



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 05:06 am 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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

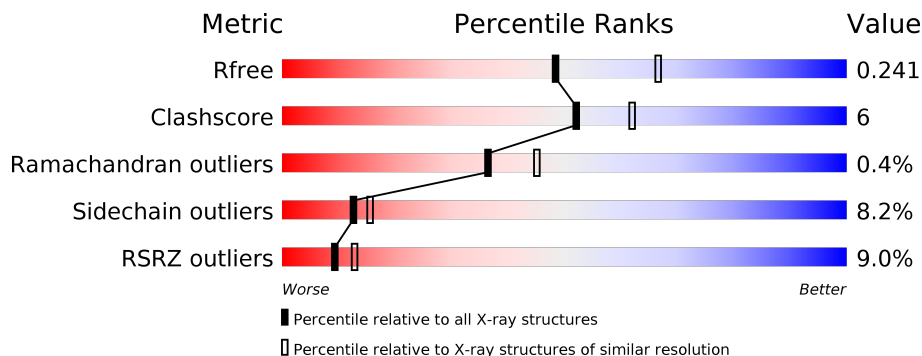
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	675	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	675	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>7%</div> </div> </div>
2	B	382	<div> <div>9%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>••</div> </div> </div>
2	D	382	<div> <div>12%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16199 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 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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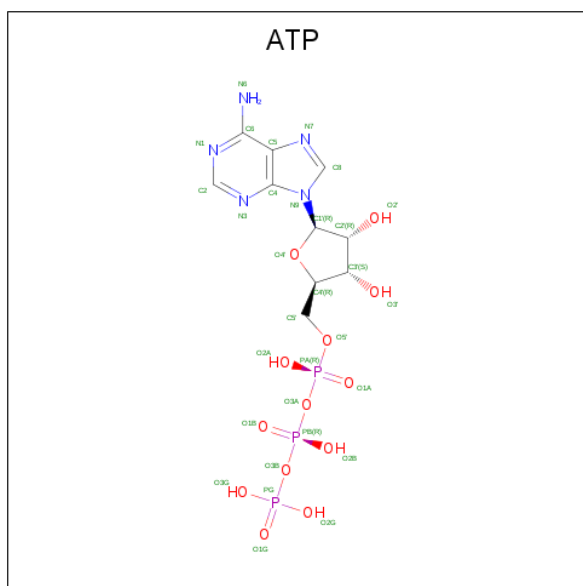
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		

- 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		

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	Depositor
R, R_{free}	0.197 , 0.244 0.196 , 0.241	Depositor DCC
R_{free} test set	6248 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 6.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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
1:C:61:ILE:O	1:C:89:THR:CG2	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:563:LEU:O	1:A:567:THR:HG22	1.88	0.73
2:D:278:THR:OG1	2:D:279:GLN:NE2	2.21	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:5:PHE:CD1	1:A:141:VAL:HG13	2.35	0.61
1:A:11:ASN:ND2	1:A:67:ASN:HA	2.14	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:11:LEU:HG	2:B:124:LEU:HD21	1.87	0.57
2:B:310:PHE:HB3	2:B:349:LEU:HD11	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:A:282:THR:HG23	7:A:3166:HOH:O	2.11	0.51
1:C:154:ARG:HH12	1:C:173:ASN:ND2	2.08	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
2:B:336:LEU:HD12	2:B:341:THR:HB	1.93	0.51
1:C:364:THR:O	1:C:364:THR:HG23	2.10	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
1:C:257:ILE:HA	1:C:292:MET:CE	2.41	0.50
2:D:310:PHE:HB3	2:D:349:LEU:HD11	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:CB	1:A:125:LYS:HG3	2.44	0.48
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
1:A:571:LYS:HB2	1:A:624:TYR:CD1	2.49	0.46
2:D:310:PHE:CD1	2:D:345:LYS:HG2	2.50	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:141:VAL:HG22	1:A:166:LEU:HB3	1.96	0.46
1:A:175:VAL:HG11	1:A:210:THR:HG21	1.97	0.46
2:D:68:PHE:HB2	7:D:1275:HOH:O	2.14	0.46
2:B:256:ASN:O	2:B:260:VAL:HG23	2.15	0.46
2:D:364:ASN:C	2:D:364:ASN:ND2	2.68	0.46
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:C:11:ASN:ND2	1:C:70:ARG:HG2	2.31	0.45
1:A:145:VAL:HB	1:A:146:PRO:HD2	1.97	0.45
1:C:330:LEU:HD12	1:C:331:SER:O	2.17	0.45
1:C:571:LYS:HE3	7:C:3205:HOH: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:46:ASP:O	2:B:108:LYS:HA	2.18	0.44
2:B:336:LEU:HD21	2:B:359:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:ILE:O	2:D:357:ARG:NH2	2.47	0.43
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:192:GLU:HA	2:D:212[A]:ILE:O	2.18	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:A:648:GLU:HG3	7:A:3267:HOH:O	2.19	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: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
1:C:629:GLU:HA	1:C:629:GLU:OE1	2.19	0.42
2:D:303:GLU:HB3	2:D:345:LYS:HD2	2.00	0.42
1:A:11:ASN:ND2	1:A:70:ARG:HG2	2.33	0.42
1:A:12:ASN:HB2	1:A:206:HIS:CG	2.54	0.42
1:C:568:GLU:HB3	2:D:279:GLN:NE2	2.35	0.42
1:A:253:TYR:HB2	1:A:255:ILE:HG12	2.02	0.42
1:A:31:VAL:O	1:A:31:VAL:HG23	2.19	0.42
1:A:448:ILE:HD13	1:A:457:GLU:HA	2.00	0.42
2:B:128:LYS:O	2:B:132:GLU:HG3	2.19	0.42
2:B:197:ILE:N	2:B:197:ILE:HD12	2.34	0.42
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:D:289:GLU:HG3	2:D:291:ILE:HD11	2.01	0.41
2:B:261:ARG:HD3	2:B:261:ARG:O	2.20	0.41
1:A:74:LEU:HB3	1:A:100:THR:HG23	2.01	0.41
1:A:238:ASP:OD1	1:A:275:LYS:CE	2.66	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:172:VAL:HG21	1:A:379:ILE:HD13	2.04	0.40
1:A:220:GLN:HA	1:A:393:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	Interatomic distance (Å)	Clash overlap (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%)	31	38
1	C	624/675 (92%)	594 (95%)	29 (5%)	1 (0%)	49	61
2	B	378/382 (99%)	365 (97%)	13 (3%)	0	100	100
2	D	380/382 (100%)	365 (96%)	11 (3%)	4 (1%)	16	17
All	All	2009/2114 (95%)	1924 (96%)	77 (4%)	8 (0%)	36	45

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

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Mol	Chain	Res	Type
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%)	9	10
1	C	512/576 (89%)	462 (90%)	50 (10%)	9	10
2	B	301/315 (96%)	292 (97%)	9 (3%)	44	60
2	D	291/315 (92%)	267 (92%)	24 (8%)	12	15
All	All	1624/1782 (91%)	1490 (92%)	134 (8%)	12	15

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	27,33,33	1.09	2 (7%)	27,52,52	1.74	4 (14%)
6	GOL	A	3002	-	5,5,5	0.63	0	5,5,5	0.78	0
5	ATP	C	1001	3,4	27,33,33	1.06	2 (7%)	27,52,52	1.72	4 (14%)

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	-	0/18/38/38	0/3/3/3
6	GOL	A	3002	-	-	0/4/4/4	0/0/0/0
5	ATP	C	1001	3,4	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1001	ATP	PG-O3B	2.31	1.63	1.60
5	A	1001	ATP	PG-O3B	2.61	1.64	1.60
5	A	1001	ATP	C5-C4	3.06	1.47	1.40
5	C	1001	ATP	C5-C4	3.31	1.48	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	ATP	N3-C2-N1	-7.03	122.85	128.86
5	C	1001	ATP	N3-C2-N1	-6.59	123.23	128.86
5	C	1001	ATP	C4-C5-N7	-2.77	106.74	109.41
5	C	1001	ATP	C1'-N9-C4	-2.63	122.09	126.64
5	A	1001	ATP	C4-C5-N7	-2.40	107.09	109.41
5	A	1001	ATP	C2-N1-C6	2.15	122.40	118.75
5	C	1001	ATP	C2-N1-C6	2.15	122.40	118.75
5	A	1001	ATP	O3G-PG-O2G	2.27	116.58	107.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	629/675 (93%)	0.25	36 (5%) 24 30	34, 43, 54, 68	0
1	C	627/675 (92%)	0.47	63 (10%) 7 10	35, 44, 55, 76	0
2	B	379/382 (99%)	0.47	36 (9%) 8 11	35, 44, 54, 79	0
2	D	379/382 (99%)	0.62	47 (12%) 4 6	38, 45, 52, 72	0
All	All	2014/2114 (95%)	0.43	182 (9%) 9 13	34, 44, 54, 79	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	226	THR	8.3
1	C	654	ARG	7.7
1	A	525	THR	7.5
2	B	226	THR	6.8
2	D	229	GLY	6.8
2	B	227	HIS	6.5
1	C	474	ASP	6.3
1	C	410	VAL	6.1
2	B	382	GLY	6.1
1	C	193	GLU	6.0
2	D	227	HIS	6.0
1	A	652	ALA	5.9
1	C	530	LYS	5.8
1	C	651	GLN	5.8
2	B	228	LEU	5.8
2	D	382	GLY	5.8
1	A	473	GLN	5.8
2	D	255	GLN	5.8
1	C	191	GLU	5.7
1	A	653	ILE	5.7
2	D	203	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
2	D	23	HIS	5.1
1	C	653	ILE	5.1
2	D	258	ARG	5.1
2	D	256	ASN	5.1
2	B	202	GLY	4.9
1	A	500	ASP	4.8
1	A	386	THR	4.7
2	D	196	LEU	4.6
1	A	385	PRO	4.6
1	C	187	THR	4.5
2	D	202	GLY	4.5
1	C	391	PRO	4.5
2	B	7	ILE	4.4
1	C	652	ALA	4.4
2	B	229	GLY	4.3
1	C	528	VAL	4.2
2	B	258	ARG	4.2
1	C	475	SER	4.1
1	A	528	VAL	4.0
1	C	471	GLU	4.0
2	B	196	LEU	4.0
1	A	527	THR	3.8
1	C	647	GLU	3.8
1	A	469	LEU	3.8
2	B	249	HIS	3.7
1	C	527	THR	3.6
1	C	649	LYS	3.6
2	B	191	GLY	3.6
1	C	450	GLN	3.5
1	A	293	ASN	3.5
1	C	655	SER	3.5
2	D	257	LYS	3.5
1	C	430	LEU	3.4
2	D	7	ILE	3.4
1	A	387	LEU	3.4
2	B	197	ILE	3.4
1	C	468	GLN	3.3
2	D	197	ILE	3.3
1	C	532	ASP	3.3
1	C	202	VAL	3.3
1	C	470	PRO	3.2
1	A	22	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	185	PHE	3.2
2	B	98	GLY	3.2
1	C	648	GLU	3.1
1	C	617	PHE	3.1
1	C	412	ASP	3.0
1	A	202	VAL	3.0
2	D	249	HIS	3.0
2	B	109	GLY	3.0
1	A	499	GLU	3.0
2	B	73	LEU	3.0
2	B	60	ALA	3.0
2	B	23	HIS	3.0
2	B	250	LYS	2.9
2	D	98	GLY	2.9
2	D	356	GLY	2.9
1	C	58	THR	2.8
1	C	376	ALA	2.8
1	C	535	ILE	2.8
2	D	8	GLY	2.8
2	B	252	ASP	2.8
1	C	333	GLU	2.8
2	B	6	ALA	2.8
1	A	193	GLU	2.7
2	B	18	VAL	2.7
2	D	198	PHE	2.7
2	B	99	ASP	2.7
1	A	141	VAL	2.7
2	D	99	ASP	2.7
1	A	204	ILE	2.7
2	B	261	ARG	2.7
1	A	142	CYS	2.7
1	C	204	ILE	2.7
2	D	4	ALA	2.7
2	B	79	GLY	2.7
1	A	200	ALA	2.7
1	C	200	ALA	2.7
2	D	355	ASN	2.7
2	D	163	VAL	2.7
2	D	9	ILE	2.6
1	C	387	LEU	2.6
1	C	329	LYS	2.6
1	C	650	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	164	ILE	2.6
1	C	377	ALA	2.6
2	D	47	THR	2.6
2	D	67	VAL	2.6
1	C	469	LEU	2.6
1	C	192	GLY	2.6
2	B	245	PHE	2.5
2	B	225	ASP	2.5
1	C	436	THR	2.5
2	D	156	GLN	2.5
2	D	250	LYS	2.5
1	C	454	ASN	2.5
2	D	15[A]	TYR	2.5
1	C	472	GLY	2.5
2	D	97	ASP	2.5
2	B	237	LEU	2.5
1	C	543	ASP	2.5
1	C	529	LYS	2.4
1	A	137	ASN	2.4
1	C	137	ASN	2.4
1	A	391	PRO	2.4
1	C	218	LYS	2.4
1	A	377	ALA	2.4
2	D	123	VAL	2.4
2	D	269	ARG	2.4
2	B	284	ILE	2.4
1	A	376	ALA	2.4
1	C	388	ARG	2.4
2	D	214	ASP	2.4
1	A	241	ILE	2.4
2	B	317	VAL	2.4
1	C	23	GLY	2.3
1	A	468	GLN	2.3
1	A	185[A]	PHE	2.3
2	D	96	ASN	2.3
1	A	531	ASP	2.3
2	B	203	GLY	2.3
2	B	108	LYS	2.3
1	A	454	ASN	2.3
1	A	5	PHE	2.3
2	D	379	ILE	2.3
1	A	478	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	253	ILE	2.2
2	D	19	GLY	2.2
1	C	534	THR	2.2
2	D	46	ASP	2.2
1	C	613	TYR	2.2
2	D	149	TYR	2.2
2	B	42	VAL	2.2
1	C	414	ASP	2.2
2	D	294	TYR	2.2
1	C	466	GLY	2.2
2	D	109	GLY	2.2
1	A	617	PHE	2.2
1	C	480	LEU	2.2
2	D	127	MET	2.2
2	B	256	ASN	2.1
1	A	605	LEU	2.1
2	D	11	LEU	2.1
2	B	255	GLN	2.1
1	C	478	VAL	2.1
1	C	531	ASP	2.1
1	C	464	ILE	2.1
1	C	413	GLU	2.1
1	C	526	LYS	2.1
1	C	533	LEU	2.1
2	D	195	VAL	2.1
2	D	110	GLU	2.1
1	A	471	GLU	2.0
1	A	530	LYS	2.0
2	D	207	VAL	2.0
1	C	22	ARG	2.0
2	D	228	LEU	2.0
1	A	21	ASN	2.0
1	C	298	SER	2.0
2	B	195	VAL	2.0
1	C	221	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	A	3002	6/6	0.80	0.20	57,60,61,62	0
3	MG	C	2002	1/1	0.89	0.11	29,29,29,29	0
3	MG	D	2001	1/1	0.91	0.14	33,33,33,33	0
3	MG	C	2001	1/1	0.94	0.06	40,40,40,40	0
3	MG	A	2002	1/1	0.96	0.16	42,42,42,42	0
3	MG	B	2001	1/1	0.96	0.14	37,37,37,37	0
3	MG	A	2001	1/1	0.98	0.10	40,40,40,40	0
4	K	C	3001	1/1	0.99	0.14	45,45,45,45	0
5	ATP	A	1001	31/31	0.99	0.10	40,42,45,47	0
5	ATP	C	1001	31/31	0.99	0.09	36,41,43,44	0
4	K	A	3001	1/1	1.00	0.12	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.