



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:32 PM GMT

PDB ID : 3C7N
Title : Structure of the Hsp110:Hsc70 Nucleotide Exchange Complex
Authors : Schuermann, J.P.; Jiang, J.; Hart, P.J.; Sousa, R.
Deposited on : 2008-02-07
Resolution : 3.12 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

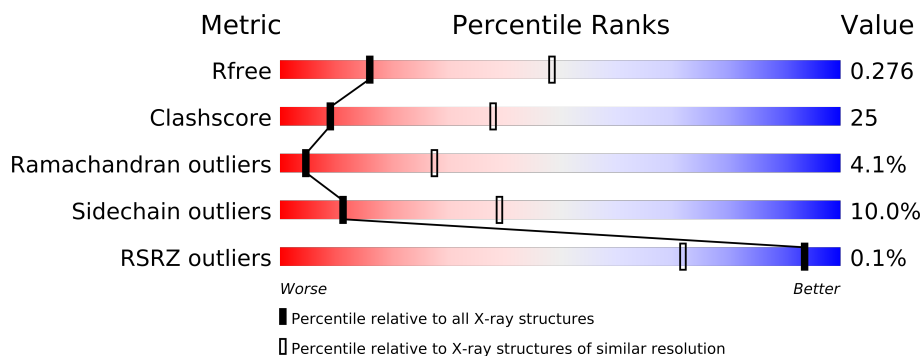
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.12 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}	66092	1466 (3.20-3.04)
Clashscore	79885	1067 (3.18-3.06)
Ramachandran outliers	78287	1034 (3.18-3.06)
Sidechain outliers	78261	1034 (3.18-3.06)
RSRZ outliers	66119	1468 (3.20-3.04)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	668	
2	B	554	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	667	-	X
3	MG	B	558	-	X
5	SO4	A	668	-	X
5	SO4	A	669	-	X
5	SO4	A	670	-	X
6	BEF	A	671	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9368 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Heat shock protein homolog SSE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5103	3227	853	1010	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P32589
A	0	PRO	-	EXPRESSION TAG	UNP P32589

- Molecule 2 is a protein called Heat shock cognate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	540	Total	C	N	O	S	0	0	0
			4182	2621	726	824	11			

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

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

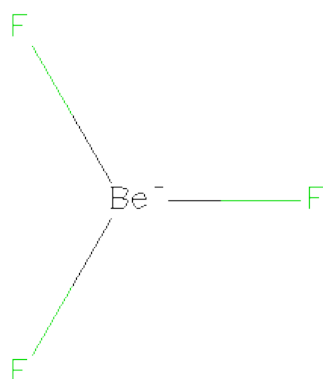
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Cl	0	0
			3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



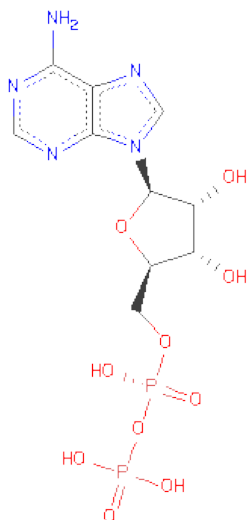
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Be	F	0	0
			4	1	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



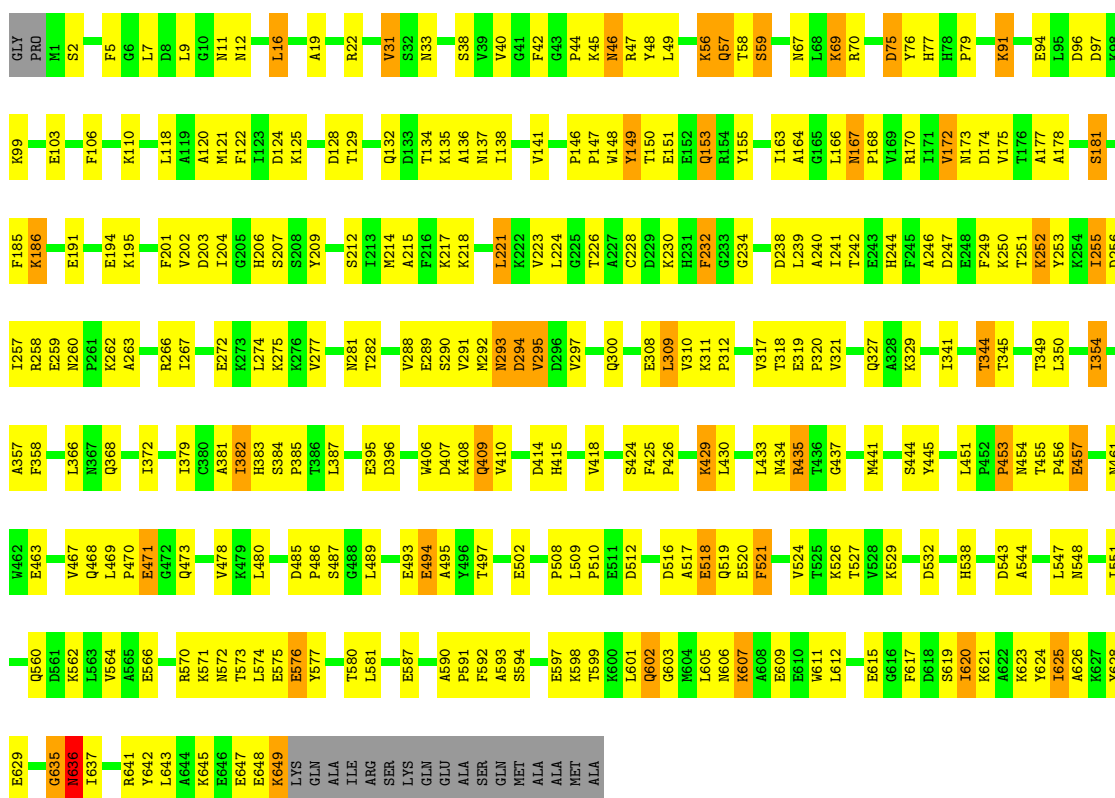
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

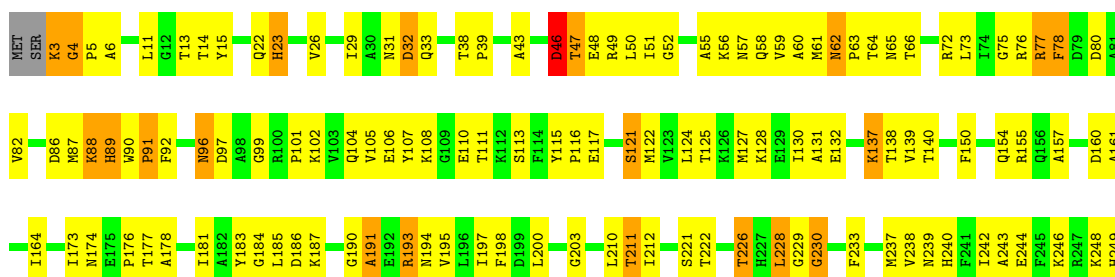
- Molecule 1: Heat shock protein homolog SSE1

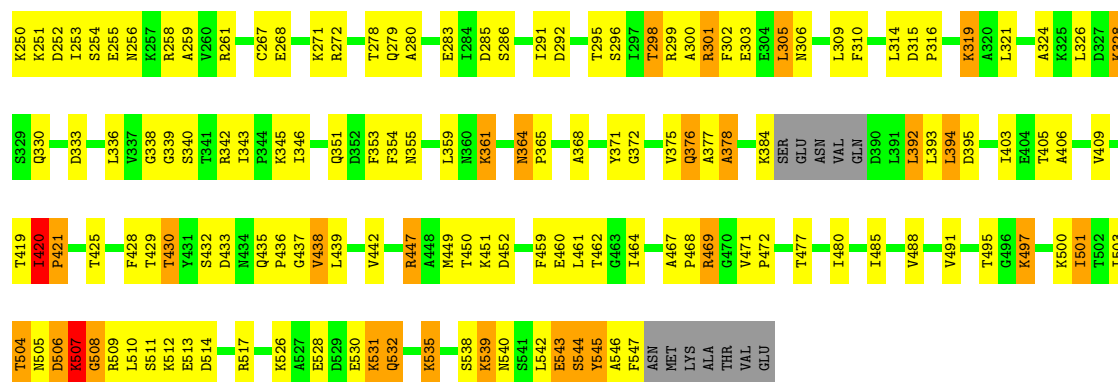
Chain A:



- Molecule 2: Heat shock cognate

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.53Å 169.50Å 87.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.38 – 3.12 42.38 – 3.12	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.38-3.12) 96.6 (42.38-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.283 0.216 , 0.276	Depositor DCC
R_{free} test set	1650 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 10.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 32506 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9368	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 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, SO4, ADP, CL

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	0.56	0/5199	0.70	0/7037
2	B	0.56	1/4242 (0.0%)	0.70	1/5728 (0.0%)
All	All	0.56	1/9441 (0.0%)	0.70	1/12765 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ARG	CG-CD	5.82	1.66	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ARG	NE-CZ-NH2	-5.67	117.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	420	ILE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5103	0	5079	245	0
2	B	4182	0	4209	243	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	3	0	0	2	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	4	0	0	0	0
7	A	27	0	12	1	0
7	B	27	0	12	5	0
All	All	9368	0	9312	473	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (473) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:420:ILE:HG23	2:B:421:PRO:CD	1.75	1.15
1:A:594:SER:HB3	1:A:597:GLU:HG2	1.32	1.11
1:A:601:LEU:O	1:A:603:GLY:HA3	1.53	1.09
1:A:141:VAL:HG21	1:A:166:LEU:HD13	1.40	1.03
2:B:405:THR:HB	2:B:409:VAL:HG23	1.44	0.97
1:A:47:ARG:NH1	1:A:121:MET:HG2	1.80	0.95
1:A:408:LYS:HB2	1:A:414:ASP:HB3	1.48	0.94
2:B:420:ILE:HG23	2:B:421:PRO:HD2	1.48	0.94
1:A:75:ASP:OD1	1:A:99:LYS:HE2	1.70	0.91
2:B:508:GLY:HA2	2:B:509:ARG:HB2	1.52	0.90
2:B:542:LEU:HD12	2:B:543:GLU:H	1.36	0.89
2:B:439:LEU:HB2	2:B:544:SER:HA	1.53	0.89
1:A:594:SER:HB3	1:A:597:GLU:CG	2.03	0.89
1:A:174:ASP:HB2	1:A:372:ILE:HG21	1.56	0.88
1:A:572:ASN:HD21	2:B:300:ALA:H	1.19	0.88
2:B:420:ILE:HG23	2:B:421:PRO:HD3	1.53	0.88
2:B:376:GLN:HE21	2:B:376:GLN:HA	1.39	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:592:PHE:CD2	1:A:642:TYR:HA	2.12	0.85
1:A:470:PRO:HB2	1:A:473:GLN:HG3	1.58	0.82
1:A:593:ALA:HA	1:A:641:ARG:HH21	1.45	0.82
2:B:258:ARG:HH21	2:B:261:ARG:HH22	1.27	0.82
1:A:575:GLU:HG2	2:B:300:ALA:HB3	1.62	0.82
2:B:110:GLU:HG2	2:B:111:THR:N	1.93	0.81
2:B:110:GLU:HG2	2:B:111:THR:H	1.46	0.81
1:A:244:HIS:HB2	1:A:309:LEU:HD21	1.64	0.80
2:B:405:THR:HB	2:B:409:VAL:CG2	2.11	0.80
1:A:434:ASN:C	1:A:435:ARG:HD2	2.02	0.80
2:B:195:VAL:HG23	2:B:333:ASP:HB2	1.62	0.79
1:A:575:GLU:OE2	2:B:301:ARG:HG3	1.82	0.79
1:A:238:ASP:OD1	1:A:275:LYS:HE2	1.83	0.78
2:B:46:ASP:HA	2:B:108:LYS:HA	1.66	0.77
1:A:602:GLN:HG3	1:A:603:GLY:CA	2.14	0.77
2:B:102:LYS:HE3	2:B:113:SER:OG	1.84	0.77
2:B:237:MET:HE3	2:B:267:CYS:HB3	1.66	0.76
1:A:395:GLU:HB3	1:A:424:SER:HB3	1.68	0.75
1:A:202:VAL:HG11	1:A:354:ILE:HD12	1.67	0.75
2:B:177:THR:HG22	2:B:210:LEU:HD13	1.68	0.75
1:A:350:LEU:O	1:A:354:ILE:HG22	1.86	0.75
2:B:546:ALA:O	2:B:547:PHE:HB2	1.86	0.75
1:A:260:ASN:HB3	1:A:263:ALA:HB3	1.69	0.74
2:B:430:THR:HG21	2:B:472:PRO:HG2	1.69	0.74
1:A:407:ASP:O	1:A:435:ARG:NH2	2.20	0.73
2:B:6:ALA:H	2:B:384:LYS:HE3	1.53	0.73
2:B:340:SER:O	2:B:343:ILE:HG12	1.87	0.73
1:A:2:SER:HB3	1:A:137:ASN:HB3	1.71	0.73
2:B:542:LEU:HD12	2:B:543:GLU:N	2.03	0.72
1:A:636:ASN:H	1:A:636:ASN:ND2	1.87	0.72
2:B:542:LEU:HG	2:B:545:TYR:HB3	1.71	0.72
1:A:602:GLN:HG3	1:A:603:GLY:HA3	1.72	0.72
2:B:38:THR:HB	2:B:127:MET:CE	2.19	0.72
1:A:147:PRO:HA	1:A:173:ASN:OD1	1.90	0.72
1:A:574:LEU:HD23	1:A:612:LEU:HD11	1.70	0.72
2:B:244:GLU:OE2	2:B:295:THR:HG21	1.90	0.72
1:A:209:TYR:CE1	1:A:320:PRO:HG2	2.25	0.71
1:A:76:TYR:CD2	1:A:94:GLU:HB2	2.25	0.71
2:B:435:GLN:HG3	2:B:543:GLU:HB3	1.73	0.71
1:A:426:PRO:HG3	1:A:486:PRO:HA	1.71	0.71
1:A:590:ALA:HB3	1:A:591:PRO:HD3	1.71	0.71
2:B:38:THR:HB	2:B:127:MET:HE3	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:76:ARG:O	2:B:101:PRO:HD3	1.91	0.70
2:B:88:LYS:HE2	2:B:89:HIS:ND1	2.06	0.70
2:B:90:TRP:HB3	2:B:92:PHE:CE2	2.27	0.69
2:B:73:LEU:CD1	2:B:116:PRO:HG3	2.23	0.69
1:A:191:GLU:OE1	1:A:218:LYS:HE3	1.93	0.69
1:A:480:LEU:HD23	1:A:495:ALA:HB2	1.72	0.69
2:B:246:LYS:HG3	2:B:252:ASP:HB2	1.74	0.68
1:A:91:LYS:HD3	1:A:103:GLU:OE1	1.93	0.68
1:A:47:ARG:HH11	1:A:121:MET:HG2	1.55	0.68
2:B:268:GLU:OE1	2:B:272:ARG:HD3	1.93	0.68
2:B:43:ALA:HB2	2:B:66:THR:HG23	1.76	0.68
1:A:444:SER:HB2	1:A:457:GLU:O	1.94	0.68
1:A:601:LEU:C	1:A:603:GLY:HA3	2.13	0.68
1:A:434:ASN:O	1:A:435:ARG:HD2	1.94	0.68
2:B:505:ASN:O	2:B:506:ASP:HB2	1.94	0.68
1:A:194:GLU:O	1:A:217:LYS:HE2	1.94	0.67
1:A:234:GLY:HA2	1:A:344:THR:HG21	1.76	0.67
2:B:64:THR:HA	2:B:91:PRO:O	1.95	0.67
1:A:575:GLU:HG2	2:B:300:ALA:CB	2.25	0.67
1:A:517:ALA:O	1:A:518:GLU:HB3	1.94	0.67
1:A:572:ASN:ND2	2:B:300:ALA:H	1.90	0.67
2:B:174:ASN:HB3	2:B:176:PRO:HD2	1.77	0.67
1:A:560:GLN:O	1:A:564:VAL:HG23	1.95	0.67
1:A:645:LYS:O	1:A:649:LYS:HB2	1.95	0.66
1:A:518:GLU:O	1:A:518:GLU:HG3	1.94	0.66
1:A:611:TRP:HE3	1:A:612:LEU:HD12	1.57	0.66
2:B:51:ILE:HD13	2:B:122:MET:O	1.96	0.66
1:A:574:LEU:CD2	1:A:612:LEU:HD11	2.25	0.66
1:A:456:PRO:O	1:A:457:GLU:CB	2.44	0.66
2:B:532:GLN:HA	2:B:535:LYS:HD3	1.78	0.66
2:B:77:ARG:O	2:B:80:ASP:HB2	1.94	0.66
1:A:118:LEU:HA	1:A:121:MET:HE3	1.77	0.65
2:B:11:LEU:HD13	2:B:124:LEU:HD11	1.78	0.65
2:B:117:GLU:O	2:B:121:SER:HB3	1.96	0.65
1:A:341:ILE:HD12	1:A:372:ILE:HD11	1.79	0.65
2:B:395:ASP:HB2	2:B:420:ILE:HG21	1.77	0.65
1:A:385:PRO:HG3	2:B:512:LYS:N	2.11	0.65
2:B:299:ARG:O	2:B:303:GLU:HG3	1.96	0.65
2:B:132:GLU:HG3	2:B:139:VAL:HG23	1.79	0.64
1:A:445:TYR:CD1	1:A:451:LEU:HD21	2.32	0.64
2:B:73:LEU:HD13	2:B:116:PRO:HG3	1.79	0.64
2:B:539:LYS:HG3	2:B:539:LYS:O	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:376:GLN:NE2	2:B:376:GLN:HA	2.13	0.63
1:A:445:TYR:CE1	1:A:451:LEU:HD21	2.32	0.63
1:A:547:LEU:O	1:A:551:ILE:HG13	1.99	0.62
2:B:50:LEU:O	2:B:55:ALA:HB2	1.99	0.62
1:A:253:TYR:HB3	1:A:255:ILE:HD13	1.82	0.62
2:B:246:LYS:HA	2:B:251:LYS:O	1.99	0.62
2:B:191:ALA:HB3	4:B:555:CL:CL	2.37	0.61
2:B:90:TRP:HB3	2:B:92:PHE:CZ	2.35	0.61
2:B:78:PHE:CD2	2:B:96:ASN:HB2	2.36	0.61
1:A:562:LYS:O	1:A:566:GLU:HB2	1.99	0.61
2:B:86:ASP:O	2:B:88:LYS:N	2.34	0.61
2:B:73:LEU:HD23	2:B:90:TRP:CZ3	2.36	0.61
1:A:594:SER:CB	1:A:597:GLU:HG2	2.21	0.60
2:B:279:GLN:HG2	2:B:280:ALA:H	1.66	0.60
2:B:531:LYS:HD3	2:B:531:LYS:O	2.01	0.60
1:A:636:ASN:HD22	1:A:636:ASN:H	1.48	0.60
1:A:435:ARG:HG2	1:A:478:VAL:HG22	1.83	0.60
2:B:467:ALA:HB1	2:B:468:PRO:CD	2.32	0.60
1:A:625:ILE:O	1:A:629:GLU:HG2	2.02	0.60
1:A:19:ALA:HB1	2:B:393:LEU:HD11	1.83	0.60
2:B:102:LYS:HD2	2:B:115:TYR:CE1	2.37	0.60
2:B:11:LEU:HD13	2:B:124:LEU:CD1	2.31	0.60
2:B:96:ASN:HD21	2:B:99:GLY:H	1.50	0.60
1:A:310:VAL:C	1:A:312:PRO:HD2	2.22	0.60
1:A:529:LYS:HE2	1:A:532:ASP:OD2	2.01	0.60
1:A:385:PRO:HG3	2:B:512:LYS:H	1.67	0.59
2:B:430:THR:CG2	2:B:472:PRO:HG2	2.32	0.59
1:A:519:GLN:HE21	1:A:520:GLU:N	2.00	0.59
1:A:203:ASP:HA	1:A:341:ILE:O	2.02	0.59
2:B:78:PHE:C	2:B:78:PHE:CD1	2.75	0.59
1:A:575:GLU:OE1	2:B:298:THR:HG21	2.03	0.59
2:B:508:GLY:CA	2:B:509:ARG:HB2	2.29	0.59
1:A:478:VAL:HG12	1:A:497:THR:CG2	2.33	0.59
1:A:291:VAL:HG23	1:A:292:MET:N	2.18	0.58
2:B:439:LEU:CB	2:B:544:SER:HA	2.31	0.58
2:B:73:LEU:HD23	2:B:90:TRP:CH2	2.38	0.58
1:A:12:ASN:HB2	1:A:206:HIS:CG	2.38	0.58
2:B:60:ALA:O	2:B:61:MET:HG3	2.02	0.58
2:B:110:GLU:CG	2:B:111:THR:H	2.11	0.58
2:B:248:LYS:C	2:B:249:HIS:CD2	2.77	0.58
2:B:117:GLU:HG2	2:B:157:ALA:HB1	1.84	0.58
2:B:539:LYS:CG	2:B:539:LYS:O	2.52	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:ASN:OD1	1:A:67:ASN:HA	2.03	0.58
1:A:581:LEU:HD23	1:A:605:LEU:HD11	1.86	0.57
1:A:317:VAL:O	1:A:320:PRO:HD2	2.04	0.57
1:A:46:ASN:HB3	1:A:564:VAL:HG21	1.85	0.57
1:A:70:ARG:NH2	1:A:230:LYS:O	2.34	0.57
1:A:344:THR:HG23	7:A:672:ADP:H1'	1.86	0.57
1:A:253:TYR:HB3	1:A:255:ILE:CD1	2.35	0.57
1:A:456:PRO:O	1:A:457:GLU:HB3	2.03	0.57
2:B:132:GLU:HG2	2:B:138:THR:HA	1.85	0.57
1:A:221:LEU:C	1:A:221:LEU:HD12	2.25	0.57
2:B:185:LEU:CD1	2:B:195:VAL:HG21	2.33	0.57
2:B:343:ILE:CD1	7:B:560:ADP:H2	2.18	0.57
2:B:62:ASN:N	2:B:63:PRO:CD	2.67	0.57
1:A:42:PHE:HB3	1:A:106:PHE:HB2	1.86	0.57
1:A:599:THR:HG22	1:A:599:THR:O	2.05	0.57
2:B:185:LEU:C	2:B:187:LYS:H	2.08	0.56
2:B:96:ASN:HD22	2:B:97:ASP:N	2.03	0.56
1:A:91:LYS:HG2	1:A:103:GLU:HB3	1.85	0.56
1:A:478:VAL:HG12	1:A:497:THR:HG22	1.86	0.56
1:A:621:LYS:O	1:A:625:ILE:HG12	2.05	0.56
1:A:426:PRO:HG3	1:A:486:PRO:CA	2.36	0.56
1:A:262:LYS:O	1:A:266:ARG:HG3	2.06	0.56
1:A:396:ASP:HB3	1:A:425:PHE:CE2	2.39	0.56
1:A:572:ASN:HD21	2:B:300:ALA:N	1.96	0.56
1:A:590:ALA:HA	1:A:598:LYS:NZ	2.21	0.56
1:A:469:LEU:HD12	1:A:469:LEU:N	2.20	0.56
1:A:150:THR:H	1:A:153:GLN:HG3	1.71	0.56
2:B:405:THR:HG23	2:B:540:ASN:H	1.72	0.55
1:A:406:TRP:CE2	1:A:433:LEU:HD21	2.42	0.55
1:A:451:LEU:CD2	1:A:455:THR:HG21	2.36	0.55
2:B:78:PHE:C	2:B:78:PHE:HD1	2.10	0.55
2:B:430:THR:HG22	2:B:472:PRO:HD2	1.88	0.55
1:A:601:LEU:O	1:A:602:GLN:CG	2.55	0.55
2:B:395:ASP:CB	2:B:420:ILE:HG21	2.36	0.54
1:A:76:TYR:CG	1:A:94:GLU:HB2	2.42	0.54
1:A:266:ARG:NH1	1:A:289:GLU:O	2.37	0.54
2:B:437:GLY:O	2:B:543:GLU:HA	2.07	0.54
1:A:641:ARG:O	1:A:645:LYS:HB2	2.07	0.54
1:A:509:LEU:N	1:A:510:PRO:HD3	2.23	0.54
2:B:248:LYS:O	2:B:249:HIS:CD2	2.61	0.54
2:B:286:SER:N	2:B:292:ASP:OD2	2.34	0.54
2:B:460:GLU:HG2	2:B:462:THR:CG2	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:436:PRO:O	2:B:464:ILE:HG13	2.08	0.54
1:A:137:ASN:O	1:A:138:ILE:HD13	2.08	0.54
2:B:3:LYS:HB2	2:B:137:LYS:HE3	1.88	0.54
1:A:246:ALA:HB2	1:A:257:ILE:HD11	1.90	0.54
2:B:338:GLY:HA2	7:B:560:ADP:O2A	2.08	0.54
1:A:451:LEU:HD22	1:A:455:THR:HG21	1.89	0.54
2:B:429:THR:CG2	2:B:540:ASN:HB3	2.38	0.54
1:A:290:SER:HA	1:A:295:VAL:O	2.07	0.54
1:A:257:ILE:C	1:A:259:GLU:H	2.10	0.53
1:A:134:THR:C	1:A:136:ALA:H	2.11	0.53
1:A:433:LEU:HB3	1:A:435:ARG:HD3	1.91	0.53
1:A:385:PRO:CD	2:B:509:ARG:HH22	2.20	0.53
1:A:150:THR:H	1:A:153:GLN:CG	2.21	0.53
2:B:351:GLN:HB2	2:B:359:LEU:HD11	1.90	0.53
1:A:571:LYS:HE2	1:A:617:PHE:O	2.07	0.53
1:A:141:VAL:CG2	1:A:166:LEU:HD13	2.25	0.53
1:A:408:LYS:HG2	1:A:408:LYS:O	2.06	0.53
1:A:636:ASN:N	1:A:636:ASN:ND2	2.51	0.53
2:B:86:ASP:C	2:B:88:LYS:H	2.12	0.53
1:A:384:SER:CB	1:A:387:LEU:HD12	2.39	0.53
1:A:623:LYS:HA	1:A:626:ALA:HB3	1.91	0.53
2:B:31:ASN:C	2:B:33:GLN:H	2.12	0.53
2:B:438:VAL:HG23	2:B:461:LEU:HB3	1.91	0.53
2:B:429:THR:HG22	2:B:540:ASN:HB3	1.90	0.53
2:B:183:TYR:OH	2:B:361:LYS:HA	2.09	0.52
2:B:240:HIS:CB	2:B:305:LEU:HD21	2.39	0.52
1:A:311:LYS:N	1:A:312:PRO:CD	2.73	0.52
1:A:643:LEU:O	1:A:647:GLU:HB2	2.08	0.52
2:B:29:ILE:HD13	2:B:131:ALA:HA	1.91	0.52
2:B:221:SER:OG	2:B:324:ALA:HB2	2.09	0.52
2:B:229:GLY:O	2:B:230:GLY:C	2.47	0.52
2:B:240:HIS:O	2:B:243:ALA:HB3	2.10	0.52
2:B:90:TRP:C	2:B:92:PHE:H	2.12	0.52
1:A:201:PHE:HE1	1:A:366:LEU:HD11	1.73	0.52
1:A:91:LYS:HD3	1:A:103:GLU:CD	2.30	0.52
1:A:260:ASN:HB3	1:A:263:ALA:CB	2.38	0.52
1:A:150:THR:OG1	1:A:153:GLN:HG2	2.10	0.52
2:B:368:ALA:O	2:B:371:TYR:HB3	2.10	0.52
1:A:635:GLY:O	1:A:636:ASN:C	2.48	0.52
1:A:170:ARG:HE	1:A:383:HIS:HE1	1.57	0.52
1:A:341:ILE:HA	1:A:368:GLN:HB2	1.91	0.51
2:B:106:GLU:O	2:B:106:GLU:HG3	2.08	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:96:ASN:HD21	2:B:99:GLY:N	2.07	0.51
2:B:253:ILE:O	2:B:255:GLU:N	2.43	0.51
1:A:256:ASP:HB3	1:A:259:GLU:CG	2.40	0.51
1:A:7:LEU:HD21	1:A:9:LEU:HD12	1.92	0.51
2:B:185:LEU:HD12	2:B:195:VAL:HG21	1.91	0.51
2:B:86:ASP:HB3	2:B:90:TRP:CH2	2.45	0.51
2:B:279:GLN:HG2	2:B:280:ALA:N	2.26	0.51
2:B:75:GLY:HA3	2:B:154:GLN:HA	1.93	0.51
2:B:405:THR:HG22	2:B:406:ALA:N	2.25	0.51
2:B:248:LYS:HB3	2:B:249:HIS:CD2	2.45	0.51
2:B:503:ILE:C	2:B:505:ASN:H	2.14	0.51
2:B:117:GLU:CG	2:B:157:ALA:HB1	2.41	0.51
1:A:649:LYS:HB3	1:A:649:LYS:NZ	2.26	0.50
1:A:214:MET:HG2	1:A:223:VAL:HG22	1.92	0.50
2:B:315:ASP:HB2	2:B:316:PRO:HD3	1.93	0.50
2:B:238:VAL:O	2:B:242:ILE:HD12	2.10	0.50
1:A:291:VAL:CG2	1:A:292:MET:H	2.24	0.50
2:B:197:ILE:N	2:B:197:ILE:HD13	2.27	0.50
1:A:146:PRO:HB2	1:A:148:TRP:CD1	2.46	0.50
2:B:542:LEU:HD21	2:B:545:TYR:HD1	1.77	0.50
2:B:430:THR:CG2	2:B:472:PRO:HD2	2.42	0.50
1:A:470:PRO:CB	1:A:473:GLN:HG3	2.35	0.50
2:B:343:ILE:HD13	7:B:560:ADP:H2	1.76	0.50
1:A:291:VAL:CG2	1:A:292:MET:N	2.75	0.50
2:B:22:GLN:O	2:B:23:HIS:HB2	2.12	0.50
1:A:212:SER:HB2	1:A:226:THR:OG1	2.12	0.50
1:A:318:THR:HG22	1:A:357:ALA:HB2	1.93	0.50
2:B:6:ALA:HB1	2:B:377:ALA:HB1	1.93	0.50
1:A:379:ILE:O	1:A:382:ILE:HB	2.12	0.50
1:A:174:ASP:HB2	1:A:372:ILE:CG2	2.34	0.49
2:B:106:GLU:HA	2:B:110:GLU:O	2.11	0.49
1:A:70:ARG:NH1	1:A:207:SER:OG	2.44	0.49
1:A:620:ILE:HD11	1:A:623:LYS:HG2	1.94	0.49
2:B:132:GLU:CG	2:B:139:VAL:HG23	2.43	0.49
2:B:324:ALA:O	2:B:326:LEU:HG	2.12	0.49
2:B:375:VAL:O	2:B:378:ALA:HB3	2.12	0.49
2:B:72:ARG:HH12	2:B:226:THR:HG22	1.76	0.49
2:B:121:SER:HB2	2:B:161:ALA:O	2.12	0.49
1:A:544:ALA:O	1:A:548:ASN:ND2	2.46	0.49
2:B:298:THR:CG2	2:B:301:ARG:H	2.24	0.49
2:B:471:VAL:HB	2:B:472:PRO:HD3	1.94	0.49
1:A:292:MET:O	1:A:294:ASP:N	2.46	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:ILE:HD13	1:A:345:THR:HG22	1.93	0.48
2:B:286:SER:HA	2:B:291:ILE:O	2.13	0.48
1:A:128:ASP:O	1:A:129:THR:C	2.52	0.48
2:B:102:LYS:HD2	2:B:115:TYR:CZ	2.49	0.48
2:B:62:ASN:H	2:B:63:PRO:CD	2.25	0.48
1:A:9:LEU:O	1:A:69:LYS:HE2	2.14	0.48
1:A:607:LYS:O	1:A:611:TRP:HB2	2.13	0.48
1:A:451:LEU:HD12	1:A:451:LEU:N	2.29	0.48
1:A:256:ASP:O	1:A:259:GLU:CG	2.62	0.48
2:B:32:ASP:OD2	2:B:32:ASP:N	2.46	0.48
1:A:2:SER:HB2	1:A:137:ASN:O	2.12	0.48
1:A:56:LYS:O	1:A:58:THR:N	2.47	0.48
1:A:150:THR:N	1:A:153:GLN:HG3	2.29	0.48
2:B:460:GLU:HG2	2:B:462:THR:HG23	1.96	0.48
2:B:26:VAL:HB	2:B:371:TYR:CE2	2.48	0.48
2:B:238:VAL:HG12	2:B:242:ILE:HD11	1.96	0.48
1:A:75:ASP:HA	1:A:99:LYS:HD3	1.96	0.48
1:A:134:THR:C	1:A:136:ALA:N	2.66	0.48
2:B:110:GLU:CG	2:B:111:THR:N	2.66	0.48
2:B:467:ALA:HB1	2:B:468:PRO:HD3	1.97	0.47
2:B:198:PHE:CD1	2:B:198:PHE:O	2.67	0.47
1:A:385:PRO:HD2	2:B:509:ARG:HH22	1.79	0.47
2:B:38:THR:HB	2:B:127:MET:HE1	1.96	0.47
2:B:500:LYS:HG3	2:B:501:ILE:N	2.29	0.47
1:A:601:LEU:O	1:A:602:GLN:HG2	2.14	0.47
2:B:364:ASN:HA	2:B:365:PRO:HD2	1.74	0.47
2:B:228:LEU:HD22	2:B:229:GLY:N	2.30	0.47
2:B:425:THR:HG23	2:B:477:THR:OG1	2.14	0.47
1:A:396:ASP:O	1:A:424:SER:HA	2.15	0.47
1:A:623:LYS:HA	1:A:626:ALA:CB	2.44	0.47
1:A:38:SER:HA	1:A:122:PHE:CE1	2.50	0.47
1:A:178:ALA:O	1:A:181:SER:HB2	2.14	0.47
2:B:298:THR:HG22	2:B:301:ARG:HB2	1.97	0.47
1:A:485:ASP:HB2	1:A:486:PRO:CD	2.45	0.47
2:B:442:VAL:HG21	2:B:488:VAL:HG21	1.97	0.47
1:A:461:ASN:ND2	1:A:538:HIS:HD2	2.13	0.47
1:A:97:ASP:OD1	1:A:99:LYS:HB2	2.15	0.46
1:A:59:SER:OG	2:B:283:GLU:OE1	2.28	0.46
2:B:543:GLU:O	2:B:545:TYR:N	2.49	0.46
2:B:107:TYR:O	2:B:108:LYS:HB2	2.15	0.46
2:B:249:HIS:ND1	2:B:291:ILE:HG21	2.31	0.46
2:B:31:ASN:HB3	2:B:130:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:VAL:H	1:A:297:VAL:HG23	1.81	0.46
1:A:327:GLN:C	1:A:329:LYS:H	2.18	0.46
2:B:233:PHE:CD1	2:B:310:PHE:HE1	2.34	0.46
2:B:531:LYS:CD	2:B:531:LYS:O	2.64	0.46
2:B:328:LYS:HE3	2:B:353:PHE:O	2.16	0.46
1:A:132:GLN:O	1:A:135:LYS:HE3	2.16	0.46
1:A:256:ASP:O	1:A:259:GLU:HG2	2.16	0.46
1:A:281:ASN:HD21	2:B:57:ASN:HB2	1.80	0.46
2:B:301:ARG:O	2:B:305:LEU:CD1	2.64	0.46
1:A:592:PHE:CE2	1:A:642:TYR:HA	2.49	0.46
2:B:339:GLY:N	7:B:560:ADP:O2A	2.45	0.46
2:B:303:GLU:OE2	2:B:345:LYS:HB2	2.16	0.46
2:B:420:ILE:CG2	2:B:421:PRO:CD	2.69	0.45
2:B:191:ALA:CB	4:B:555:CL:CL	3.01	0.45
2:B:200:LEU:HD11	2:B:228:LEU:HD13	1.99	0.45
2:B:526:LYS:O	2:B:530:GLU:HB2	2.16	0.45
2:B:339:GLY:O	2:B:342:ARG:HG3	2.17	0.45
2:B:49:ARG:O	2:B:50:LEU:HD23	2.15	0.45
1:A:174:ASP:OD1	1:A:175:VAL:N	2.45	0.45
1:A:232:PHE:C	1:A:232:PHE:CD2	2.90	0.45
1:A:204:ILE:HG13	1:A:209:TYR:CD2	2.51	0.45
1:A:606:ASN:O	1:A:609:GLU:HB3	2.17	0.45
2:B:436:PRO:HG2	2:B:437:GLY:H	1.81	0.45
1:A:602:GLN:HG3	1:A:603:GLY:HA2	1.93	0.45
1:A:487:SER:HB2	1:A:489:LEU:HG	1.98	0.45
2:B:480:ILE:HA	2:B:485:ILE:O	2.17	0.45
1:A:172:VAL:HG21	1:A:379:ILE:CD1	2.46	0.45
2:B:459:PHE:CE1	2:B:501:ILE:HG22	2.52	0.45
1:A:16:LEU:N	1:A:16:LEU:CD1	2.79	0.45
2:B:249:HIS:C	2:B:251:LYS:H	2.20	0.44
1:A:291:VAL:HG23	1:A:292:MET:H	1.79	0.44
2:B:392:LEU:C	2:B:392:LEU:HD12	2.38	0.44
2:B:508:GLY:HA2	2:B:509:ARG:CB	2.34	0.44
1:A:203:ASP:C	1:A:203:ASP:OD2	2.56	0.44
1:A:381:ALA:O	1:A:382:ILE:C	2.55	0.44
1:A:40:VAL:HG22	1:A:49:LEU:HD22	2.00	0.44
2:B:279:GLN:NE2	2:B:296:SER:HB2	2.33	0.44
1:A:31:VAL:CG2	1:A:33:ASN:ND2	2.80	0.44
2:B:449:MET:O	2:B:451:LYS:N	2.51	0.44
1:A:577:TYR:HA	1:A:580:THR:HG22	2.00	0.44
1:A:418:VAL:O	1:A:429:LYS:HE3	2.17	0.44
1:A:406:TRP:O	1:A:414:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:46:ASP:CA	2:B:108:LYS:HA	2.43	0.44
1:A:249:PHE:O	1:A:255:ILE:O	2.35	0.44
2:B:256:ASN:HB3	2:B:259:ALA:HB3	2.00	0.44
1:A:56:LYS:O	1:A:57:GLN:C	2.56	0.44
2:B:542:LEU:HG	2:B:545:TYR:CB	2.42	0.44
1:A:48:TYR:CD2	1:A:56:LYS:HG2	2.53	0.44
2:B:469:ARG:HG2	2:B:469:ARG:O	2.18	0.44
2:B:405:THR:CG2	2:B:406:ALA:N	2.81	0.43
2:B:435:GLN:CG	2:B:543:GLU:HB3	2.45	0.43
1:A:310:VAL:C	1:A:312:PRO:CD	2.86	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.74	0.43
2:B:104:GLN:HG3	2:B:113:SER:HB3	2.00	0.43
1:A:146:PRO:HG2	1:A:149:TYR:CD1	2.53	0.43
1:A:174:ASP:O	1:A:177:ALA:N	2.50	0.43
1:A:110:LYS:HA	1:A:110:LYS:HD3	1.80	0.43
1:A:167:ASN:HA	1:A:168:PRO:HD3	1.83	0.43
2:B:174:ASN:HB2	2:B:177:THR:OG1	2.18	0.43
1:A:560:GLN:O	1:A:560:GLN:HG2	2.17	0.43
1:A:647:GLU:HB3	1:A:648:GLU:OE2	2.18	0.43
1:A:573:THR:HG22	1:A:628:TYR:CE1	2.54	0.43
2:B:505:ASN:O	2:B:506:ASP:CB	2.64	0.43
1:A:151:GLU:O	1:A:155:TYR:HD1	2.01	0.43
1:A:135:LYS:HE2	1:A:135:LYS:HA	1.99	0.43
1:A:239:LEU:O	1:A:240:ALA:C	2.57	0.43
1:A:406:TRP:HB3	1:A:441:MET:HG2	2.01	0.43
2:B:185:LEU:C	2:B:187:LYS:N	2.72	0.43
2:B:511:SER:O	2:B:514:ASP:N	2.51	0.43
1:A:469:LEU:N	1:A:469:LEU:CD1	2.81	0.43
2:B:510:LEU:HD22	2:B:514:ASP:HB3	2.01	0.43
2:B:178:ALA:O	2:B:372:GLY:HA3	2.19	0.43
1:A:453:PRO:O	1:A:454:ASN:HB2	2.19	0.43
1:A:521:PHE:CD1	1:A:521:PHE:N	2.87	0.43
1:A:247:ASP:O	1:A:250:LYS:HB3	2.18	0.43
2:B:240:HIS:HB2	2:B:305:LEU:HD21	2.01	0.43
1:A:425:PHE:HA	1:A:426:PRO:C	2.40	0.43
1:A:185:PHE:O	1:A:186:LYS:C	2.57	0.43
1:A:463:GLU:OE2	1:A:538:HIS:NE2	2.33	0.42
2:B:319:LYS:O	2:B:319:LYS:HG3	2.18	0.42
2:B:301:ARG:O	2:B:305:LEU:HD12	2.19	0.42
2:B:343:ILE:HD11	7:B:560:ADP:H2	1.84	0.42
2:B:59:VAL:O	2:B:60:ALA:HB3	2.19	0.42
1:A:435:ARG:HG2	1:A:478:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:31:ASN:O	2:B:33:GLN:N	2.52	0.42
2:B:181:ILE:O	2:B:184:GLY:N	2.47	0.42
1:A:22:ARG:HH11	2:B:394:LEU:HD12	1.84	0.42
2:B:251:LYS:HA	2:B:251:LYS:HD3	1.89	0.42
2:B:309:LEU:HD23	2:B:309:LEU:HA	1.80	0.42
2:B:403:ILE:HD11	2:B:428:PHE:CZ	2.54	0.42
2:B:543:GLU:O	2:B:544:SER:C	2.58	0.42
2:B:238:VAL:HG12	2:B:242:ILE:CD1	2.49	0.42
2:B:459:PHE:CD1	2:B:501:ILE:HG22	2.55	0.42
1:A:120:ALA:O	1:A:164:ALA:HB2	2.20	0.42
2:B:513:GLU:HG2	2:B:517:ARG:NH2	2.34	0.42
1:A:395:GLU:HB3	1:A:424:SER:CB	2.44	0.42
1:A:576:GLU:O	1:A:580:THR:HG22	2.19	0.42
1:A:249:PHE:CD1	1:A:249:PHE:N	2.86	0.42
2:B:237:MET:HE1	2:B:271:LYS:HB2	2.01	0.42
2:B:238:VAL:O	2:B:239:ASN:C	2.58	0.42
2:B:237:MET:CE	2:B:267:CYS:HB3	2.42	0.42
2:B:5:PRO:HB3	2:B:384:LYS:CE	2.50	0.42
2:B:86:ASP:C	2:B:88:LYS:N	2.72	0.42
2:B:505:ASN:HB3	2:B:507:LYS:HD3	2.01	0.42
1:A:564:VAL:O	1:A:564:VAL:HG12	2.20	0.42
2:B:65:ASN:OD1	2:B:106:GLU:HB3	2.20	0.42
1:A:251:THR:HG22	1:A:252:LYS:N	2.35	0.42
1:A:602:GLN:CG	1:A:603:GLY:HA3	2.45	0.41
1:A:414:ASP:O	1:A:415:HIS:HB3	2.20	0.41
1:A:77:HIS:CD2	1:A:94:GLU:OE1	2.73	0.41
2:B:291:ILE:HG22	2:B:292:ASP:N	2.35	0.41
1:A:46:ASN:N	1:A:46:ASN:HD22	2.18	0.41
2:B:78:PHE:CE2	2:B:96:ASN:HB2	2.55	0.41
1:A:274:LEU:O	1:A:277:VAL:HB	2.20	0.41
1:A:437:GLY:HA2	1:A:467:VAL:HG11	2.02	0.41
2:B:268:GLU:CD	2:B:272:ARG:HH11	2.23	0.41
1:A:571:LYS:HA	1:A:624:TYR:CD1	2.55	0.41
2:B:495:THR:OG1	2:B:497:LYS:HG2	2.20	0.41
1:A:409:GLN:HG3	1:A:435:ARG:NH2	2.33	0.41
1:A:103:GLU:OE2	1:A:110:LYS:HD2	2.20	0.41
2:B:336:LEU:HD11	2:B:359:LEU:HD22	2.03	0.41
2:B:193:ARG:O	2:B:211:THR:HA	2.20	0.41
2:B:150:PHE:O	2:B:155:ARG:NH2	2.51	0.41
2:B:56:LYS:O	2:B:59:VAL:HG12	2.20	0.41
2:B:39:PRO:O	2:B:52:GLY:HA2	2.21	0.41
1:A:215:ALA:HB2	1:A:224:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:LYS:O	1:A:564:VAL:HG21	2.20	0.41
1:A:623:LYS:HA	1:A:623:LYS:HD3	1.74	0.41
1:A:120:ALA:HB1	1:A:163:ILE:CG2	2.51	0.41
1:A:502:GLU:HA	1:A:524:VAL:O	2.20	0.41
2:B:543:GLU:C	2:B:545:TYR:N	2.73	0.41
1:A:203:ASP:HB2	1:A:341:ILE:HG13	2.03	0.41
1:A:252:LYS:HG3	1:A:252:LYS:O	2.21	0.41
2:B:15:TYR:CE2	2:B:39:PRO:HG3	2.56	0.41
2:B:508:GLY:CA	2:B:509:ARG:CB	2.95	0.41
1:A:350:LEU:O	1:A:350:LEU:HD12	2.20	0.41
1:A:251:THR:O	1:A:253:TYR:N	2.52	0.41
1:A:251:THR:C	1:A:253:TYR:H	2.24	0.41
2:B:459:PHE:CD1	2:B:501:ILE:CG2	3.03	0.41
1:A:321:VAL:HG22	1:A:358:PHE:CE2	2.56	0.41
1:A:241:ILE:O	1:A:242:THR:C	2.58	0.41
1:A:526:LYS:HA	1:A:526:LYS:HD3	1.74	0.41
2:B:125:THR:O	2:B:128:LYS:HB3	2.21	0.41
1:A:611:TRP:CE2	1:A:615:GLU:O	2.75	0.41
2:B:160:ASP:C	2:B:164:ILE:HD12	2.42	0.41
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.74	0.41
1:A:516:ASP:O	1:A:517:ALA:HB2	2.21	0.40
2:B:198:PHE:O	2:B:198:PHE:HD1	2.04	0.40
2:B:419:THR:O	2:B:420:ILE:O	2.40	0.40
1:A:570:ARG:C	1:A:572:ASN:N	2.74	0.40
1:A:194:GLU:O	1:A:217:LYS:CE	2.65	0.40
1:A:125:LYS:O	1:A:128:ASP:HB3	2.20	0.40
1:A:267:ILE:HD13	1:A:288:VAL:HG21	2.03	0.40
2:B:447:ARG:HG3	2:B:452:ASP:HB3	2.03	0.40
2:B:4:GLY:HA2	2:B:5:PRO:HD3	1.78	0.40
2:B:343:ILE:HB	2:B:346:ILE:HB	2.04	0.40
1:A:493:GLU:O	1:A:494:GLU:HB2	2.21	0.40
2:B:302:PHE:O	2:B:306:ASN:ND2	2.55	0.40
1:A:12:ASN:HB2	1:A:206:HIS:CB	2.52	0.40
1:A:571:LYS:HG2	1:A:571:LYS:O	2.20	0.40
2:B:354:PHE:O	2:B:355:ASN:HB2	2.22	0.40
2:B:194:ASN:HB2	2:B:330:GLN:O	2.21	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	647/668 (97%)	546 (84%)	80 (12%)	21 (3%)	6	35
2	B	536/554 (97%)	442 (82%)	67 (12%)	27 (5%)	3	22
All	All	1183/1222 (97%)	988 (84%)	147 (12%)	48 (4%)	4	27

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	457	GLU
1	A	471	GLU
1	A	636	ASN
1	A	637	ILE
2	B	46	ASP
2	B	190	GLY
2	B	230	GLY
2	B	420	ILE
2	B	421	PRO
2	B	543	GLU
1	A	57	GLN
1	A	252	LYS
1	A	508	PRO
1	A	518	GLU
1	A	635	GLY
2	B	62	ASN
2	B	186	ASP
2	B	191	ALA
2	B	254	SER
2	B	469	ARG
2	B	506	ASP
2	B	508	GLY
2	B	538	SER
2	B	23	HIS
2	B	32	ASP
2	B	87	MET

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Mol	Chain	Res	Type
2	B	450	THR
2	B	504	THR
2	B	507	LYS
1	A	44	PRO
1	A	258	ARG
1	A	409	GLN
1	A	602	GLN
2	B	47	THR
2	B	305	LEU
1	A	494	GLU
1	A	619	SER
2	B	203	GLY
2	B	378	ALA
2	B	532	GLN
1	A	56	LYS
1	A	294	ASP
1	A	453	PRO
2	B	4	GLY
2	B	91	PRO
1	A	79	PRO
1	A	382	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/573 (98%)	511 (91%)	49 (9%)	14	50
2	B	455/468 (97%)	403 (89%)	52 (11%)	8	32
All	All	1015/1041 (98%)	914 (90%)	101 (10%)	11	39

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	16	LEU
1	A	31	VAL
1	A	46	ASN

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Mol	Chain	Res	Type
1	A	59	SER
1	A	69	LYS
1	A	75	ASP
1	A	91	LYS
1	A	96	ASP
1	A	124	ASP
1	A	149	TYR
1	A	153	GLN
1	A	167	ASN
1	A	172	VAL
1	A	181	SER
1	A	186	LYS
1	A	195	LYS
1	A	221	LEU
1	A	228	CYS
1	A	232	PHE
1	A	255	ILE
1	A	272	GLU
1	A	282	THR
1	A	293	ASN
1	A	295	VAL
1	A	300	GLN
1	A	308	GLU
1	A	309	LEU
1	A	319	GLU
1	A	344	THR
1	A	349	THR
1	A	354	ILE
1	A	410	VAL
1	A	429	LYS
1	A	430	LEU
1	A	435	ARG
1	A	468	GLN
1	A	471	GLU
1	A	512	ASP
1	A	521	PHE
1	A	527	THR
1	A	543	ASP
1	A	576	GLU
1	A	587	GLU
1	A	607	LYS
1	A	620	ILE

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Mol	Chain	Res	Type
1	A	625	ILE
1	A	636	ASN
1	A	649	LYS
2	B	3	LYS
2	B	13	THR
2	B	14	THR
2	B	46	ASP
2	B	47	THR
2	B	48	GLU
2	B	58	GLN
2	B	77	ARG
2	B	78	PHE
2	B	82	VAL
2	B	88	LYS
2	B	89	HIS
2	B	96	ASN
2	B	105	VAL
2	B	121	SER
2	B	137	LYS
2	B	140	THR
2	B	173	ILE
2	B	193	ARG
2	B	211	THR
2	B	212	ILE
2	B	222	THR
2	B	226	THR
2	B	228	LEU
2	B	250	LYS
2	B	278	THR
2	B	285	ASP
2	B	298	THR
2	B	314	LEU
2	B	319	LYS
2	B	328	LYS
2	B	361	LYS
2	B	364	ASN
2	B	376	GLN
2	B	392	LEU
2	B	394	LEU
2	B	430	THR
2	B	432	SER
2	B	433	ASP

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Mol	Chain	Res	Type
2	B	438	VAL
2	B	447	ARG
2	B	491	VAL
2	B	497	LYS
2	B	501	ILE
2	B	504	THR
2	B	507	LYS
2	B	528	GLU
2	B	531	LYS
2	B	535	LYS
2	B	539	LYS
2	B	544	SER
2	B	545	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	46	ASN
1	A	77	HIS
1	A	87	HIS
1	A	153	GLN
1	A	244	HIS
1	A	281	ASN
1	A	300	GLN
1	A	383	HIS
1	A	415	HIS
1	A	461	ASN
1	A	519	GLN
1	A	572	ASN
1	A	606	ASN
1	A	636	ASN
2	B	57	ASN
2	B	84	GLN
2	B	96	ASN
2	B	227	HIS
2	B	249	HIS
2	B	279	GLN
2	B	376	GLN
2	B	505	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\# Z > 2$
5	SO4	A	668	-	4,4,4	0.13	0	6,6,6	0.15	0
5	SO4	A	669	-	4,4,4	0.19	0	6,6,6	0.41	0
5	SO4	A	670	-	4,4,4	0.42	0	6,6,6	0.43	0
6	BEF	A	671	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	A	672	3,6	29,29,29	1.08	2 (6%)	45,45,45	2.00	9 (20%)
5	SO4	B	559	-	4,4,4	0.17	0	6,6,6	0.25	0
7	ADP	B	560	-	29,29,29	1.26	4 (13%)	45,45,45	2.19	12 (26%)

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
5	SO4	A	668	-	-	0/0/0/0	0/0/0/0
5	SO4	A	669	-	-	0/0/0/0	0/0/0/0
5	SO4	A	670	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BEF	A	671	7	-	0/0/0/0	0/0/0/0
7	ADP	A	672	3,6	-	0/16/32/32	0/1/3/3
5	SO4	B	559	-	-	0/0/0/0	0/0/0/0
7	ADP	B	560	-	-	0/16/32/32	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	672	ADP	C5-C4	3.34	1.48	1.40
7	B	560	ADP	C4-N9	-3.28	1.33	1.37
7	B	560	ADP	C5-C4	2.99	1.47	1.40
7	A	672	ADP	C4-N9	-2.61	1.33	1.37
7	B	560	ADP	PB-O3A	2.11	1.63	1.60
7	B	560	ADP	C8-N9	-2.05	1.33	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	560	ADP	N3-C2-N1	-7.14	122.74	128.71
7	A	672	ADP	O4'-C1'-N9	6.75	114.72	108.44
7	A	672	ADP	N3-C2-N1	-5.68	123.96	128.71
7	B	560	ADP	C4-C5-N7	-5.40	104.89	109.52
7	A	672	ADP	N3-C4-N9	5.11	134.66	125.43
7	B	560	ADP	N3-C4-N9	4.70	133.92	125.43
7	B	560	ADP	C8-N9-C4	3.84	109.83	106.90
7	B	560	ADP	PA-O3A-PB	-3.52	121.36	131.68
7	A	672	ADP	C5-C4-N3	-3.20	118.74	125.70
7	A	672	ADP	PA-O3A-PB	-3.07	122.68	131.68
7	A	672	ADP	C4-C5-N7	-3.05	106.91	109.52
7	B	560	ADP	C5-C4-N3	-2.96	119.25	125.70
7	B	560	ADP	C2-N1-C6	2.91	124.03	118.77
7	A	672	ADP	C3'-C2'-C1'	2.78	105.25	100.91
7	B	560	ADP	O4'-C1'-N9	2.67	110.92	108.44
7	B	560	ADP	C4'-O4'-C1'	-2.59	106.94	109.75
7	B	560	ADP	C2-N3-C4	2.44	120.97	114.01
7	B	560	ADP	O3B-PB-O2B	2.39	116.90	107.61
7	A	672	ADP	C2-N3-C4	2.34	120.68	114.01
7	A	672	ADP	C2'-C1'-N9	-2.29	107.39	113.27
7	B	560	ADP	C1'-N9-C4	-2.06	123.07	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	649/668 (97%)	-0.23	0 100 100	10, 42, 114, 147	0
2	B	540/554 (97%)	-0.19	0 100 100	22, 50, 99, 136	0
All	All	1189/1222 (97%)	-0.21	0 93 100	10, 47, 107, 147	0

There are no RSRZ outliers to report.

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	667	1/1	0.40	12.11	14,14,14,14	0
5	SO4	A	669	5/5	0.31	11.58	76,79,80,82	0
6	BEF	A	671	4/4	0.34	6.67	39,39,39,39	0
3	MG	B	558	1/1	0.30	5.17	27,27,27,27	0
5	SO4	A	670	5/5	0.24	3.87	103,106,108,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	668	5/5	0.32	3.07	81,83,85,86	0
4	CL	B	556	1/1	0.20	1.61	65,65,65,65	0
7	ADP	A	672	27/27	0.24	1.50	44,44,44,44	0
7	ADP	B	560	27/27	0.23	1.48	60,60,60,60	0
4	CL	B	557	1/1	0.17	0.57	48,48,48,48	0
5	SO4	B	559	5/5	0.21	0.12	70,72,74,75	0
4	CL	B	555	1/1	0.12	-1.73	69,69,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.