WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 11:58 AM EDT

PDB ID	:	1Q7Q
Title	:	Cobalamin-dependent methionine synthase (1-566) from T. maritima (Oxidized, Orthorhombic)
Authors	:	Evans, J.C.; Huddler, D.P.; Hilgers, M.T.; Romanchuk, G.; Matthews, R.G.; Ludwig, M.L.
Deposited on	:	2003-08-19
Resolution	:	3.10 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

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 3.10 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		29
Ramachandran outliers		2.6%
Sidechain outliers		7.5%
RSRZ outliers		1.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
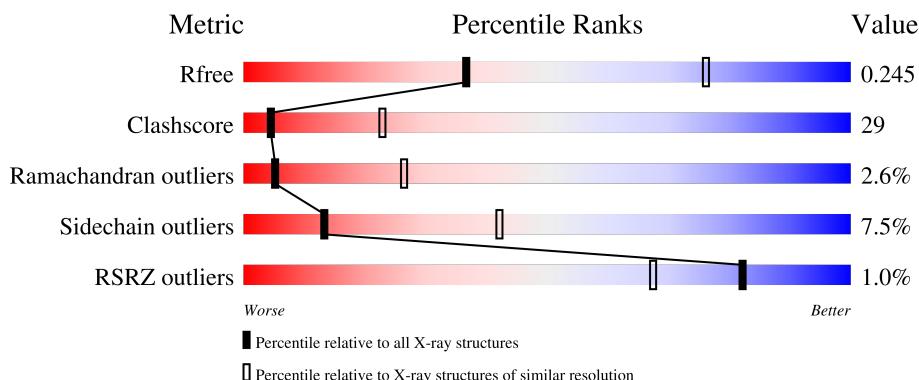
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	566	52% 42% 5%
1	B	566	49% 42% 6% ··
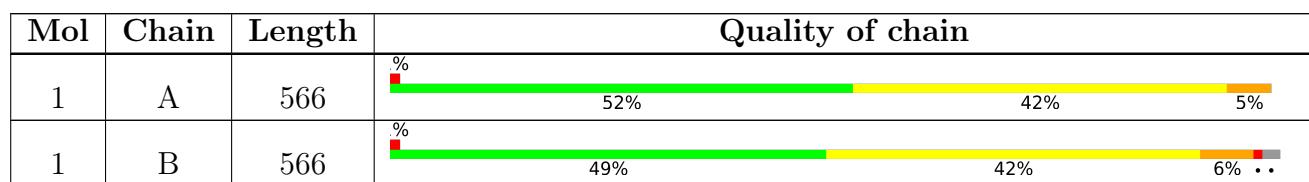
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9031 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 5-methyltetrahydrofolate S-homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4467	2866	747	841	13			
1	B	552	Total	C	N	O	S	0	0	0
			4370	2805	731	821	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	103	Total	O	0	0
			103	103		
2	B	91	Total	O	0	0
			91	91		

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: 5-methyltetrahydrofolate S-homocysteine methyltransferase
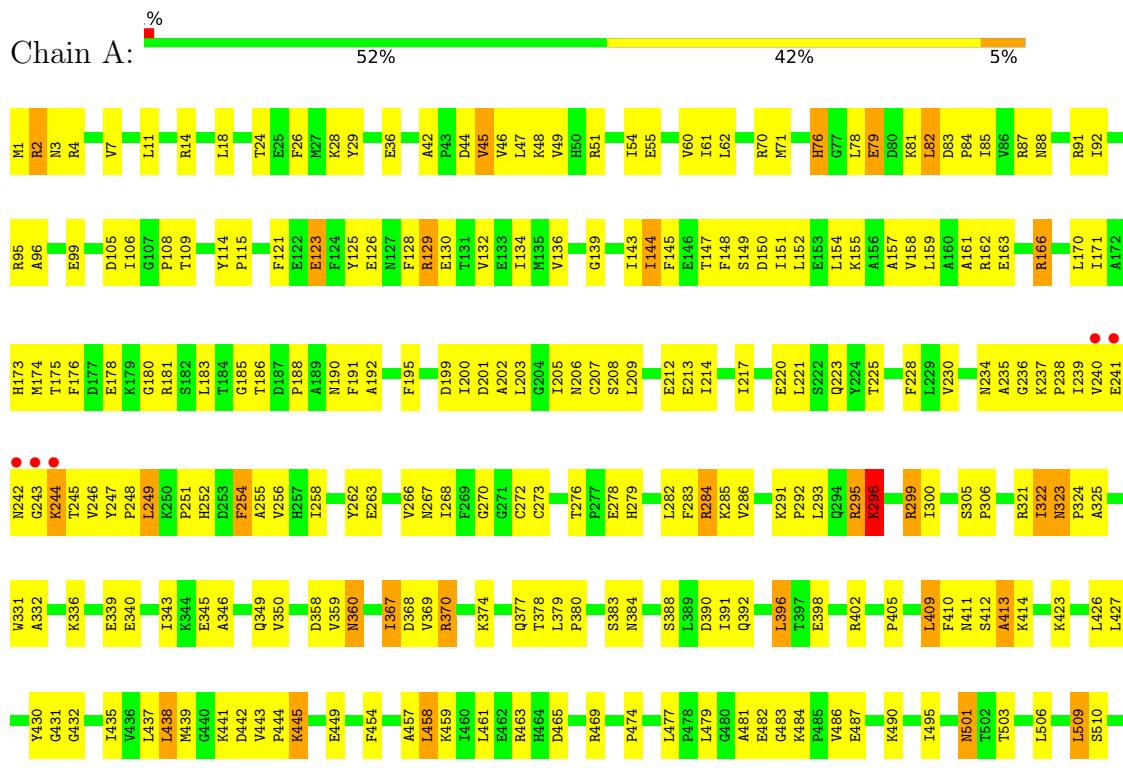
• Molecule 1: 5-methyltetrahydrofolate S-homocysteine methyltransferase
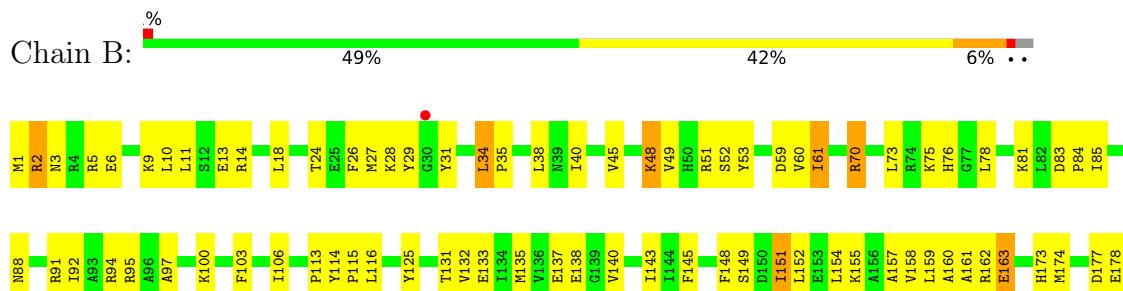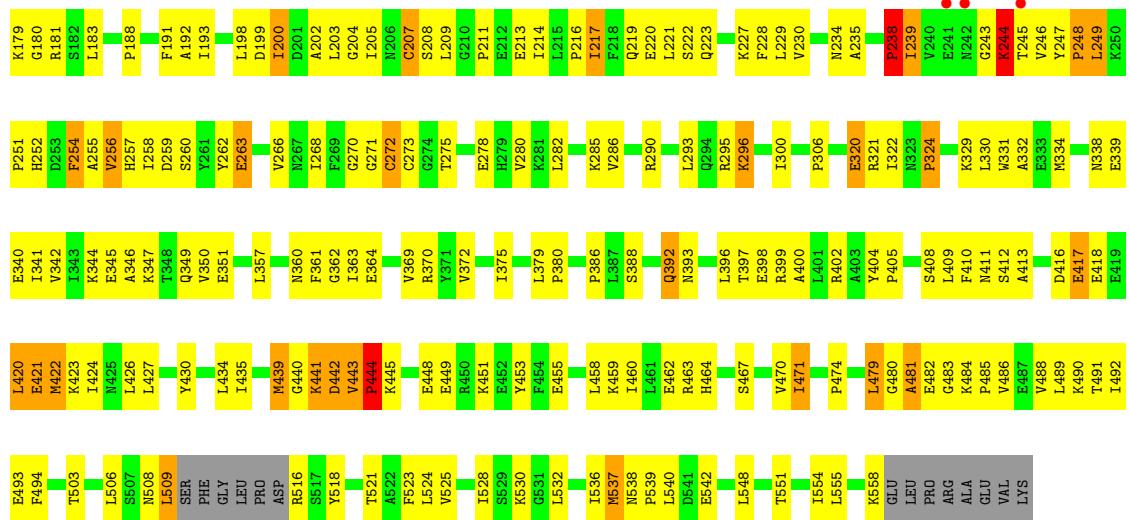
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.58Å 169.02Å 174.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10	Depositor
	46.39 – 3.10	EDS
% Data completeness	(Not available) (50.00-3.10)	Depositor
(in resolution range)	90.6 (46.39-3.10)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.265	Depositor
	0.204 , 0.245	DCC
R_{free} test set	4583 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 73.8	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.031 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9031	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.39	0/4550	0.66	0/6145
1	B	0.41	0/4449	0.66	0/6005
All	All	0.40	0/8999	0.66	0/12150

There are no bond length outliers.

There are no bond angle outliers.

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	4467	0	4553	254	0
1	B	4370	0	4467	257	0
2	A	103	0	0	26	0
2	B	91	0	0	7	0
All	All	9031	0	9020	510	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 (510) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ASP:O	1:B:263:GLU:HG2	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HH21	1:A:166:ARG:HB2	1.29	0.93
1:A:296:LYS:HA	1:A:296:LYS:NZ	1.89	0.87
1:B:271:GLY:HA3	1:B:275:THR:HG21	1.57	0.86
1:A:54:ILE:HD11	1:A:61:ILE:HD13	1.57	0.86
1:B:372:VAL:HG11	1:B:396:LEU:HD11	1.59	0.84
1:A:558:LYS:HG3	1:A:559:GLU:N	1.91	0.83
1:B:455:GLU:O	1:B:459:LYS:HG3	1.79	0.82
1:B:439:MET:HG2	1:B:440:GLY:H	1.44	0.82
1:A:444:PRO:HB3	1:A:449:GLU:HG2	1.62	0.82
1:A:70:ARG:HB3	2:A:636:HOH:O	1.80	0.81
1:A:242:ASN:HB2	1:A:244:LYS:HE3	1.60	0.81
1:B:479:LEU:HA	1:B:483:GLY:HA2	1.63	0.81
1:A:151:ILE:HD11	1:A:306:PRO:HA	1.63	0.80
1:A:284:ARG:HE	1:A:284:ARG:HA	1.46	0.80
1:B:230:VAL:HG22	1:B:268:ILE:HB	1.64	0.79
1:B:151:ILE:HD11	1:B:306:PRO:HG3	1.64	0.79
1:A:209:LEU:HB2	1:A:214:ILE:HG12	1.64	0.78
1:A:390:ASP:HA	2:A:574:HOH:O	1.83	0.76
1:A:54:ILE:HD13	1:A:96:ALA:O	1.85	0.76
1:A:114:TYR:CD1	1:A:115:PRO:HA	2.21	0.76
1:A:515:ASP:HB3	1:A:518:TYR:HD1	1.52	0.75
1:B:409:LEU:HD21	1:B:435:ILE:HD11	1.68	0.74
1:B:370:ARG:HH21	1:B:370:ARG:HB2	1.52	0.73
1:A:402:ARG:HG2	1:A:430:TYR:CE1	2.23	0.73
1:A:171:ILE:HG12	1:A:202:ALA:HB3	1.69	0.73
1:A:166:ARG:HB2	1:A:166:ARG:NH2	2.03	0.73
1:A:244:LYS:HG3	1:A:245:THR:H	1.54	0.73
1:A:360:ASN:HB2	1:A:390:ASP:HB3	1.68	0.72
1:A:562:ARG:CZ	1:A:562:ARG:HA	2.19	0.72
1:A:212:GLU:HG2	2:A:624:HOH:O	1.88	0.72
1:B:435:ILE:HD13	1:B:471:ILE:HG12	1.71	0.72
1:B:364:GLU:OE2	1:B:392:GLN:HG2	1.89	0.71
1:A:213:GLU:HG2	2:A:630:HOH:O	1.90	0.71
1:B:29:TYR:CE1	1:B:48:LYS:HD3	2.26	0.70
1:B:244:LYS:NZ	1:B:244:LYS:HA	2.06	0.70
1:A:1:MET:HG3	1:A:139:GLY:HA3	1.72	0.70
1:A:445:LYS:H	1:A:445:LYS:HD2	1.57	0.70
1:B:1:MET:HG3	1:B:140:VAL:O	1.92	0.69
1:B:439:MET:CG	1:B:440:GLY:H	2.03	0.69
1:A:255:ALA:O	1:A:286:VAL:HG11	1.92	0.69
1:A:296:LYS:HA	1:A:296:LYS:HZ3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLU:HB3	1:B:536:ILE:HG22	1.74	0.69
1:B:132:VAL:HG13	1:B:143:ILE:CD1	2.22	0.69
1:A:411:ASN:HB3	2:A:574:HOH:O	1.92	0.69
1:A:18:LEU:HD23	1:A:60:VAL:HG13	1.75	0.68
1:A:4:ARG:HD3	1:A:201:ASP:OD2	1.94	0.68
1:A:482:GLU:HB3	1:A:484:LYS:HE3	1.74	0.68
1:A:180:GLY:O	1:A:188:PRO:HD3	1.94	0.68
1:B:324:PRO:HG2	1:B:362:GLY:N	2.09	0.67
1:B:151:ILE:HD13	1:B:151:ILE:H	1.59	0.67
1:A:549:ASN:O	1:A:553:VAL:HG23	1.93	0.67
1:B:244:LYS:HA	1:B:244:LYS:HZ3	1.59	0.67
1:B:244:LYS:HZ2	1:B:245:THR:H	1.43	0.67
1:A:299:ARG:HD2	1:A:300:ILE:N	2.10	0.66
1:B:479:LEU:HD22	1:B:509:LEU:HG	1.77	0.66
1:B:537:MET:HE1	1:B:548:LEU:HD22	1.78	0.66
1:A:562:ARG:HA	1:A:562:ARG:NE	2.10	0.66
1:A:128:PHE:O	1:A:132:VAL:HG23	1.96	0.66
1:A:145:PHE:CE2	1:A:157:ALA:HB1	2.31	0.65
1:B:3:ASN:OD1	1:B:6:GLU:HG3	1.96	0.65
1:A:515:ASP:HB3	1:A:518:TYR:CD1	2.31	0.65
1:A:285:LYS:HA	2:A:658:HOH:O	1.95	0.65
1:B:463:ARG:HB2	1:B:463:ARG:HH21	1.62	0.65
1:A:442:ASP:HB3	2:A:587:HOH:O	1.95	0.65
1:B:364:GLU:CD	1:B:392:GLN:HG2	2.17	0.65
1:A:132:VAL:HG11	1:A:161:ALA:HA	1.79	0.64
1:A:87:ARG:O	1:A:91:ARG:HG3	1.97	0.64
1:A:42:ALA:O	1:A:45:VAL:HG23	1.97	0.64
1:B:463:ARG:HB2	1:B:463:ARG:NH2	2.12	0.64
1:A:132:VAL:O	1:A:136:VAL:HG23	1.98	0.64
1:B:202:ALA:HB2	1:B:228:PHE:HB2	1.79	0.64
1:B:133:GLU:O	1:B:137:GLU:HG3	1.97	0.63
1:A:132:VAL:HG13	1:A:143:ILE:HD13	1.80	0.63
1:B:9:LYS:O	1:B:13:GLU:HG3	1.98	0.63
1:B:48:LYS:C	1:B:48:LYS:HE2	2.19	0.63
1:B:370:ARG:HB2	1:B:370:ARG:NH2	2.13	0.63
1:A:79:GLU:HB3	2:A:577:HOH:O	1.99	0.63
1:A:88:ASN:O	1:A:92:ILE:HG12	1.99	0.63
1:B:471:ILE:HD11	1:B:503:THR:HB	1.81	0.63
1:B:49:VAL:O	1:B:52:SER:HB3	1.99	0.63
1:B:320:GLU:HB3	1:B:536:ILE:CG2	2.29	0.63
1:B:296:LYS:HA	1:B:296:LYS:HE3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ASP:CB	2:A:587:HOH:O	2.48	0.62
1:B:238:PRO:O	1:B:239:ILE:HB	2.00	0.62
1:B:402:ARG:HB3	1:B:430:TYR:CE1	2.35	0.62
1:B:540:LEU:N	1:B:540:LEU:HD12	2.14	0.62
1:A:564:GLU:HG2	1:A:565:VAL:N	2.15	0.61
1:B:18:LEU:CD1	1:B:60:VAL:HB	2.30	0.61
1:B:439:MET:HG2	1:B:440:GLY:N	2.14	0.61
1:A:132:VAL:HG13	1:A:143:ILE:CD1	2.31	0.61
1:A:291:LYS:HG3	1:A:292:PRO:HD2	1.81	0.61
1:A:29:TYR:CE2	1:A:48:LYS:HD2	2.35	0.61
1:A:558:LYS:HG3	1:A:559:GLU:H	1.65	0.61
1:B:539:PRO:HG2	1:B:540:LEU:HD12	1.83	0.61
1:A:81:LYS:O	1:A:85:ILE:HG12	2.00	0.61
1:B:106:ILE:HD11	1:B:135:MET:SD	2.41	0.61
1:A:346:ALA:O	1:A:350:VAL:HG23	2.01	0.60
1:A:295:ARG:HG2	1:A:295:ARG:HH21	1.67	0.60
1:A:521:THR:O	1:A:525:VAL:HG23	2.02	0.60
1:A:70:ARG:NE	2:A:636:HOH:O	2.35	0.60
1:A:108:PRO:HB2	2:A:661:HOH:O	2.01	0.60
1:B:349:GLN:HB2	1:B:357:LEU:HD21	1.83	0.60
1:A:186:THR:HA	2:A:609:HOH:O	2.01	0.59
1:B:106:ILE:HD12	1:B:131:THR:HG21	1.83	0.59
1:B:372:VAL:HG11	1:B:396:LEU:CD1	2.29	0.59
1:B:70:ARG:HH21	1:B:70:ARG:HG3	1.67	0.59
1:B:440:GLY:O	1:B:442:ASP:N	2.35	0.59
1:B:445:LYS:HG2	1:B:482:GLU:OE1	2.02	0.59
1:A:174:MET:HG3	1:A:191:PHE:CE1	2.37	0.59
1:B:2:ARG:HD3	1:B:2:ARG:N	2.16	0.59
1:A:145:PHE:HB3	1:A:148:PHE:CE1	2.37	0.59
1:A:178:GLU:HG2	2:A:666:HOH:O	2.03	0.59
1:A:479:LEU:HG	1:A:509:LEU:HD22	1.84	0.59
1:B:88:ASN:O	1:B:92:ILE:HG13	2.02	0.58
1:A:565:VAL:HG13	1:A:565:VAL:O	2.03	0.58
1:A:438:LEU:HD12	1:A:474:PRO:HA	1.85	0.58
1:A:360:ASN:CB	1:A:390:ASP:HB3	2.34	0.58
1:B:320:GLU:HG3	1:B:537:MET:O	2.04	0.58
1:B:479:LEU:CD2	1:B:479:LEU:H	2.16	0.58
1:A:162:ARG:NH1	1:A:170:LEU:HB2	2.18	0.58
1:B:444:PRO:HD3	1:B:453:TYR:HE1	1.68	0.58
1:A:166:ARG:HH21	1:A:166:ARG:CB	2.09	0.57
1:A:147:THR:HG22	1:A:147:THR:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASP:O	1:B:443:VAL:HG23	2.02	0.57
1:B:27:MET:HE3	2:B:639:HOH:O	2.03	0.57
1:A:345:GLU:O	1:A:349:GLN:HG3	2.05	0.57
1:A:99:GLU:HA	1:A:99:GLU:OE1	2.03	0.57
1:A:252:HIS:O	1:A:256:VAL:HG13	2.05	0.57
1:A:70:ARG:HD3	1:A:130:GLU:CD	2.24	0.57
1:B:209:LEU:HB2	1:B:214:ILE:CD1	2.34	0.57
1:A:483:GLY:O	1:A:484:LYS:HD2	2.04	0.57
1:B:243:GLY:O	1:B:244:LYS:O	2.22	0.57
1:A:207:CYS:O	1:A:208:SER:HB2	2.05	0.57
1:B:439:MET:CG	1:B:440:GLY:N	2.68	0.57
1:B:412:SER:H	1:B:435:ILE:HB	1.69	0.56
1:B:26:PHE:O	1:B:31:TYR:HB2	2.06	0.56
1:A:276:THR:HG22	2:A:589:HOH:O	2.05	0.56
1:B:479:LEU:HA	1:B:483:GLY:CA	2.36	0.56
1:B:341:ILE:HG23	1:B:342:VAL:N	2.21	0.56
1:B:435:ILE:CD1	1:B:471:ILE:HG12	2.34	0.56
1:A:551:THR:HG22	1:A:555:LEU:HD12	1.88	0.56
1:A:3:ASN:O	1:A:7:VAL:HG23	2.06	0.56
1:A:192:ALA:HB2	1:A:221:LEU:HD12	1.86	0.56
1:B:205:ILE:HD13	1:B:217:ILE:HG22	1.87	0.56
1:B:125:TYR:CE1	1:B:160:ALA:HA	2.41	0.55
1:A:370:ARG:NH2	1:A:370:ARG:HB2	2.20	0.55
1:A:92:ILE:O	1:A:95:ARG:HB2	2.06	0.55
1:A:441:LYS:HG3	2:A:571:HOH:O	2.05	0.55
1:A:209:LEU:HB2	1:A:214:ILE:CG1	2.35	0.55
1:B:484:LYS:N	1:B:485:PRO:HD3	2.21	0.55
1:B:155:LYS:O	1:B:159:LEU:HB2	2.06	0.55
1:A:251:PRO:O	1:A:282:LEU:HD22	2.07	0.55
1:A:4:ARG:NH1	1:A:162:ARG:CZ	2.69	0.55
1:B:29:TYR:HE1	1:B:48:LYS:HD3	1.71	0.55
1:B:295:ARG:HH21	1:B:295:ARG:HG3	1.72	0.55
1:A:332:ALA:O	1:A:336:LYS:HG3	2.07	0.55
1:B:252:HIS:O	1:B:256:VAL:HG13	2.07	0.54
1:B:18:LEU:HD12	1:B:60:VAL:HB	1.88	0.54
1:B:209:LEU:HB3	1:B:213:GLU:HB2	1.89	0.54
1:B:114:TYR:CD1	1:B:115:PRO:HA	2.43	0.54
1:A:121:PHE:HZ	1:A:159:LEU:HD12	1.73	0.54
1:A:162:ARG:NH1	1:A:170:LEU:HD12	2.22	0.54
1:B:3:ASN:OD1	1:B:5:ARG:HB2	2.08	0.54
1:A:513:LEU:O	1:A:516:ARG:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLU:HG2	1:B:464:HIS:NE2	2.23	0.54
1:B:95:ARG:HG2	1:B:95:ARG:HH11	1.72	0.53
1:B:192:ALA:HB2	1:B:221:LEU:HD12	1.90	0.53
1:A:266:VAL:HG22	1:A:267:ASN:N	2.23	0.53
1:A:398:GLU:HG3	1:A:426:LEU:HD22	1.90	0.53
1:A:438:LEU:HD11	1:A:495:ILE:HD11	1.91	0.53
1:A:176:PHE:CE1	1:A:205:ILE:HD12	2.44	0.53
1:B:208:SER:H	1:B:234:ASN:HD21	1.57	0.53
1:B:416:ASP:O	1:B:418:GLU:N	2.41	0.53
1:B:458:LEU:O	1:B:462:GLU:HB2	2.07	0.53
1:A:151:ILE:HG22	1:A:195:PHE:HE1	1.74	0.53
1:A:358:ASP:HA	1:A:388:SER:HB3	1.90	0.53
1:B:474:PRO:HD2	1:B:503:THR:O	2.09	0.53
1:B:551:THR:HG22	1:B:555:LEU:CD2	2.38	0.53
1:A:321:ARG:HD2	1:A:540:LEU:HD22	1.90	0.53
1:A:151:ILE:O	1:A:155:LYS:HB2	2.08	0.53
1:A:240:VAL:HG23	1:A:240:VAL:O	2.09	0.53
1:A:383:SER:O	1:A:384:ASN:HB2	2.09	0.53
1:B:413:ALA:HB2	1:B:434:LEU:HD11	1.91	0.53
1:A:235:ALA:HB3	1:A:247:TYR:HB3	1.90	0.53
1:A:284:ARG:HE	1:A:284:ARG:CA	2.18	0.53
1:B:191:PHE:CZ	1:B:203:LEU:HD12	2.44	0.53
1:B:404:TYR:CD1	1:B:408:SER:HB3	2.44	0.53
1:A:251:PRO:HB3	1:A:282:LEU:HD13	1.90	0.52
1:B:61:ILE:HD11	1:B:97:ALA:HB2	1.91	0.52
1:A:202:ALA:HB2	1:A:228:PHE:HB2	1.91	0.52
1:A:296:LYS:HA	1:A:296:LYS:HZ2	1.69	0.52
1:A:126:GLU:OE1	1:A:129:ARG:NH1	2.42	0.52
1:A:345:GLU:HG2	2:A:651:HOH:O	2.08	0.52
1:B:282:LEU:HD23	1:B:282:LEU:O	2.09	0.52
1:B:173:HIS:CD2	1:B:204:GLY:HA3	2.44	0.52
1:B:479:LEU:H	1:B:479:LEU:HD23	1.74	0.52
1:B:524:LEU:O	1:B:528:ILE:HG13	2.09	0.52
1:A:151:ILE:HD11	1:A:306:PRO:CA	2.36	0.52
1:A:151:ILE:HG22	1:A:195:PHE:CE1	2.45	0.52
1:B:538:ASN:OD1	1:B:540:LEU:HB2	2.10	0.52
1:B:14:ARG:HA	1:B:290:ARG:O	2.08	0.52
1:B:81:LYS:C	1:B:84:PRO:HD2	2.30	0.52
1:B:106:ILE:O	1:B:145:PHE:HA	2.10	0.52
1:A:176:PHE:HE1	1:A:205:ILE:HD12	1.75	0.52
1:B:508:ASN:O	1:B:509:LEU:HD13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:THR:HG22	1:B:555:LEU:HD23	1.92	0.51
1:A:212:GLU:HB3	1:A:213:GLU:OE2	2.10	0.51
1:A:411:ASN:O	1:A:412:SER:HB2	2.09	0.51
1:B:479:LEU:HD23	1:B:479:LEU:N	2.26	0.51
1:A:11:LEU:HD21	1:A:268:ILE:HD11	1.91	0.51
1:A:46:VAL:HG12	1:A:92:ILE:HG21	1.91	0.51
1:A:188:PRO:HB2	1:A:220:GLU:HB3	1.92	0.51
1:A:487:GLU:OE1	1:A:487:GLU:HA	2.11	0.51
1:B:422:MET:HE3	1:B:426:LEU:HD12	1.91	0.51
1:A:62:LEU:HD22	1:A:144:ILE:HG21	1.93	0.51
1:B:18:LEU:HB3	1:B:270:GLY:HA3	1.93	0.51
1:B:31:TYR:CE2	1:B:45:VAL:HG21	2.45	0.51
1:B:83:ASP:HB3	1:B:84:PRO:HD3	1.92	0.51
1:B:131:THR:O	1:B:135:MET:HG3	2.11	0.51
1:A:262:TYR:O	1:A:293:LEU:HD22	2.11	0.51
1:B:213:GLU:O	1:B:216:PRO:HD2	2.11	0.51
1:A:282:LEU:O	1:A:285:LYS:N	2.43	0.51
1:A:410:PHE:HE2	1:A:423:LYS:HD2	1.75	0.51
1:B:205:ILE:CD1	1:B:217:ILE:HG22	2.41	0.51
1:A:439:MET:HG3	1:A:439:MET:O	2.11	0.51
1:A:539:PRO:HG2	1:A:540:LEU:HD12	1.93	0.51
1:B:125:TYR:OH	1:B:163:GLU:HG2	2.11	0.51
1:A:379:LEU:HB2	1:A:380:PRO:HD3	1.92	0.50
1:A:323:ASN:CG	1:A:323:ASN:O	2.49	0.50
1:A:70:ARG:HG2	2:A:578:HOH:O	2.12	0.50
1:A:241:GLU:HB2	1:A:246:VAL:HG21	1.92	0.50
1:A:510:SER:HA	1:A:513:LEU:HD21	1.94	0.50
1:B:480:GLY:O	1:B:481:ALA:HB2	2.12	0.50
1:B:48:LYS:HE2	1:B:49:VAL:N	2.26	0.50
1:B:91:ARG:NE	1:B:138:GLU:OE2	2.44	0.50
1:B:441:LYS:HE3	1:B:453:TYR:HE2	1.76	0.50
1:B:521:THR:O	1:B:525:VAL:HG23	2.11	0.50
1:B:324:PRO:HB3	1:B:331:TRP:HE3	1.75	0.50
1:A:62:LEU:HB3	1:A:105:ASP:HB2	1.94	0.50
1:A:251:PRO:C	1:A:282:LEU:HD22	2.31	0.50
1:B:322:ILE:HG22	1:B:322:ILE:O	2.11	0.50
1:B:467:SER:O	1:B:470:VAL:HG22	2.11	0.50
1:B:492:ILE:HD12	1:B:532:LEU:HD13	1.93	0.50
1:A:378:THR:HG22	1:A:379:LEU:N	2.27	0.50
1:A:391:ILE:HG21	1:A:396:LEU:HB3	1.94	0.50
1:A:292:PRO:HA	2:A:602:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HG2	1:A:321:ARG:HH21	1.77	0.50
1:B:34:LEU:HD11	1:B:76:HIS:CD2	2.47	0.50
1:B:479:LEU:HD22	1:B:509:LEU:CG	2.41	0.49
1:A:149:SER:HB3	1:A:183:LEU:HB3	1.94	0.49
1:B:238:PRO:O	1:B:239:ILE:CB	2.60	0.49
1:A:158:VAL:HG23	1:A:159:LEU:N	2.26	0.49
1:A:244:LYS:O	1:A:245:THR:HG23	2.12	0.49
1:A:263:GLU:HA	1:A:293:LEU:CD2	2.42	0.49
1:B:338:ASN:HD22	1:B:339:GLU:H	1.59	0.49
1:B:200:ILE:H	1:B:200:ILE:HD13	1.75	0.49
1:A:95:ARG:HD2	2:A:569:HOH:O	2.11	0.49
1:A:487:GLU:OE1	1:A:490:LYS:HD3	2.12	0.49
1:B:149:SER:HB3	1:B:183:LEU:HB3	1.93	0.49
1:B:331:TRP:HH2	1:B:363:ILE:O	1.96	0.49
1:A:295:ARG:HG2	1:A:295:ARG:NH2	2.26	0.49
1:B:486:VAL:HG22	1:B:490:LYS:HZ2	1.78	0.49
1:A:188:PRO:CG	1:A:217:ILE:HG23	2.43	0.49
1:B:427:LEU:CD1	1:B:434:LEU:HB2	2.43	0.49
1:B:151:ILE:HD11	1:B:306:PRO:CG	2.39	0.49
1:A:306:PRO:HG3	1:A:405:PRO:HB2	1.94	0.48
1:A:409:LEU:HD22	1:A:435:ILE:HG13	1.95	0.48
1:B:70:ARG:HH21	1:B:70:ARG:CG	2.25	0.48
1:B:259:ASP:O	1:B:263:GLU:CG	2.49	0.48
1:B:422:MET:HE2	1:B:423:LYS:HG3	1.95	0.48
1:B:528:ILE:HD11	1:B:548:LEU:CD1	2.43	0.48
1:A:130:GLU:O	1:A:134:ILE:HG12	2.13	0.48
1:A:486:VAL:O	1:A:490:LYS:HG3	2.13	0.48
1:B:207:CYS:HG	1:B:272:CYS:HG	1.60	0.48
1:B:410:PHE:HE2	1:B:423:LYS:HD3	1.78	0.48
1:A:47:LEU:HD12	1:A:96:ALA:HB2	1.94	0.48
1:A:295:ARG:HG3	2:A:659:HOH:O	2.11	0.48
1:A:36:GLU:O	1:A:85:ILE:HG23	2.13	0.48
1:B:211:PRO:HG3	1:B:254:PHE:CE1	2.48	0.48
1:B:420:LEU:C	1:B:424:ILE:HD13	2.34	0.48
1:A:255:ALA:O	1:A:258:ILE:HD13	2.14	0.48
1:A:255:ALA:HB1	1:A:286:VAL:HG21	1.96	0.48
1:A:561:PRO:O	1:A:562:ARG:HB2	2.14	0.48
1:A:114:TYR:HE2	1:A:374:LYS:HZ1	1.55	0.48
1:B:3:ASN:CG	1:B:5:ARG:HD3	2.34	0.48
1:B:338:ASN:ND2	1:B:339:GLU:N	2.61	0.48
1:B:489:LEU:HD21	1:B:523:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLY:O	1:A:469:ARG:NH2	2.45	0.48
1:B:211:PRO:HD3	1:B:234:ASN:O	2.14	0.48
1:B:238:PRO:O	1:B:246:VAL:O	2.32	0.48
1:B:321:ARG:HG3	1:B:540:LEU:HD13	1.95	0.48
1:A:45:VAL:O	1:A:49:VAL:HG23	2.13	0.48
1:A:46:VAL:CG1	1:A:92:ILE:HG21	2.43	0.48
1:A:155:LYS:O	1:A:159:LEU:HG	2.14	0.48
1:B:486:VAL:HG22	1:B:490:LYS:NZ	2.29	0.48
1:A:54:ILE:HD13	1:A:96:ALA:C	2.34	0.47
1:A:186:THR:HG23	1:A:190:ASN:HB3	1.94	0.47
1:A:521:THR:CG2	1:A:547:THR:HG21	2.44	0.47
1:B:306:PRO:HD3	1:B:405:PRO:O	2.14	0.47
1:B:379:LEU:HB2	1:B:380:PRO:HD3	1.96	0.47
1:A:454:PHE:CE2	1:A:458:LEU:HD12	2.50	0.47
1:B:402:ARG:HB3	1:B:430:TYR:CD1	2.48	0.47
1:A:221:LEU:O	1:A:225:THR:HG22	2.14	0.47
1:A:237:LYS:HE3	2:A:630:HOH:O	2.14	0.47
1:A:114:TYR:CE2	1:A:374:LYS:NZ	2.75	0.47
1:A:414:LYS:HB3	1:A:439:MET:O	2.15	0.47
1:A:560:LEU:HA	1:A:561:PRO:HD3	1.56	0.47
1:B:420:LEU:HD12	1:B:460:ILE:HD12	1.97	0.47
1:A:564:GLU:HG2	1:A:565:VAL:H	1.79	0.47
1:A:200:ILE:CD1	1:A:203:LEU:HD21	2.44	0.47
1:A:244:LYS:HG3	1:A:245:THR:N	2.28	0.47
1:A:321:ARG:HD2	1:A:540:LEU:HD13	1.95	0.47
1:A:427:LEU:O	1:A:431:GLY:N	2.46	0.47
1:B:324:PRO:HB3	1:B:331:TRP:CE3	2.50	0.47
1:B:338:ASN:HD22	1:B:339:GLU:N	2.12	0.47
1:A:444:PRO:CB	1:A:449:GLU:HG2	2.39	0.47
1:B:445:LYS:HB2	1:B:449:GLU:OE2	2.15	0.47
1:A:324:PRO:O	1:A:331:TRP:HB2	2.15	0.46
1:A:564:GLU:O	1:A:565:VAL:HG12	2.15	0.46
1:B:29:TYR:HD2	1:B:29:TYR:N	2.13	0.46
1:B:145:PHE:HB3	1:B:148:PHE:CE1	2.49	0.46
1:B:558:LYS:HB2	2:B:641:HOH:O	2.15	0.46
1:A:412:SER:O	1:A:413:ALA:HB2	2.14	0.46
1:B:188:PRO:HG3	1:B:217:ILE:HG23	1.97	0.46
1:B:222:SER:HB3	1:B:229:LEU:CD1	2.45	0.46
1:A:208:SER:O	1:A:209:LEU:HD23	2.15	0.46
1:A:150:ASP:OD2	1:A:152:LEU:HB3	2.14	0.46
1:A:151:ILE:CD1	1:A:306:PRO:HA	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ILE:HG22	1:A:392:GLN:N	2.31	0.46
1:B:60:VAL:HG11	1:B:103:PHE:CD2	2.50	0.46
1:A:321:ARG:O	1:A:323:ASN:N	2.49	0.46
1:A:551:THR:HG22	1:A:555:LEU:CD1	2.45	0.46
1:A:81:LYS:O	1:A:85:ILE:CG1	2.63	0.46
1:A:228:PHE:HD2	1:A:267:ASN:ND2	2.13	0.46
1:A:441:LYS:NZ	1:A:441:LYS:HB3	2.31	0.46
1:A:546:LYS:HD2	1:B:518:TYR:CZ	2.51	0.46
1:A:239:ILE:HG13	1:A:248:PRO:HD3	1.98	0.46
1:A:24:THR:O	1:A:28:LYS:HG3	2.16	0.46
1:A:155:LYS:O	1:A:158:VAL:HG22	2.16	0.46
1:B:341:ILE:CG2	1:B:342:VAL:N	2.79	0.46
1:B:38:LEU:C	1:B:40:ILE:N	2.69	0.46
1:B:346:ALA:O	1:B:350:VAL:HG23	2.16	0.46
1:B:113:PRO:O	1:B:116:LEU:N	2.49	0.45
1:B:95:ARG:HG2	1:B:95:ARG:NH1	2.30	0.45
1:B:188:PRO:HB2	1:B:220:GLU:HB3	1.99	0.45
1:A:173:HIS:ND1	1:A:206:ASN:OD1	2.42	0.45
1:A:238:PRO:HB3	1:A:247:TYR:CE1	2.51	0.45
1:B:18:LEU:HD12	1:B:60:VAL:O	2.17	0.45
1:B:81:LYS:O	1:B:85:ILE:HG13	2.17	0.45
1:A:402:ARG:HG2	1:A:430:TYR:CZ	2.51	0.45
1:B:1:MET:CA	2:B:580:HOH:O	2.64	0.45
1:B:34:LEU:HD11	1:B:76:HIS:HD2	1.82	0.45
1:B:208:SER:N	1:B:234:ASN:HD21	2.15	0.45
1:B:420:LEU:O	1:B:423:LYS:N	2.48	0.45
1:A:367:ILE:HD13	1:A:368:ASP:N	2.31	0.45
1:B:145:PHE:HZ	1:B:161:ALA:HB2	1.82	0.45
1:A:230:VAL:HG22	1:A:268:ILE:HB	1.98	0.45
1:B:260:SER:HA	1:B:263:GLU:HG3	1.98	0.45
1:A:457:ALA:O	1:A:461:LEU:HG	2.16	0.45
1:B:416:ASP:O	1:B:417:GLU:C	2.56	0.45
1:A:249:LEU:HD23	1:A:254:PHE:CD2	2.51	0.44
1:A:531:GLY:O	1:A:532:LEU:C	2.55	0.44
1:B:29:TYR:N	1:B:29:TYR:CD2	2.84	0.44
1:B:479:LEU:CD2	1:B:479:LEU:N	2.80	0.44
1:A:409:LEU:CD2	1:A:435:ILE:HG13	2.47	0.44
1:B:397:THR:O	1:B:400:ALA:HB3	2.16	0.44
1:A:51:ARG:O	1:A:55:GLU:HG3	2.18	0.44
1:A:71:MET:SD	1:A:109:THR:HG21	2.57	0.44
1:B:324:PRO:HG2	1:B:362:GLY:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:HB2	2:B:574:HOH:O	2.17	0.44
1:A:445:LYS:HE3	1:A:449:GLU:OE2	2.18	0.44
1:B:73:LEU:HD22	1:B:78:LEU:HB2	1.99	0.44
1:B:506:LEU:HD12	1:B:506:LEU:HA	1.86	0.44
1:B:255:ALA:HB2	1:B:282:LEU:HD22	1.98	0.44
1:B:282:LEU:HD23	1:B:286:VAL:HG23	2.00	0.44
1:A:188:PRO:HG3	1:A:217:ILE:HG23	1.99	0.44
1:B:145:PHE:CD2	1:B:157:ALA:HB1	2.52	0.44
1:B:180:GLY:O	1:B:181:ARG:HG2	2.16	0.44
1:B:70:ARG:CG	1:B:70:ARG:NH2	2.79	0.44
1:B:235:ALA:HB3	1:B:247:TYR:HB3	2.00	0.44
1:B:282:LEU:CD2	1:B:286:VAL:HG23	2.48	0.44
1:A:44:ASP:OD2	1:A:44:ASP:N	2.51	0.44
1:A:524:LEU:HD21	1:A:548:LEU:HG	1.99	0.44
1:B:145:PHE:CE2	1:B:157:ALA:HB1	2.53	0.44
1:A:76:HIS:ND1	1:A:76:HIS:N	2.66	0.43
1:A:236:GLY:HA3	1:A:249:LEU:HB2	2.01	0.43
1:A:258:ILE:N	1:A:258:ILE:HD12	2.33	0.43
1:B:75:LYS:C	1:B:76:HIS:ND1	2.71	0.43
1:B:177:ASP:OD1	1:B:179:LYS:N	2.51	0.43
1:B:324:PRO:HD3	1:B:360:ASN:O	2.18	0.43
1:A:125:TYR:CD1	1:A:125:TYR:C	2.91	0.43
1:A:340:GLU:OE2	1:A:340:GLU:HA	2.18	0.43
1:B:24:THR:HG22	1:B:28:LYS:HE3	2.01	0.43
1:B:61:ILE:CD1	1:B:97:ALA:HB2	2.48	0.43
1:B:441:LYS:HE3	1:B:453:TYR:CE2	2.52	0.43
1:A:369:VAL:HG12	2:A:628:HOH:O	2.18	0.43
1:B:45:VAL:O	1:B:49:VAL:HG23	2.19	0.43
1:B:207:CYS:O	1:B:208:SER:HB2	2.18	0.43
1:A:209:LEU:HD12	1:A:214:ILE:HD13	2.00	0.43
1:A:322:ILE:HG21	1:A:359:VAL:HG13	2.00	0.43
1:A:323:ASN:ND2	1:A:325:ALA:HB3	2.34	0.43
1:A:410:PHE:CE2	1:A:423:LYS:HD2	2.53	0.43
1:B:347:LYS:O	1:B:351:GLU:HG3	2.17	0.43
1:A:561:PRO:O	1:A:562:ARG:CB	2.67	0.43
1:B:1:MET:HA	2:B:580:HOH:O	2.17	0.43
1:B:484:LYS:N	1:B:485:PRO:CD	2.82	0.43
1:B:154:LEU:O	1:B:158:VAL:HG22	2.19	0.43
1:B:174:MET:HG3	1:B:191:PHE:CE1	2.53	0.43
1:B:255:ALA:HB1	1:B:286:VAL:HG21	2.00	0.43
1:A:154:LEU:HG	1:A:195:PHE:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLU:O	1:B:402:ARG:HG2	2.18	0.43
1:A:248:PRO:O	1:A:249:LEU:C	2.56	0.43
1:B:340:GLU:O	1:B:344:LYS:HB2	2.19	0.43
1:B:420:LEU:HD22	1:B:424:ILE:HD11	2.01	0.43
1:B:463:ARG:HD3	2:B:635:HOH:O	2.19	0.43
1:B:199:ASP:CG	1:B:199:ASP:O	2.55	0.43
1:B:219:GLN:HG2	1:B:223:GLN:HE21	1.84	0.43
1:A:339:GLU:O	1:A:343:ILE:HG13	2.19	0.42
1:B:493:GLU:HB2	1:B:530:LYS:HD2	2.00	0.42
1:B:422:MET:CE	1:B:426:LEU:HD12	2.48	0.42
1:B:537:MET:CE	1:B:548:LEU:HD22	2.48	0.42
1:A:26:PHE:CE1	1:A:49:VAL:HG21	2.54	0.42
1:A:234:ASN:OD1	1:A:273:CYS:HB2	2.18	0.42
1:A:325:ALA:HB2	1:A:360:ASN:HD21	1.84	0.42
1:A:443:VAL:HG11	1:A:477:LEU:HD11	2.01	0.42
1:A:532:LEU:HD11	1:A:534:SER:O	2.18	0.42
1:A:541:ASP:CG	1:A:544:LEU:HB2	2.39	0.42
1:B:386:PRO:HA	1:B:404:TYR:OH	2.20	0.42
1:A:162:ARG:HA	1:A:162:ARG:HD3	1.85	0.42
1:A:175:THR:O	1:A:175:THR:HG23	2.19	0.42
1:A:437:LEU:HG	1:A:439:MET:HG2	2.01	0.42
1:B:149:SER:HB3	1:B:183:LEU:CB	2.49	0.42
1:B:251:PRO:C	1:B:282:LEU:HD13	2.39	0.42
1:B:479:LEU:O	1:B:481:ALA:N	2.51	0.42
1:B:488:VAL:O	1:B:491:THR:N	2.52	0.42
1:A:503:THR:HA	1:A:534:SER:O	2.19	0.42
1:B:540:LEU:N	1:B:540:LEU:CD1	2.82	0.42
1:A:266:VAL:HG22	1:A:267:ASN:H	1.85	0.42
1:B:257:HIS:O	1:B:258:ILE:C	2.57	0.42
1:B:451:LYS:HG3	1:B:494:PHE:CE2	2.54	0.42
1:B:38:LEU:C	1:B:40:ILE:H	2.23	0.42
1:B:151:ILE:O	1:B:155:LYS:HB2	2.20	0.42
1:B:420:LEU:HD23	1:B:420:LEU:HA	1.91	0.42
1:A:255:ALA:HA	1:A:258:ILE:HD13	2.00	0.42
1:B:247:TYR:O	1:B:248:PRO:O	2.38	0.42
1:B:411:ASN:O	1:B:412:SER:HB3	2.20	0.42
1:B:255:ALA:HA	1:B:258:ILE:HD13	2.02	0.42
1:B:263:GLU:HG2	1:B:263:GLU:H	1.48	0.42
1:A:82:LEU:O	1:A:82:LEU:HD22	2.20	0.42
1:A:445:LYS:HB3	2:A:605:HOH:O	2.20	0.42
1:A:479:LEU:HD12	1:A:513:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:C	1:B:29:TYR:HD2	2.23	0.42
1:B:393:ASN:HD22	1:B:396:LEU:HB2	1.85	0.42
1:B:132:VAL:HG13	1:B:143:ILE:HD13	1.99	0.41
1:B:321:ARG:HB3	1:B:345:GLU:OE2	2.20	0.41
1:B:330:LEU:C	1:B:332:ALA:N	2.73	0.41
1:B:388:SER:HA	1:B:409:LEU:O	2.19	0.41
1:A:295:ARG:O	1:A:296:LYS:O	2.37	0.41
1:B:10:LEU:HD12	1:B:10:LEU:O	2.20	0.41
1:B:53:TYR:CD2	1:B:280:VAL:HG21	2.56	0.41
1:A:162:ARG:CZ	1:A:170:LEU:HD12	2.50	0.41
1:B:162:ARG:HA	1:B:162:ARG:HD3	1.78	0.41
1:B:375:ILE:HD13	1:B:375:ILE:HA	1.88	0.41
1:A:249:LEU:HD23	1:A:254:PHE:CG	2.55	0.41
1:A:258:ILE:HD12	1:A:258:ILE:H	1.85	0.41
1:B:81:LYS:HA	1:B:81:LYS:HD3	1.78	0.41
1:A:279:HIS:HB3	1:A:283:PHE:CZ	2.54	0.41
1:A:562:ARG:NE	1:A:562:ARG:CA	2.81	0.41
1:B:11:LEU:HD12	1:B:11:LEU:HA	1.96	0.41
1:B:321:ARG:NH1	1:B:538:ASN:HB2	2.35	0.41
1:A:1:MET:O	1:A:2:ARG:HB2	2.20	0.41
1:A:145:PHE:O	1:A:173:HIS:HB2	2.21	0.41
1:A:255:ALA:HA	1:A:258:ILE:CD1	2.50	0.41
1:B:26:PHE:CE1	1:B:49:VAL:HG21	2.56	0.41
1:B:324:PRO:HG3	1:B:334:MET:CE	2.51	0.41
1:B:255:ALA:HA	1:B:258:ILE:CD1	2.50	0.41
1:B:463:ARG:HD2	2:B:613:HOH:O	2.20	0.41
1:A:152:LEU:CD2	1:A:377:GLN:HG3	2.50	0.41
1:A:200:ILE:HD11	1:A:203:LEU:HD21	2.03	0.41
1:B:443:VAL:O	1:B:443:VAL:HG12	2.21	0.41
1:A:282:LEU:O	1:A:283:PHE:C	2.59	0.41
1:B:59:ASP:HA	1:B:100:LYS:HG3	2.02	0.41
1:B:73:LEU:HD22	1:B:78:LEU:CB	2.51	0.41
1:B:262:TYR:CZ	1:B:293:LEU:HD13	2.56	0.41
1:B:262:TYR:HA	1:B:266:VAL:HG12	2.02	0.41
1:B:409:LEU:HD11	1:B:435:ILE:CD1	2.51	0.41
1:B:439:MET:CG	1:B:443:VAL:HG22	2.51	0.41
1:A:18:LEU:HB2	1:A:270:GLY:HA3	2.02	0.41
1:A:28:LYS:NZ	2:A:665:HOH:O	2.44	0.41
1:A:240:VAL:HB	1:A:243:GLY:CA	2.51	0.41
1:A:501:ASN:HD22	1:A:501:ASN:HA	1.54	0.41
1:B:369:VAL:O	1:B:369:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HG3	2:A:635:HOH:O	2.20	0.40
1:B:40:ILE:HD13	1:B:88:ASN:ND2	2.36	0.40
1:B:329:LYS:HD2	1:B:329:LYS:HA	1.91	0.40
1:B:361:PHE:CE1	1:B:372:VAL:HG13	2.56	0.40
1:A:76:HIS:O	1:A:78:LEU:HG	2.22	0.40
1:A:83:ASP:HB3	1:A:84:PRO:CD	2.51	0.40
1:A:123:GLU:HB2	2:A:618:HOH:O	2.20	0.40
1:A:391:ILE:CG2	1:A:396:LEU:HB3	2.51	0.40
1:A:540:LEU:HD12	1:A:540:LEU:N	2.36	0.40
1:B:51:ARG:HG2	1:B:51:ARG:HH11	1.85	0.40
1:B:83:ASP:N	1:B:84:PRO:CD	2.84	0.40
1:B:272:CYS:HB3	1:B:273:CYS:H	1.55	0.40
1:B:345:GLU:O	1:B:349:GLN:HG3	2.21	0.40
1:B:404:TYR:CE1	1:B:408:SER:HB3	2.56	0.40
1:B:193:ILE:HD11	1:B:300:ILE:HD11	2.03	0.40
1:A:181:ARG:HD2	1:A:185:GLY:O	2.20	0.40
1:A:539:PRO:HG2	1:A:540:LEU:CD1	2.51	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	563/566 (100%)	490 (87%)	61 (11%)	12 (2%)	7	30
1	B	548/566 (97%)	462 (84%)	69 (13%)	17 (3%)	4	23
All	All	1111/1132 (98%)	952 (86%)	130 (12%)	29 (3%)	5	26

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS

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Mol	Chain	Res	Type
1	A	413	ALA
1	B	238	PRO
1	B	244	LYS
1	B	248	PRO
1	B	417	GLU
1	B	443	VAL
1	B	444	PRO
1	B	481	ALA
1	A	296	LYS
1	A	438	LEU
1	A	481	ALA
1	A	562	ARG
1	B	239	ILE
1	B	249	LEU
1	B	441	LYS
1	A	2	ARG
1	A	199	ASP
1	B	227	LYS
1	A	295	ARG
1	B	324	PRO
1	B	420	LEU
1	A	79	GLU
1	A	322	ILE
1	A	465	ASP
1	B	421	GLU
1	B	439	MET
1	B	542	GLU
1	B	35	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	492/494 (100%)	456 (93%)	36 (7%)	14	43
1	B	482/494 (98%)	445 (92%)	37 (8%)	13	41
All	All	974/988 (99%)	901 (92%)	73 (8%)	13	42

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	45	VAL
1	A	76	HIS
1	A	82	LEU
1	A	106	ILE
1	A	123	GLU
1	A	129	ARG
1	A	144	ILE
1	A	163	GLU
1	A	166	ARG
1	A	223	GLN
1	A	249	LEU
1	A	254	PHE
1	A	272	CYS
1	A	278	GLU
1	A	284	ARG
1	A	296	LYS
1	A	299	ARG
1	A	305	SER
1	A	323	ASN
1	A	360	ASN
1	A	367	ILE
1	A	370	ARG
1	A	396	LEU
1	A	409	LEU
1	A	445	LYS
1	A	458	LEU
1	A	459	LYS
1	A	463	ARG
1	A	501	ASN
1	A	506	LEU
1	A	509	LEU
1	A	513	LEU
1	A	548	LEU
1	A	558	LYS
1	A	562	ARG
1	B	2	ARG
1	B	34	LEU
1	B	48	LYS
1	B	61	ILE
1	B	70	ARG
1	B	94	ARG

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Mol	Chain	Res	Type
1	B	151	ILE
1	B	152	LEU
1	B	163	GLU
1	B	178	GLU
1	B	198	LEU
1	B	200	ILE
1	B	207	CYS
1	B	217	ILE
1	B	238	PRO
1	B	244	LYS
1	B	249	LEU
1	B	254	PHE
1	B	256	VAL
1	B	263	GLU
1	B	272	CYS
1	B	278	GLU
1	B	285	LYS
1	B	296	LYS
1	B	320	GLU
1	B	392	GLN
1	B	399	ARG
1	B	422	MET
1	B	442	ASP
1	B	444	PRO
1	B	448	GLU
1	B	471	ILE
1	B	479	LEU
1	B	509	LEU
1	B	516	ARG
1	B	537	MET
1	B	554	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	335	GLN
1	A	520	ASN
1	B	338	ASN
1	B	393	ASN
1	B	425	ASN
1	B	508	ASN

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 ⓘ

There are no ligands in this entry.

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	565/566 (99%)	-0.42	7 (1%)	79	61	30, 51, 85, 100	0
1	B	552/566 (97%)	-0.40	4 (0%)	87	75	29, 49, 81, 100	0
All	All	1117/1132 (98%)	-0.41	11 (0%)	82	67	29, 50, 82, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	GLY	4.7
1	A	241	GLU	2.9
1	A	561	PRO	2.9
1	A	242	ASN	2.7
1	B	242	ASN	2.6
1	A	240	VAL	2.5
1	A	563	ALA	2.4
1	B	241	GLU	2.4
1	B	30	GLY	2.3
1	B	245	THR	2.1
1	A	244	LYS	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.