	2:B:296:GLU:HB2	2.37	0.40
2:B:403:ALA:HA	2:B:445:THR:HB	2.02	0.40
2:B:543:ALA:CB	4:B:843:HOH:O	2.69	0.40
2:B:728:PHE:O	2:B:729:ASP:HB2	2.20	0.40
2:B:728:PHE:CG	2:B:746:HIS:CE1	3.08	0.40
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.95	0.40
1:A:206:GLU:HG3	1:A:207:GLN:N	2.36	0.40
1:A:316:GLY:N	3:A:351:DAH:CD2	2.84	0.40
2:B:277:ALA:O	2:B:295:PRO:HA	2.21	0.40
2:B:434:ARG:O	2:B:444:VAL:HA	2.22	0.40
2:B:517:ASP:CG	2:B:540:GLU:HA	2.47	0.40
2:B:569:LEU:HD12	2:B:569:LEU:HA	1.94	0.40
1:A:234:LYS:HG2	1:A:253:PHE:CE1	2.55	0.40
1:A:288:PRO:HG2	2:B:457:GLU:HG3	2.02	0.40
1:A:322:LEU:HD22	1:A:322:LEU:HA	1.90	0.40
2:B:278:ARG:HD3	2:B:278:ARG:HA	1.91	0.40
2:B:334:GLU:CD	4:B:932:HOH:O	2.65	0.40
2:B:502:LEU:HD12	2:B:502:LEU:HA	1.93	0.40
2:B:40:PRO:HD2	4:B:827:HOH:O	2.21	0.40
2:B:163:ASN:C	2:B:165:PRO:HD3	2.46	0.40
2:B:196:LEU:O	2:B:196:LEU:HD12	2.20	0.40
2:B:567:ARG:HH12	2:B:594:VAL:HG12	1.84	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PRO:O	4:B:884:HOH:O[5_665]	2.00	0.20
1:A:191:THR:OG1	4:B:884:HOH:O[5_665]	2.12	0.08
4:B:821:HOH:O	4:B:821:HOH:O[5_555]	2.17	0.03

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	264/350 (75%)	240 (91%)	20 (8%)	4 (2%)	8	18
2	B	783/785 (100%)	706 (90%)	57 (7%)	20 (3%)	4	9
All	All	1047/1135 (92%)	946 (90%)	77 (7%)	24 (2%)	5	11

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	VAL
2	B	244	ASN
2	B	253	MET
2	B	738	GLU
2	B	99	LEU
2	B	449	HIS
2	B	545	ARG
2	B	737	PRO
2	B	754	ARG
1	A	337	GLY
2	B	357	SER
2	B	590	PHE
2	B	740	HIS
1	A	93	ALA
1	A	208	THR
2	B	770	GLU
2	B	243	ASN
2	B	741	LYS
2	B	534	LEU
2	B	100	GLY
2	B	687	PRO
2	B	632	PRO
2	B	752	PRO
2	B	535	ASN

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	214/277 (77%)	175 (82%)	39 (18%)	2	2
2	B	630/630 (100%)	521 (83%)	109 (17%)	2	3
All	All	844/907 (93%)	696 (82%)	148 (18%)	2	3

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	88	VAL
1	A	105	LEU
1	A	110	LEU
1	A	111	VAL
1	A	115	ARG
1	A	139	ILE
1	A	157	GLU
1	A	161	LEU
1	A	162	GLU
1	A	165	LEU
1	A	174	LEU
1	A	178	HIS
1	A	179	THR
1	A	191	THR
1	A	197	VAL
1	A	198	VAL
1	A	201	ARG
1	A	202	VAL
1	A	204	ARG
1	A	207	GLN
1	A	208	THR
1	A	215	VAL
1	A	222	LEU
1	A	240	LEU
1	A	250	LYS
1	A	256	VAL
1	A	261	VAL
1	A	286	VAL
1	A	294	VAL
1	A	301	LEU
1	A	308	ARG
1	A	317	LEU
1	A	319	VAL
1	A	322	LEU

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Mol	Chain	Res	Type
1	A	325	LEU
1	A	329	ILE
1	A	341	LYS
1	A	350	LEU
2	B	12	VAL
2	B	19	GLU
2	B	20	VAL
2	B	21	LEU
2	B	28	LEU
2	B	32	THR
2	B	38	VAL
2	B	60	ARG
2	B	62	LYS
2	B	80	ASN
2	B	83	LYS
2	B	99	LEU
2	B	111	VAL
2	B	112	ARG
2	B	132	LEU
2	B	133	LEU
2	B	134	GLU
2	B	140	LEU
2	B	144	THR
2	B	147	SER
2	B	154	VAL
2	B	155	VAL
2	B	173	LEU
2	B	184	LEU
2	B	196	LEU
2	B	204	VAL
2	B	222	ARG
2	B	228	LEU
2	B	245	VAL
2	B	248	VAL
2	B	253	MET
2	B	260	MET
2	B	274	VAL
2	B	276	ARG
2	B	282	ARG
2	B	289	VAL
2	B	313	LEU
2	B	329	GLU

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Mol	Chain	Res	Type
2	B	333	LEU
2	B	359	ARG
2	B	364	VAL
2	B	375	ARG
2	B	377	LEU
2	B	379	LEU
2	B	388	VAL
2	B	393	LEU
2	B	428	LEU
2	B	435	VAL
2	B	438	GLU
2	B	441	THR
2	B	444	VAL
2	B	445	THR
2	B	451	LEU
2	B	454	ARG
2	B	457	GLU
2	B	460	VAL
2	B	462	GLU
2	B	463	VAL
2	B	467	GLN
2	B	470	GLU
2	B	474	LEU
2	B	493	ARG
2	B	497	ARG
2	B	498	LEU
2	B	502	LEU
2	B	503	SER
2	B	505	LEU
2	B	509	GLU
2	B	510	VAL
2	B	526	LEU
2	B	530	ARG
2	B	532	LEU
2	B	537	LEU
2	B	548	LEU
2	B	557	LYS
2	B	559	ASN
2	B	560	LEU
2	B	562	LEU
2	B	576	VAL
2	B	578	ARG

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Mol	Chain	Res	Type
2	B	583	THR
2	B	585	LEU
2	B	600	LYS
2	B	601	GLU
2	B	609	LEU
2	B	619	ARG
2	B	622	LEU
2	B	626	VAL
2	B	638	VAL
2	B	642	VAL
2	B	644	VAL
2	B	647	GLU
2	B	658	GLU
2	B	661	GLN
2	B	665	LEU
2	B	670	LEU
2	B	675	LEU
2	B	694	PHE
2	B	695	ARG
2	B	697	LEU
2	B	727	LEU
2	B	730	LEU
2	B	732	GLN
2	B	740	HIS
2	B	754	ARG
2	B	756	LEU
2	B	760	GLU
2	B	765	VAL
2	B	768	VAL

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

Mol	Chain	Res	Type
1	A	142	HIS
1	A	178	HIS
1	A	207	GLN
1	A	218	GLN
2	B	54	HIS
2	B	80	ASN
2	B	101	GLN
2	B	178	HIS
2	B	212	HIS

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Mol	Chain	Res	Type
2	B	231	GLN
2	B	244	ASN
2	B	258	GLN
2	B	261	HIS
2	B	350	HIS
2	B	381	GLN
2	B	467	GLN
2	B	485	ASN
2	B	732	GLN
2	B	751	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.10	12 (4%)	38 29	45, 60, 106, 148	0
2	B	779/785 (99%)	0.31	48 (6%)	26 19	41, 63, 133, 173	0
All	All	1044/1135 (91%)	0.26	60 (5%)	29 22	41, 62, 128, 173	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	779	LEU	5.9
2	B	739	GLY	5.8
2	B	737	PRO	5.1
1	A	350	LEU	4.6
2	B	738	GLU	4.6
2	B	695	ARG	4.4
2	B	703	ALA	3.9
2	B	756	LEU	3.8
2	B	777	PHE	3.8
2	B	697	LEU	3.7
2	B	778	GLY	3.6
2	B	731	TYR	3.6
1	A	86	VAL	3.5
2	B	740	HIS	3.3
2	B	203	LYS	3.2
2	B	693	ALA	3.2
2	B	692	ALA	3.2
2	B	694	PHE	3.1
2	B	698	ALA	3.0
2	B	689	ARG	2.9
2	B	702	PRO	2.8
1	A	271	TRP	2.8
2	B	736	LEU	2.8
2	B	633	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	734	PRO	2.8
2	B	753	LYS	2.6
2	B	530	ARG	2.5
2	B	43	ARG	2.5
2	B	628	ALA	2.5
2	B	278	ARG	2.5
2	B	771	ALA	2.5
2	B	761	VAL	2.4
2	B	700	VAL	2.4
1	A	321	ARG	2.4
2	B	745	PHE	2.4
1	A	143	HIS	2.4
1	A	158	GLY	2.4
2	B	749	PHE	2.4
1	A	349	VAL	2.3
2	B	741	LYS	2.3
2	B	768	VAL	2.3
2	B	513	TYR	2.3
1	A	272	PRO	2.3
2	B	752	PRO	2.3
1	A	339	ARG	2.2
2	B	724	SER	2.2
2	B	776	GLY	2.2
2	B	636	PRO	2.2
2	B	60	ARG	2.2
2	B	773	ARG	2.2
2	B	662	GLU	2.2
2	B	101	GLN	2.1
2	B	643	LEU	2.1
2	B	625	ARG	2.1
2	B	486	ARG	2.1
2	B	755	THR	2.1
1	A	308	ARG	2.1
1	A	144	PRO	2.1
1	A	316	GLY	2.1
2	B	642	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DAH	B	786	14/14	0.64	0.34	20,20,20,20	0
3	DAH	A	351	14/14	0.74	0.26	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.