



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:08 PM GMT

PDB ID : 3D2F
Title : Crystal structure of a complex of Sse1p and Hsp70
Authors : Polier, S.; Bracher, A.
Deposited on : 2008-05-08
Resolution : 2.30 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>

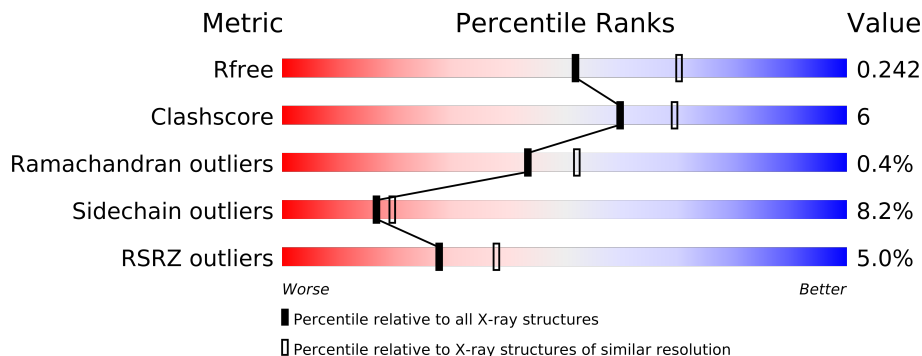
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	675	
1	C	675	
2	B	382	
2	D	382	

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	2001	-	X
4	K	A	3001	-	X
6	GOL	A	3002	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16199 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	629	Total	C	N	O	S	0	2	0
			4874	3085	817	960	12			
1	C	627	Total	C	N	O	S	0	1	0
			4828	3050	810	956	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	ALA	-	LINKER	UNP P32589
A	504	GLY	-	LINKER	UNP P32589
A	505	SER	-	LINKER	UNP P32589
A	506	ASP	-	LINKER	UNP P32589
C	503	ALA	-	LINKER	UNP P32589
C	504	GLY	-	LINKER	UNP P32589
C	505	SER	-	LINKER	UNP P32589
C	506	ASP	-	LINKER	UNP P32589

- Molecule 2 is a protein called Heat shock 70 kDa protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	1	0
			2895	1824	505	559	7			
2	D	379	Total	C	N	O	S	0	3	0
			2865	1806	490	562	7			

- 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	2	Total	Mg	0	0
			2	2		

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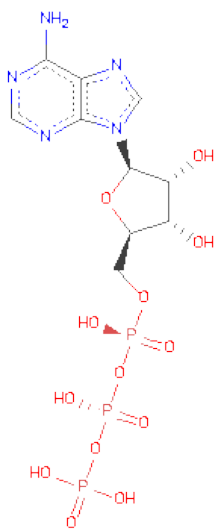
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

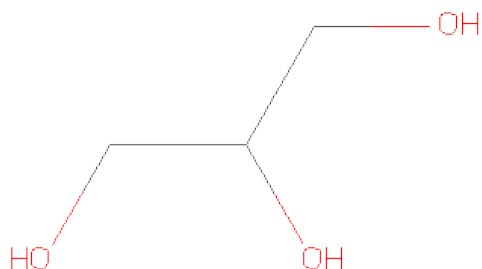
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

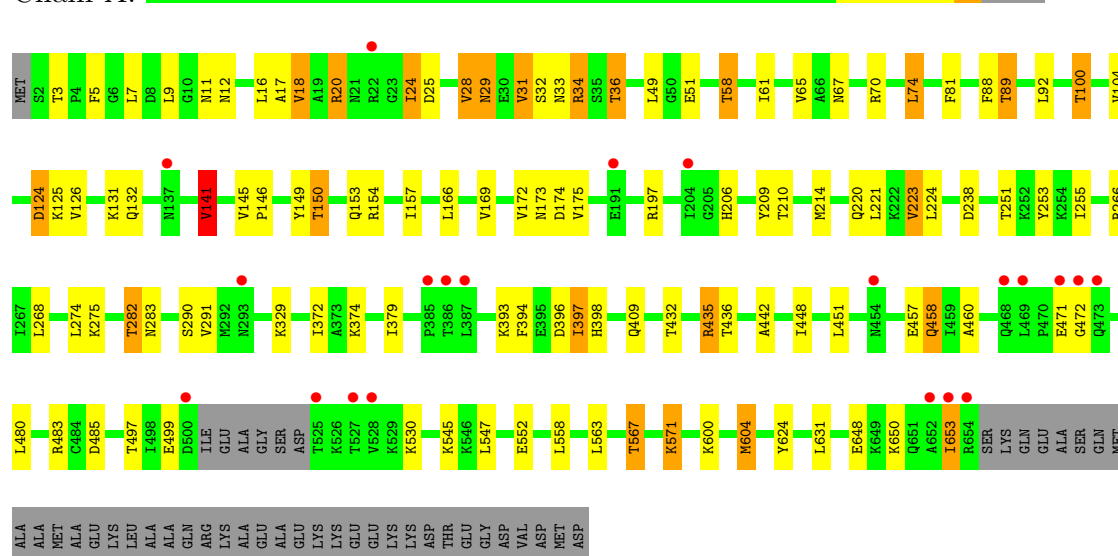
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	272	Total	O	0	0
			272	272		
7	B	102	Total	O	0	0
			102	102		
7	C	207	Total	O	0	0
			207	207		
7	D	80	Total	O	0	0
			80	80		

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.

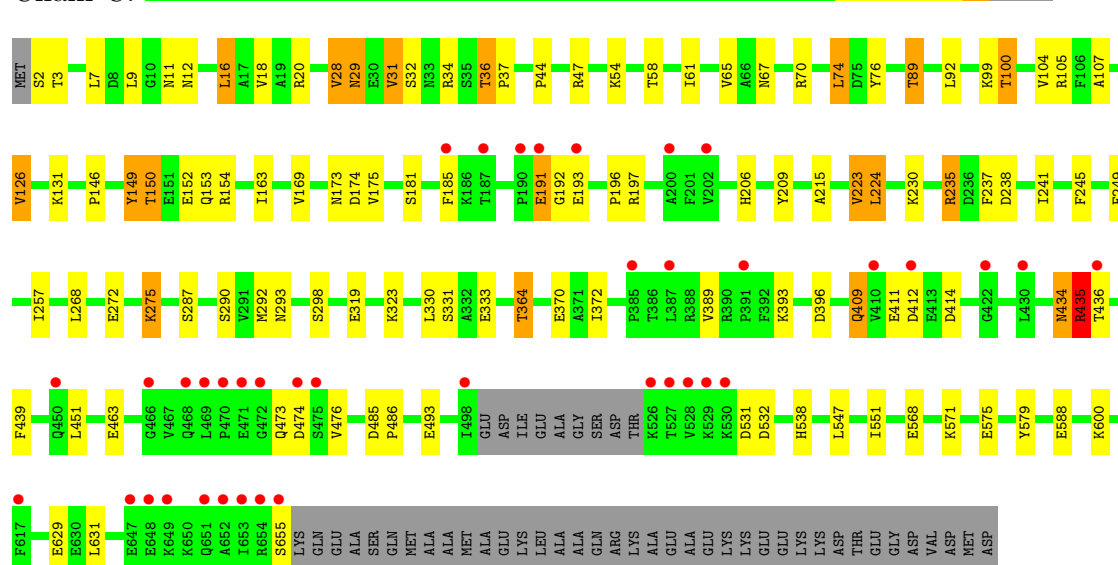
- Molecule 1: Heat shock protein homolog SSE1

Chain A:



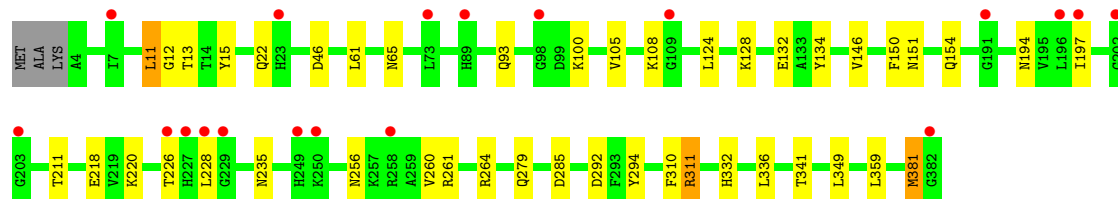
- Molecule 1: Heat shock protein homolog SSE1

Chain C:



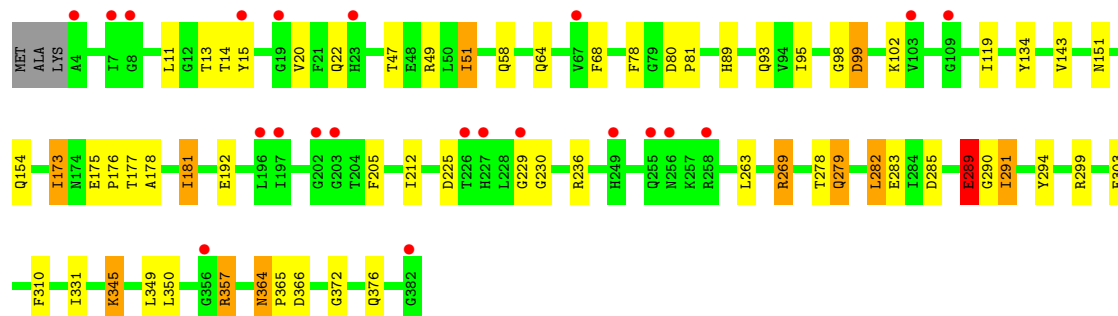
- Molecule 2: Heat shock 70 kDa protein 1

Chain B: 



- Molecule 2: Heat shock 70 kDa protein 1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	129.50Å 141.90Å 151.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 100.0 (19.93-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.244 0.197 , 0.242	Depositor DCC
R_{free} test set	6248 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 124106 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16199	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

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	0.59	1/4965 (0.0%)	0.73	5/6731 (0.1%)
1	C	0.79	13/4917 (0.3%)	0.75	4/6673 (0.1%)
2	B	0.55	0/2943	0.63	0/3988
2	D	1.21	7/2913 (0.2%)	0.67	5/3958 (0.1%)
All	All	0.80	21/15738 (0.1%)	0.71	14/21350 (0.1%)

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
1	C	0	1
2	B	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	289	GLU	CD-OE1	55.35	1.86	1.25
1	C	435	ARG	CZ-NH1	19.98	1.59	1.33
1	C	411	GLU	CD-OE1	14.87	1.42	1.25
1	C	434	ASN	CG-OD1	14.74	1.56	1.24
2	D	289	GLU	CD-OE2	-13.50	1.10	1.25
1	C	655	SER	C-O	13.40	1.48	1.23
1	C	414	ASP	CG-OD1	8.72	1.45	1.25
1	C	409	GLN	CD-NE2	7.94	1.52	1.32
1	C	435	ARG	NE-CZ	7.26	1.42	1.33
2	D	289	GLU	CG-CD	6.41	1.61	1.51
2	D	99	ASP	CG-OD1	6.33	1.40	1.25
2	D	289	GLU	C-N	5.99	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	474	ASP	CG-OD2	5.76	1.38	1.25
1	A	471	GLU	C-O	5.70	1.34	1.23
1	C	412	ASP	CG-OD2	5.35	1.37	1.25
2	D	99	ASP	CG-OD2	5.35	1.37	1.25
1	C	193	GLU	CG-CD	5.33	1.59	1.51
2	D	290	GLY	C-O	5.29	1.32	1.23
1	C	193	GLU	CD-OE2	5.26	1.31	1.25
1	C	435	ARG	CZ-NH2	5.12	1.39	1.33
1	C	414	ASP	CG-OD2	5.06	1.36	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	435	ARG	NE-CZ-NH2	-18.75	110.92	120.30
1	C	435	ARG	NE-CZ-NH1	11.00	125.80	120.30
2	D	289	GLU	CG-CD-OE2	8.11	134.53	118.30
1	A	141	VAL	CB-CA-C	-7.16	97.80	111.40
1	A	34	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	D	99	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	34	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	141	VAL	CG1-CB-CG2	5.69	120.00	110.90
2	D	289	GLU	CG-CD-OE1	-5.67	106.95	118.30
1	A	274	LEU	CA-CB-CG	5.47	127.89	115.30
2	D	282	LEU	CA-CB-CG	5.39	127.69	115.30
2	D	289	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	C	435	ARG	CD-NE-CZ	-5.32	116.16	123.60
1	C	224	LEU	CA-CB-CG	5.31	127.50	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	226	THR	Peptide
1	C	434	ASN	Sidechain

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	4874	0	4770	70	0
1	C	4828	0	4693	55	1
2	B	2895	0	2846	27	0
2	D	2865	0	2748	36	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	31	0	12	0	0
5	C	31	0	12	0	0
6	A	6	0	8	0	0
7	A	272	0	0	9	1
7	B	102	0	0	0	0
7	C	207	0	0	7	0
7	D	80	0	0	1	0
All	All	16199	0	15089	185	1

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 6.

All (185) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:289:GLU:CD	2:D:289:GLU:OE1	1.86	1.13
2:B:311:ARG:HH21	2:B:311:ARG:HG2	1.13	1.09
1:A:17:ALA:HB1	1:A:24[A]:ILE:HD11	1.40	1.02
1:C:61:ILE:O	1:C:89:THR:HG23	1.65	0.95
2:B:194:ASN:H	2:B:332:HIS:HD2	1.15	0.89
1:C:150:THR:HG22	1:C:153:GLN:H	1.43	0.84
2:B:311:ARG:HH21	2:B:311:ARG:CG	1.92	0.82
1:A:61:ILE:O	1:A:89:THR:HG23	1.77	0.82
1:C:238:ASP:OD1	1:C:275:LYS:HE3	1.79	0.81
1:A:266:ARG:NH2	1:A:290:SER:O	2.17	0.77
1:C:463:GLU:OE1	1:C:538:HIS:HE1	1.66	0.77
1:A:150:THR:HG21	7:A:3030:HOH:O	1.84	0.77
1:C:150:THR:HG21	7:C:3030:HOH:O	1.85	0.76
1:A:20:ARG:HD2	1:A:25:ASP:OD2	1.85	0.76
1:C:11:ASN:HD21	1:C:67:ASN:HA	1.51	0.76
1:C:36:THR:HG22	7:C:3015:HOH:O	1.85	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:61:ILE:O	1:C:89:THR:CG2	2.34	0.75
2:B:311:ARG:HG2	2:B:311:ARG:NH2	1.92	0.74
2:D:205:PHE:HB3	2:D:225:ASP:HB3	1.69	0.74
2:D:151:ASN:H	2:D:154:GLN:HE21	1.35	0.73
1:A:58:THR:HG22	7:A:3178:HOH:O	1.88	0.73
2:D:278:THR:OG1	2:D:279:GLN:NE2	2.21	0.73
1:A:563:LEU:O	1:A:567:THR:HG22	1.88	0.73
1:A:238:ASP:OD1	1:A:275:LYS:HE2	1.90	0.72
2:B:194:ASN:H	2:B:332:HIS:CD2	2.06	0.71
1:A:497:THR:HG22	1:A:530:LYS:HB3	1.73	0.71
2:D:364:ASN:C	2:D:364:ASN:HD22	1.96	0.69
1:A:175:VAL:HG13	7:A:3094:HOH:O	1.92	0.69
1:A:11:ASN:HD21	1:A:67:ASN:HA	1.57	0.68
2:D:181:ILE:HD13	2:D:376:GLN:HE21	1.58	0.68
2:D:14:THR:HG22	2:D:15[A]:TYR:CD1	2.31	0.66
1:A:61:ILE:O	1:A:89:THR:CG2	2.43	0.65
1:C:58:THR:HG21	2:D:269:ARG:HH22	1.61	0.65
1:A:31:VAL:HG13	1:A:51:GLU:HG3	1.79	0.64
1:A:49:LEU:HB2	1:A:125:LYS:HG3	1.80	0.64
2:D:310:PHE:CG	2:D:345:LYS:HG2	2.32	0.64
1:C:223:VAL:HG13	1:C:396:ASP:HA	1.80	0.62
1:A:150:THR:HG23	7:A:3144:HOH:O	1.99	0.62
1:A:150:THR:HG22	1:A:153:GLN:H	1.63	0.62
1:A:409:GLN:NE2	1:A:436:THR:H	1.97	0.62
1:A:154:ARG:HH22	1:A:173:ASN:HD21	1.46	0.62
1:A:223:VAL:HG13	1:A:396:ASP:HA	1.82	0.62
1:A:11:ASN:ND2	1:A:67:ASN:HA	2.14	0.61
1:A:5:PHE:CD1	1:A:141:VAL:HG13	2.35	0.61
2:D:289:GLU:H	2:D:291:ILE:HD12	1.65	0.61
1:A:24[A]:ILE:HD12	1:A:374:LYS:HG2	1.82	0.61
1:C:11:ASN:ND2	1:C:67:ASN:HA	2.15	0.60
2:D:177:THR:O	2:D:181:ILE:HG23	2.00	0.60
2:D:14:THR:HG22	2:D:15[A]:TYR:HD1	1.65	0.60
1:C:150:THR:HG23	7:C:3145:HOH:O	2.00	0.60
1:A:571:LYS:HB2	1:A:624:TYR:CE1	2.37	0.60
1:C:206:HIS:O	1:C:235:ARG:HB2	2.02	0.60
2:D:364:ASN:ND2	2:D:366:ASP:H	1.99	0.60
2:B:235:ASN:ND2	2:B:264:ARG:HH22	2.00	0.59
1:C:181:SER:O	1:C:185:PHE:HB3	2.03	0.58
2:D:364:ASN:HD22	2:D:366:ASP:H	1.50	0.57
2:B:310:PHE:HB3	2:B:349:LEU:HD11	1.84	0.57
2:B:11:LEU:HG	2:B:124:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:283:GLU:HG2	2:D:294:TYR:CD2	2.40	0.57
1:A:442:ALA:HB1	1:A:458:GLN:HE22	1.70	0.56
1:A:483:ARG:NH1	7:A:3233:HOH:O	2.06	0.56
2:B:211:THR:HG22	2:B:218:GLU:HB3	1.88	0.56
2:B:151:ASN:H	2:B:154:GLN:HE21	1.54	0.56
1:C:31:VAL:O	1:C:32:SER:HB2	2.06	0.55
2:B:381:MET:HE3	2:B:381:MET:HA	1.87	0.55
1:A:29:ASN:HD22	1:A:29:ASN:C	2.09	0.55
1:C:28:VAL:HG13	1:C:32:SER:HA	1.89	0.55
1:C:154:ARG:HH22	1:C:173:ASN:HD21	1.54	0.55
1:C:34:ARG:NH1	1:C:370:GLU:OE2	2.41	0.54
1:C:174:ASP:HB2	1:C:372:ILE:HD13	1.88	0.54
1:A:124:ASP:OD2	1:A:558:LEU:HD11	2.08	0.53
1:A:28:VAL:HG13	1:A:32:SER:HA	1.90	0.53
1:A:563:LEU:O	1:A:567:THR:CG2	2.56	0.53
2:D:49:ARG:HD2	2:D:51:ILE:HD11	1.91	0.52
2:B:381:MET:CE	2:B:381:MET:HA	2.38	0.52
1:A:600:LYS:O	1:A:604:MET:HG2	2.10	0.52
1:C:485:ASP:HB2	1:C:486:PRO:CD	2.40	0.51
1:A:74:LEU:O	1:A:100:THR:HG23	2.10	0.51
1:C:154:ARG:HH12	1:C:173:ASN:ND2	2.08	0.51
1:A:282:THR:HG23	7:A:3166:HOH:O	2.11	0.51
1:C:12:ASN:HB2	1:C:206:HIS:CG	2.46	0.51
1:A:24[A]:ILE:HD13	1:A:25:ASP:N	2.26	0.51
1:C:364:THR:O	1:C:364:THR:HG23	2.10	0.51
2:B:336:LEU:HD12	2:B:341:THR:HB	1.93	0.51
1:C:74:LEU:O	1:C:100:THR:HG22	2.10	0.51
1:C:196:PRO:HB2	1:C:215:ALA:HB1	1.92	0.50
1:A:18:VAL:HG13	1:A:20:ARG:HG2	1.93	0.50
1:A:17:ALA:CB	1:A:24[A]:ILE:HD11	2.27	0.50
2:D:310:PHE:HB3	2:D:349:LEU:HD11	1.93	0.50
1:C:257:ILE:HA	1:C:292:MET:CE	2.41	0.50
1:A:36:THR:HG22	7:A:3015:HOH:O	2.11	0.50
1:C:409:GLN:OE1	1:C:435:ARG:HG3	2.12	0.50
1:C:319:GLU:O	1:C:323:LYS:HG3	2.13	0.49
1:A:24[A]:ILE:C	1:A:24[A]:ILE:HD13	2.32	0.49
1:A:81:PHE:HE1	1:A:100:THR:HG21	1.78	0.49
1:C:29:ASN:C	1:C:29:ASN:HD22	2.16	0.49
1:A:650:LYS:HA	1:A:653:ILE:HD12	1.95	0.48
1:A:67:ASN:HB2	1:A:88:PHE:CZ	2.49	0.48
1:C:237:PHE:O	1:C:241:ILE:HG13	2.14	0.48
1:A:49:LEU:CB	1:A:125:LYS:HG3	2.44	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:146:PRO:O	1:C:149:TYR:HB2	2.14	0.48
2:B:235:ASN:HD21	2:B:264:ARG:HH22	1.61	0.48
1:C:131:LYS:HE3	7:C:3113:HOH:O	2.13	0.47
1:C:74:LEU:HB3	1:C:100:THR:HG23	1.96	0.47
1:A:29:ASN:ND2	1:A:33:ASN:H	2.12	0.47
1:C:76:TYR:HD1	1:C:100:THR:HB	1.78	0.47
2:D:78:PHE:N	2:D:99:ASP:O	2.47	0.47
2:B:22:GLN:NE2	2:B:134:TYR:OH	2.48	0.47
2:B:285:ASP:OD1	2:B:294:TYR:OH	2.22	0.47
1:C:435:ARG:HG2	1:C:439:PHE:CD1	2.50	0.46
1:A:31:VAL:HG22	1:A:33:ASN:ND2	2.29	0.46
2:D:310:PHE:CD1	2:D:345:LYS:HG2	2.50	0.46
1:A:571:LYS:HB2	1:A:624:TYR:CD1	2.49	0.46
1:A:458:GLN:NE2	1:A:460:ALA:O	2.48	0.46
1:A:175:VAL:HG11	1:A:210:THR:CG2	2.46	0.46
1:A:175:VAL:HG11	1:A:210:THR:HG21	1.97	0.46
1:A:141:VAL:HG22	1:A:166:LEU:HB3	1.96	0.46
2:D:68:PHE:HB2	7:D:1275:HOH:O	2.14	0.46
2:D:364:ASN:C	2:D:364:ASN:ND2	2.68	0.46
2:B:256:ASN:O	2:B:260:VAL:HG23	2.15	0.46
1:C:11:ASN:ND2	1:C:70:ARG:HG2	2.31	0.45
1:A:214:MET:HG2	1:A:223:VAL:HB	1.97	0.45
1:C:163:ILE:HA	1:C:551:ILE:HG12	1.98	0.45
1:A:145:VAL:HB	1:A:146:PRO:HD2	1.97	0.45
1:C:571:LYS:HE3	7:C:3205:HOH:O	2.17	0.45
1:C:330:LEU:HD12	1:C:331:SER:O	2.17	0.45
1:C:44:PRO:O	1:C:107:ALA:HA	2.16	0.45
1:C:16:LEU:HD11	1:C:126:VAL:HG22	1.99	0.45
1:C:191:GLU:HB3	1:C:192:GLY:H	1.57	0.45
2:B:146:VAL:HB	2:B:150:PHE:CD1	2.51	0.45
1:C:154:ARG:HH12	1:C:173:ASN:HD21	1.63	0.45
1:A:31:VAL:O	1:A:32:SER:HB2	2.17	0.44
2:D:143:VAL:HG11	2:D:173:ILE:HD12	1.98	0.44
1:C:37:PRO:HB3	1:C:54:LYS:HG3	1.99	0.44
2:D:364:ASN:HD22	2:D:365:PRO:N	2.15	0.44
1:A:409:GLN:HE22	1:A:435:ARG:HG3	1.83	0.44
2:B:292:ASP:HB3	2:B:294:TYR:CE2	2.53	0.44
1:A:24[A]:ILE:HD12	1:A:374:LYS:CG	2.48	0.44
2:B:336:LEU:HD21	2:B:359:LEU:HD22	1.99	0.44
2:B:46:ASP:O	2:B:108:LYS:HA	2.18	0.44
2:D:331:ILE:O	2:D:357:ARG:NH2	2.47	0.43
2:D:192:GLU:HA	2:D:212[A]:ILE:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:221:LEU:O	1:A:394:PHE:HA	2.18	0.43
1:A:397:ILE:HG13	1:A:398:HIS:N	2.33	0.43
2:D:151:ASN:H	2:D:154:GLN:NE2	2.07	0.43
2:B:65:ASN:HA	2:B:105:VAL:HG22	2.01	0.43
2:B:12:GLY:HA3	2:B:15[B]:TYR:O	2.19	0.43
1:C:175:VAL:HG13	7:C:3093:HOH:O	2.17	0.43
1:C:364:THR:O	1:C:364:THR:CG2	2.66	0.43
2:D:175:GLU:N	2:D:176:PRO:HD2	2.33	0.43
1:A:648:GLU:HG3	7:A:3267:HOH:O	2.19	0.43
1:C:2:SER:N	7:C:3185:HOH:O	2.51	0.42
1:C:575:GLU:HG2	1:C:579:TYR:CE1	2.53	0.42
2:D:303:GLU:HB3	2:D:345:LYS:HD2	2.00	0.42
1:C:629:GLU:HA	1:C:629:GLU:OE1	2.19	0.42
1:A:11:ASN:ND2	1:A:70:ARG:HG2	2.33	0.42
1:C:568:GLU:HB3	2:D:279:GLN:NE2	2.35	0.42
1:A:12:ASN:HB2	1:A:206:HIS:CG	2.54	0.42
1:A:31:VAL:HG23	1:A:31:VAL:O	2.19	0.42
1:A:253:TYR:HB2	1:A:255:ILE:HG12	2.02	0.42
1:A:448:ILE:HD13	1:A:457:GLU:HA	2.00	0.42
2:B:197:ILE:N	2:B:197:ILE:HD12	2.34	0.42
2:B:128:LYS:O	2:B:132:GLU:HG3	2.19	0.42
2:D:289:GLU:HG3	2:D:291:ILE:HD11	2.01	0.41
1:A:34:ARG:HD3	7:A:3018:HOH:O	2.20	0.41
2:D:20:VAL:HG13	2:D:22:GLN:HG2	2.01	0.41
2:B:261:ARG:HD3	2:B:261:ARG:O	2.20	0.41
1:A:238:ASP:OD1	1:A:275:LYS:CE	2.66	0.41
1:A:74:LEU:HB3	1:A:100:THR:HG23	2.01	0.41
1:C:245:PHE:HB3	1:C:249:PHE:CE2	2.56	0.41
2:D:95:ILE:HG13	2:D:102:LYS:HB2	2.03	0.41
1:A:174:ASP:HB2	1:A:372:ILE:HD13	2.02	0.41
1:A:29:ASN:HD21	1:A:33:ASN:H	1.68	0.41
2:D:143:VAL:CG1	2:D:173:ILE:CD1	2.99	0.41
1:C:257:ILE:HA	1:C:292:MET:HE3	2.03	0.41
1:C:31:VAL:O	1:C:31:VAL:CG2	2.69	0.41
2:D:22:GLN:NE2	2:D:134:TYR:OH	2.52	0.41
1:A:497:THR:HG21	1:A:530:LYS:HD3	2.03	0.41
2:B:93:GLN:HE21	2:D:89:HIS:HD2	1.69	0.40
1:A:220:GLN:HA	1:A:393:LYS:O	2.21	0.40
1:A:172:VAL:HG21	1:A:379:ILE:HD13	2.04	0.40
1:C:36:THR:HA	1:C:37:PRO:HD3	1.97	0.40
1:A:157:ILE:HD12	1:A:157:ILE:HA	1.87	0.40
2:D:178:ALA:O	2:D:372:GLY:HA3	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:99:LYS:HE3	1:C:152:GLU:OE1	2.21	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:C:293:ASN:OD1	7:A:3056:HOH:O[4_467]	2.13	0.07

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	627/675 (93%)	600 (96%)	24 (4%)	3 (0%)	38	45
1	C	624/675 (92%)	594 (95%)	29 (5%)	1 (0%)	56	68
2	B	378/382 (99%)	365 (97%)	13 (3%)	0	100	100
2	D	380/382 (100%)	365 (96%)	11 (3%)	4 (1%)	21	21
All	All	2009/2114 (95%)	1924 (96%)	77 (4%)	8 (0%)	43	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	499	GLU
1	A	472	GLY
1	C	473	GLN
2	D	230	GLY
2	D	98	GLY
1	A	653	ILE
2	D	229	GLY
2	D	81	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	520/576 (90%)	469 (90%)	51 (10%)	12	13
1	C	512/576 (89%)	462 (90%)	50 (10%)	12	13
2	B	301/315 (96%)	292 (97%)	9 (3%)	53	70
2	D	291/315 (92%)	267 (92%)	24 (8%)	17	19
All	All	1624/1782 (91%)	1490 (92%)	134 (8%)	17	19

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	7	LEU
1	A	9	LEU
1	A	16	LEU
1	A	18	VAL
1	A	20	ARG
1	A	24[A]	ILE
1	A	24[B]	ILE
1	A	28	VAL
1	A	29	ASN
1	A	31	VAL
1	A	36	THR
1	A	58	THR
1	A	65	VAL
1	A	74	LEU
1	A	89	THR
1	A	92	LEU
1	A	100	THR
1	A	104	VAL
1	A	124	ASP
1	A	126	VAL
1	A	131	LYS
1	A	132	GLN
1	A	141	VAL
1	A	149	TYR
1	A	150	THR

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Mol	Chain	Res	Type
1	A	169	VAL
1	A	197	ARG
1	A	209	TYR
1	A	223	VAL
1	A	224	LEU
1	A	251	THR
1	A	268	LEU
1	A	282	THR
1	A	283	ASN
1	A	291	VAL
1	A	329	LYS
1	A	397	ILE
1	A	432	THR
1	A	435	ARG
1	A	451	LEU
1	A	458	GLN
1	A	480	LEU
1	A	485	ASP
1	A	545	LYS
1	A	547	LEU
1	A	552	GLU
1	A	567	THR
1	A	571	LYS
1	A	604	MET
1	A	631	LEU
2	B	11	LEU
2	B	13	THR
2	B	61	LEU
2	B	100	LYS
2	B	220	LYS
2	B	228	LEU
2	B	279	GLN
2	B	311	ARG
2	B	381	MET
1	C	3	THR
1	C	7	LEU
1	C	9	LEU
1	C	16	LEU
1	C	18	VAL
1	C	20	ARG
1	C	28	VAL
1	C	29	ASN

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Mol	Chain	Res	Type
1	C	31	VAL
1	C	36	THR
1	C	47	ARG
1	C	65	VAL
1	C	74	LEU
1	C	89	THR
1	C	92	LEU
1	C	100	THR
1	C	104	VAL
1	C	105	ARG
1	C	126	VAL
1	C	149	TYR
1	C	150	THR
1	C	169	VAL
1	C	191	GLU
1	C	197	ARG
1	C	209	TYR
1	C	223	VAL
1	C	224	LEU
1	C	230	LYS
1	C	235	ARG
1	C	268	LEU
1	C	272	GLU
1	C	275	LYS
1	C	287	SER
1	C	290	SER
1	C	298	SER
1	C	333	GLU
1	C	364	THR
1	C	389	VAL
1	C	393	LYS
1	C	435	ARG
1	C	436	THR
1	C	451	LEU
1	C	476	VAL
1	C	493	GLU
1	C	531	ASP
1	C	532	ASP
1	C	547	LEU
1	C	588	GLU
1	C	600	LYS
1	C	631	LEU

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Mol	Chain	Res	Type
2	D	11	LEU
2	D	13	THR
2	D	47	THR
2	D	51	ILE
2	D	58	GLN
2	D	64	GLN
2	D	80	ASP
2	D	93	GLN
2	D	119	ILE
2	D	173	ILE
2	D	181	ILE
2	D	236	ARG
2	D	263	LEU
2	D	269	ARG
2	D	279	GLN
2	D	282	LEU
2	D	285	ASP
2	D	289	GLU
2	D	291	ILE
2	D	299	ARG
2	D	345	LYS
2	D	350	LEU
2	D	357	ARG
2	D	364	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	13	ASN
1	A	21	ASN
1	A	29	ASN
1	A	60	ASN
1	A	156	ASN
1	A	173	ASN
1	A	409	GLN
1	A	454	ASN
1	A	458	GLN
1	A	548	ASN
1	A	555	ASN
1	A	602	GLN
2	B	22	GLN

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Mol	Chain	Res	Type
2	B	84	GLN
2	B	154	GLN
2	B	235	ASN
2	B	279	GLN
2	B	332	HIS
2	B	376	GLN
1	C	11	ASN
1	C	13	ASN
1	C	29	ASN
1	C	60	ASN
1	C	111	HIS
1	C	117	GLN
1	C	156	ASN
1	C	173	ASN
1	C	352	GLN
1	C	538	HIS
1	C	548	ASN
1	C	555	ASN
1	C	602	GLN
2	D	22	GLN
2	D	64	GLN
2	D	89	HIS
2	D	93	GLN
2	D	154	GLN
2	D	194	ASN
2	D	279	GLN
2	D	364	ASN
2	D	376	GLN

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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	ATP	A	1001	3,4	33,33,33	1.20	4 (12%)	52,52,52	1.89	10 (19%)
6	GOL	A	3002	-	5,5,5	0.57	0	5,5,5	0.82	0
5	ATP	C	1001	3,4	33,33,33	1.07	3 (9%)	52,52,52	1.80	9 (17%)

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	ATP	A	1001	3,4	-	0/22/38/38	0/1/3/3
6	GOL	A	3002	-	-	0/4/4/4	0/0/0/0
5	ATP	C	1001	3,4	-	0/22/38/38	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1001	ATP	C5-C4	3.31	1.48	1.40
5	A	1001	ATP	C5-C4	3.06	1.47	1.40
5	A	1001	ATP	C4-N9	-2.76	1.33	1.37
5	A	1001	ATP	PB-O3B	2.59	1.64	1.59
5	C	1001	ATP	C4-N9	-2.34	1.34	1.37
5	A	1001	ATP	PG-O3B	2.20	1.64	1.60
5	C	1001	ATP	PB-O3B	2.15	1.63	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	ATP	N3-C2-N1	-7.01	122.85	128.71
5	C	1001	ATP	N3-C2-N1	-6.56	123.23	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	ATP	N3-C4-N9	5.34	135.08	125.43
5	A	1001	ATP	O4'-C1'-N9	4.91	113.00	108.44
5	C	1001	ATP	N3-C4-N9	4.83	134.16	125.43
5	C	1001	ATP	O4'-C1'-N9	4.53	112.65	108.44
5	A	1001	ATP	C8-N9-C4	3.54	109.60	106.90
5	C	1001	ATP	C8-N9-C4	3.32	109.43	106.90
5	C	1001	ATP	C4-C5-N7	-3.25	106.74	109.52
5	A	1001	ATP	C5-C4-N3	-2.87	119.45	125.70
5	A	1001	ATP	C4-C5-N7	-2.84	107.09	109.52
5	C	1001	ATP	C1'-N9-C4	-2.63	122.09	126.64
5	C	1001	ATP	C5-C4-N3	-2.54	120.17	125.70
5	A	1001	ATP	C2-N3-C4	2.49	121.08	114.01
5	A	1001	ATP	O3A-PB-O3B	-2.45	96.69	101.66
5	A	1001	ATP	O3G-PG-O2G	2.30	116.58	107.61
5	C	1001	ATP	C2-N3-C4	2.23	120.37	114.01
5	A	1001	ATP	C2-N1-C6	2.01	122.40	118.77
5	C	1001	ATP	C2-N1-C6	2.01	122.40	118.77

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	629/675 (93%)	-0.05	21 (3%)	44	54	34, 43, 54, 68	0
1	C	627/675 (92%)	0.15	39 (6%)	20	28	35, 44, 55, 76	0
2	B	379/382 (99%)	0.14	19 (5%)	28	38	35, 44, 54, 79	0
2	D	379/382 (99%)	0.31	22 (5%)	22	31	38, 45, 52, 72	0
All	All	2014/2114 (95%)	0.11	101 (5%)	28	38	34, 44, 54, 79	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	226	THR	8.4
2	B	227	HIS	6.4
1	C	527	THR	6.3
1	C	654	ARG	6.1
2	D	382	GLY	5.9
2	B	228	LEU	5.7
2	D	227	HIS	5.7
1	A	473	GLN	5.5
1	A	525	THR	5.5
2	D	255	GLN	5.3
1	C	474	ASP	5.2
2	D	229	GLY	5.2
2	B	229	GLY	5.1
1	A	653	ILE	5.1
1	A	500	ASP	5.0
1	C	653	ILE	4.8
1	A	652	ALA	4.7
1	C	191	GLU	4.7
1	A	386	THR	4.5
1	C	528	VAL	4.4
1	C	193	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	226	THR	4.3
1	C	471	GLU	4.1
1	C	410	VAL	4.1
2	D	202	GLY	4.0
1	C	652	ALA	4.0
1	A	527	THR	4.0
2	B	382	GLY	4.0
2	D	196	LEU	3.9
1	C	530	LYS	3.8
2	B	202	GLY	3.8
1	A	528	VAL	3.8
1	A	385	PRO	3.7
1	C	187	THR	3.7
2	D	203	GLY	3.7
2	D	23	HIS	3.7
1	A	387	LEU	3.6
1	C	651	GLN	3.6
1	C	475	SER	3.5
2	D	258	ARG	3.4
2	B	7	ILE	3.4
1	C	648	GLU	3.3
1	A	293	ASN	3.3
2	B	109	GLY	3.2
2	B	196	LEU	3.2
1	C	649	LYS	3.2
2	D	4	ALA	3.2
1	A	22	ARG	3.2
2	D	256	ASN	3.2
2	B	250	LYS	3.1
1	A	469	LEU	3.1
1	C	202	VAL	3.1
2	B	98	GLY	3.1
2	D	109	GLY	3.0
1	A	471	GLU	3.0
1	C	647	GLU	2.9
1	C	617	PHE	2.8
2	D	249	HIS	2.8
1	C	200	ALA	2.7
1	C	470	PRO	2.7
1	C	412	ASP	2.7
2	B	203	GLY	2.7
1	C	469	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	466	GLY	2.6
1	C	185	PHE	2.6
2	B	197	ILE	2.6
1	C	450	GLN	2.5
1	C	391	PRO	2.5
2	B	249	HIS	2.5
1	A	654	ARG	2.5
2	D	7	ILE	2.5
2	D	356	GLY	2.4
1	C	526	LYS	2.4
1	A	137	ASN	2.4
1	A	454	ASN	2.4
2	D	197	ILE	2.4
1	C	655	SER	2.4
2	B	191	GLY	2.3
1	C	387	LEU	2.3
1	C	190	PRO	2.3
1	C	498	ILE	2.3
1	C	529	LYS	2.3
2	D	103	VAL	2.3
2	B	258	ARG	2.3
1	C	472	GLY	2.2
2	D	15[A]	TYR	2.2
1	A	468	GLN	2.2
1	C	430	LEU	2.2
1	C	468	GLN	2.2
2	B	23	HIS	2.2
1	A	472	GLY	2.2
2	D	19	GLY	2.1
2	D	67	VAL	2.1
1	C	422	GLY	2.1
2	B	89	HIS	2.1
1	A	204	ILE	2.1
1	C	385	PRO	2.0
2	D	8	GLY	2.0
1	A	191	GLU	2.0
2	B	73	LEU	2.0
1	C	436	THR	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 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
4	K	A	3001	1/1	0.22	6.63	44,44,44,44	0
6	GOL	A	3002	6/6	0.20	5.28	57,60,61,62	0
3	MG	A	2001	1/1	0.18	2.09	40,40,40,40	0
5	ATP	A	1001	31/31	0.17	1.55	40,42,45,47	0
4	K	C	3001	1/1	0.17	1.32	45,45,45,45	0
5	ATP	C	1001	31/31	0.13	0.35	36,41,43,44	0
3	MG	C	2001	1/1	0.10	-0.35	40,40,40,40	0
3	MG	A	2002	1/1	0.14	-0.58	42,42,42,42	0
3	MG	C	2002	1/1	0.14	-0.59	29,29,29,29	0
3	MG	B	2001	1/1	0.11	-0.89	37,37,37,37	0
3	MG	D	2001	1/1	0.11	-1.00	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.