



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2017 – 08:27 PM EDT

PDB ID : 3D2E
Title : Crystal structure of a complex of Sse1p and Hsp70, Selenomethionine-labeled crystals
Authors : Polier, S.; Bracher, A.
Deposited on : unknown
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

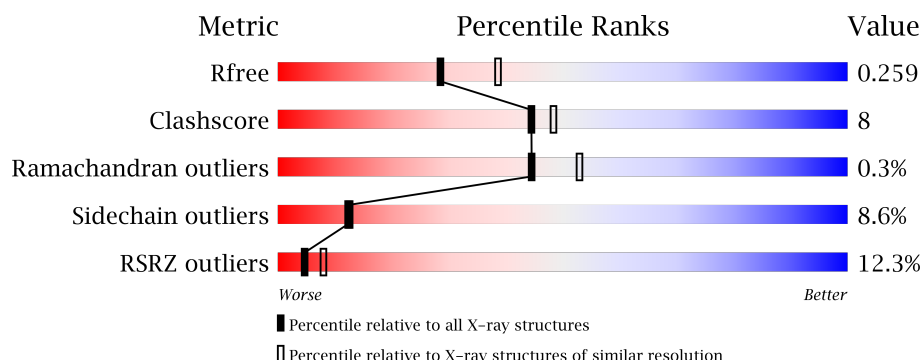
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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>10%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	C	675	<div> <div>12%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 7%</div> </div> </div>
2	B	382	<div> <div>12%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>••</div> </div> </div>
2	D	382	<div> <div>13%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>••</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15834 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	Se	0	1	0
			4835	3056	813	954	5	7			
1	C	627	Total	C	N	O	S	Se	0	0	0
			4812	3040	808	952	5	7			

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

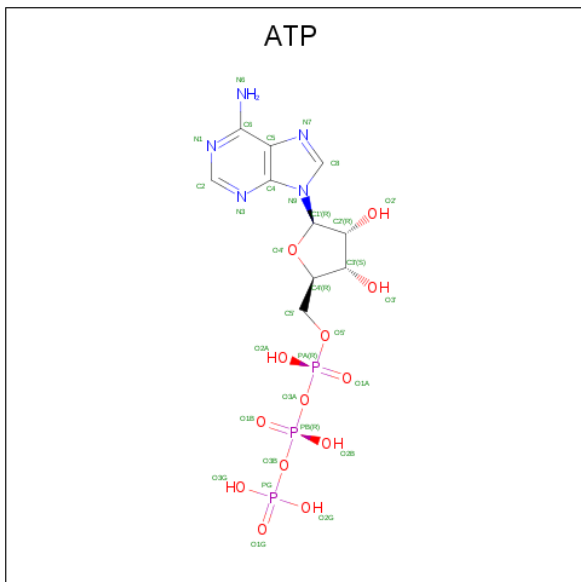
- Molecule 2 is a protein called Heat shock 70 kDa protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	Se	0	0	0
			2869	1811	497	554	3	4			
2	D	379	Total	C	N	O	S	Se	0	0	0
			2820	1775	486	552	3	4			

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

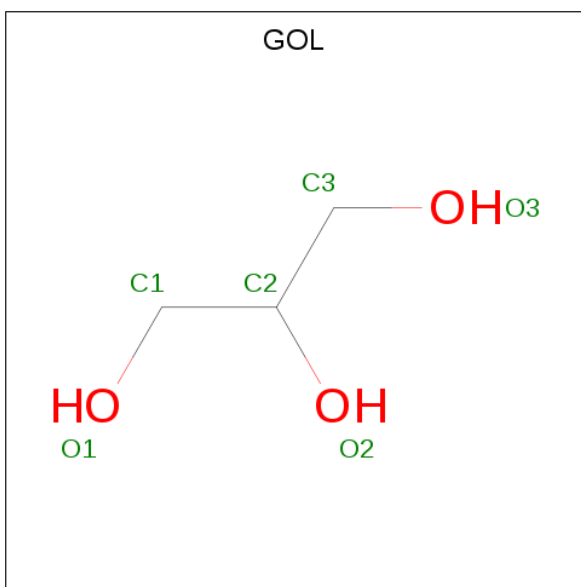
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	161	Total	O	0	0
			161	161		
6	B	65	Total	O	0	0
			65	65		
6	C	144	Total	O	0	0
			144	144		
6	D	58	Total	O	0	0
			58	58		

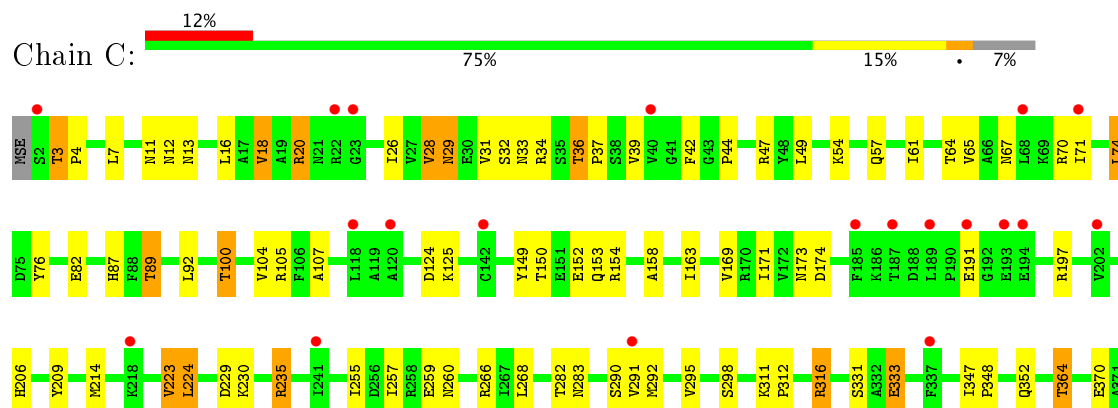
3 Residue-property plots [i](#)

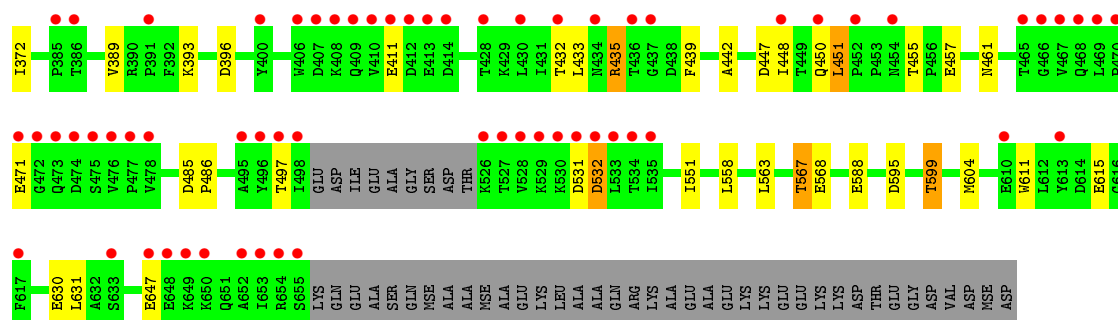
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Heat shock protein homolog SSE1

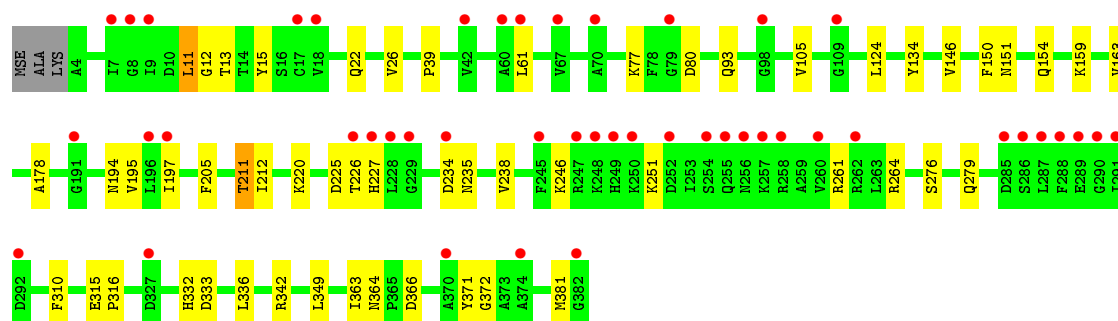
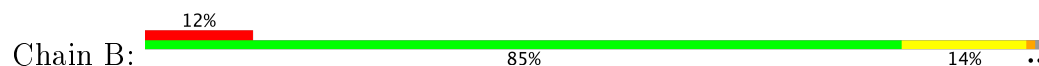


- Molecule 1: Heat shock protein homolog SSE1

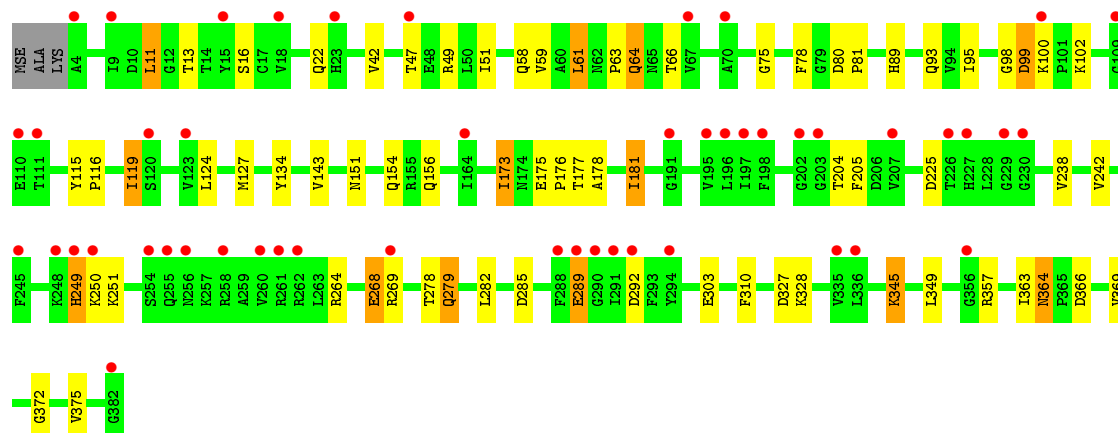
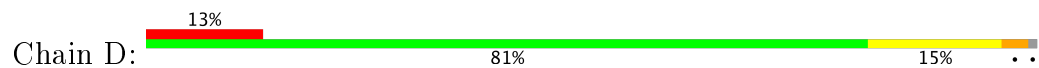




- Molecule 2: Heat shock 70 kDa protein 1



- Molecule 2: Heat shock 70 kDa protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	129.84Å 141.65Å 150.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 99.8 (20.00-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.262 0.209 , 0.259	Depositor DCC
R_{free} test set	5797 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15834	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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, 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	0.60	2/4918 (0.0%)	0.74	3/6663 (0.0%)
1	C	0.54	0/4894	0.70	2/6630 (0.0%)
2	B	0.54	0/2913	0.62	0/3944
2	D	0.76	2/2862 (0.1%)	0.66	2/3882 (0.1%)
All	All	0.60	4/15587 (0.0%)	0.69	7/21119 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	289	GLU	CD-OE1	25.64	1.53	1.25
2	D	289	GLU	CD-OE2	15.77	1.43	1.25
1	A	473	GLN	CD-OE1	5.70	1.36	1.24
1	A	473	GLN	CD-NE2	5.34	1.46	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	289	GLU	OE1-CD-OE2	6.54	131.15	123.30
1	A	141	VAL	CB-CA-C	-6.26	99.50	111.40
1	C	316	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	274	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	203	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	224	LEU	CA-CB-CG	5.11	127.06	115.30
2	D	61	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4835	0	4692	84	0
1	C	4812	0	4667	75	0
2	B	2869	0	2813	28	0
2	D	2820	0	2700	43	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	31	0	12	0	0
4	C	31	0	12	0	0
5	A	6	0	8	0	0
6	A	161	0	0	5	0
6	B	65	0	0	1	0
6	C	144	0	0	2	0
6	D	58	0	0	1	0
All	All	15834	0	14904	228	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:CE2	1:A:557:MSE:HE3	1.81	1.15
1:C:61:ILE:O	1:C:89:THR:HG23	1.64	0.95
1:A:61:ILE:O	1:A:89:THR:HG23	1.73	0.89
1:A:106:PHE:HE2	1:A:557:MSE:HE3	1.35	0.89
1:A:47:ARG:HD3	1:A:557:MSE:HE2	1.56	0.84
1:A:150:THR:HG21	6:A:2031:HOH:O	1.78	0.83
1:C:150:THR:HG21	6:C:2030:HOH:O	1.78	0.82
2:D:16:SER:HB2	2:D:127:MSE:HE3	1.62	0.80
1:A:106:PHE:CE2	1:A:557:MSE:CE	2.66	0.77
1:A:563:LEU:O	1:A:567:THR:HG22	1.88	0.74
1:C:260:ASN:HB3	1:C:292:MSE:HE2	1.70	0.73
2:D:205:PHE:HB3	2:D:225:ASP:HB3	1.69	0.73
1:A:36:THR:HG22	6:A:2016:HOH:O	1.88	0.73
1:A:49:LEU:HB2	1:A:125:LYS:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:ASN:HD21	2:B:264:ARG:HH22	1.36	0.73
1:C:206:HIS:O	1:C:235:ARG:HB2	1.87	0.73
1:C:11:ASN:HD21	1:C:67:ASN:HA	1.54	0.72
1:C:36:THR:HG22	6:C:2015:HOH:O	1.88	0.72
2:D:364:ASN:HD22	2:D:366:ASP:H	1.35	0.72
2:D:357:ARG:HG3	6:D:1188:HOH:O	1.90	0.72
1:C:563:LEU:O	1:C:567:THR:CG2	2.37	0.72
1:A:11:ASN:HD21	1:A:67:ASN:HA	1.53	0.71
1:A:20:ARG:HD2	1:A:25:ASP:OD2	1.89	0.71
1:A:31:VAL:HG13	1:A:51:GLU:HG3	1.73	0.71
2:B:151:ASN:H	2:B:154:GLN:HE21	1.39	0.71
1:A:497:THR:HG22	1:A:530:LYS:HB3	1.73	0.70
1:A:150:THR:HG22	1:A:153:GLN:H	1.57	0.70
1:C:223:VAL:HG13	1:C:396:ASP:HA	1.73	0.69
1:C:563:LEU:O	1:C:567:THR:HG22	1.93	0.69
1:A:583:GLY:O	1:A:587:GLU:HG3	1.93	0.69
1:A:451:LEU:HD22	1:A:455:THR:HG21	1.75	0.69
1:C:257:ILE:HA	1:C:292:MSE:CE	2.24	0.67
2:B:205:PHE:CE2	2:B:316:PRO:HG2	2.30	0.66
1:A:24:ILE:CD1	1:A:374:LYS:HG2	2.26	0.65
1:C:595:ASP:O	1:C:599:THR:HG23	1.96	0.65
1:A:61:ILE:O	1:A:89:THR:CG2	2.44	0.65
1:A:442:ALA:HB1	1:A:458:GLN:HE22	1.61	0.64
1:A:600:LYS:O	1:A:604:MSE:HG2	1.97	0.64
2:D:364:ASN:ND2	2:D:366:ASP:H	1.94	0.64
1:A:150:THR:HG23	6:A:2159:HOH:O	1.97	0.63
1:A:67:ASN:HB2	1:A:88:PHE:CZ	2.33	0.63
1:C:154:ARG:HH12	1:C:173:ASN:ND2	1.96	0.63
1:A:24:ILE:HD12	1:A:374:LYS:HG2	1.81	0.63
1:A:432:THR:HB	1:A:479:LYS:HG2	1.82	0.62
1:C:11:ASN:ND2	1:C:67:ASN:HA	2.14	0.62
1:A:469:LEU:HD13	1:A:473:GLN:HG3	1.82	0.62
1:A:24:ILE:HD13	1:A:24:ILE:C	2.20	0.61
1:A:223:VAL:HG13	1:A:396:ASP:HA	1.81	0.61
1:C:49:LEU:CB	1:C:125:LYS:HG3	2.30	0.61
1:A:11:ASN:ND2	1:A:67:ASN:HA	2.16	0.61
1:C:364:THR:CG2	1:C:364:THR:O	2.49	0.61
1:C:485:ASP:HB2	1:C:486:PRO:CD	2.31	0.60
2:D:364:ASN:C	2:D:364:ASN:HD22	2.05	0.60
2:B:194:ASN:H	2:B:332:HIS:HD2	1.50	0.60
1:C:49:LEU:HB2	1:C:125:LYS:HG3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASP:OD2	1:C:316:ARG:HD2	2.02	0.59
2:D:310:PHE:CG	2:D:345:LYS:HG2	2.37	0.59
2:D:143:VAL:HG11	2:D:173:ILE:HD12	1.85	0.59
1:C:28:VAL:HG13	1:C:32:SER:HA	1.85	0.59
1:C:568:GLU:HB3	2:D:279:GLN:NE2	2.18	0.59
2:B:194:ASN:H	2:B:332:HIS:CD2	2.21	0.58
1:A:174:ASP:HB2	1:A:372:ILE:HD13	1.85	0.58
2:D:278:THR:OG1	2:D:279:GLN:NE2	2.36	0.58
2:D:175:GLU:HG2	2:D:369:VAL:HG11	1.85	0.58
1:A:28:VAL:HG13	1:A:32:SER:HA	1.86	0.57
2:D:238:VAL:O	2:D:242:VAL:HG23	2.03	0.57
1:A:29:ASN:HD22	1:A:29:ASN:C	2.07	0.57
1:C:154:ARG:HH22	1:C:173:ASN:HD21	1.53	0.57
2:D:264:ARG:O	2:D:268:GLU:HB2	2.05	0.57
2:B:12:GLY:HA3	2:B:15:TYR:O	2.04	0.57
1:C:34:ARG:NH1	1:C:370:GLU:OE2	2.38	0.57
2:D:151:ASN:H	2:D:154:GLN:HE21	1.51	0.56
2:D:249:HIS:O	2:D:251:LYS:N	2.36	0.56
1:A:481:LYS:HE3	1:A:493:GLU:OE1	2.06	0.56
1:A:76:TYR:CD2	1:A:94:GLU:HB2	2.40	0.56
1:A:266:ARG:NH2	1:A:290:SER:O	2.39	0.56
1:C:174:ASP:HB2	1:C:372:ILE:HD13	1.86	0.56
1:A:79:PRO:HG2	1:A:454:ASN:HD21	1.71	0.56
1:C:154:ARG:HH12	1:C:173:ASN:HD21	1.52	0.55
1:C:163:ILE:HA	1:C:551:ILE:HG12	1.88	0.55
1:C:331:SER:HB3	1:C:333:GLU:OE2	2.06	0.55
2:D:95:ILE:HG13	2:D:102:LYS:HB2	1.89	0.55
1:A:564:VAL:O	1:A:568:GLU:HG3	2.07	0.55
2:D:100:LYS:HE2	2:D:115:TYR:HE2	1.71	0.55
1:A:16:LEU:HD11	1:A:126:VAL:HG22	1.89	0.54
1:C:257:ILE:HA	1:C:292:MSE:HE3	1.89	0.54
1:C:563:LEU:O	1:C:567:THR:HG23	2.06	0.54
2:D:100:LYS:HE2	2:D:115:TYR:CE2	2.42	0.54
2:D:59:VAL:HG23	2:D:66:THR:HG21	1.89	0.54
2:B:93:GLN:HE21	2:D:89:HIS:HD2	1.55	0.54
1:A:409:GLN:HE22	1:A:435:ARG:HG3	1.72	0.54
1:A:571:LYS:HB2	1:A:624:TYR:CE1	2.43	0.54
2:D:11:LEU:HG	2:D:124:LEU:HD21	1.90	0.54
2:B:310:PHE:HB3	2:B:349:LEU:HD11	1.90	0.54
1:C:37:PRO:HB3	1:C:54:LYS:HG3	1.90	0.53
1:A:5:PHE:CD1	1:A:141:VAL:HG13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ILE:HG22	1:C:292:MSE:HE3	1.89	0.53
1:A:563:LEU:O	1:A:567:THR:CG2	2.55	0.53
2:D:151:ASN:OD1	2:D:154:GLN:HG3	2.10	0.52
1:A:17:ALA:HB1	1:A:24:ILE:HD11	1.91	0.52
1:C:74:LEU:HB3	1:C:100:THR:HG23	1.91	0.52
1:A:220:GLN:HA	1:A:393:LYS:O	2.10	0.52
1:C:57:GLN:HG3	1:C:64:THR:HG21	1.93	0.51
2:D:177:THR:O	2:D:181:ILE:HG23	2.11	0.51
1:C:29:ASN:HD22	1:C:29:ASN:C	2.14	0.51
1:C:87:HIS:CE1	1:C:235:ARG:HG2	2.45	0.51
1:C:447:ASP:O	1:C:450:GLN:HG2	2.10	0.51
2:B:178:ALA:O	2:B:372:GLY:HA3	2.11	0.51
1:C:158:ALA:HB2	1:C:171:ILE:HD13	1.93	0.50
2:B:195:VAL:HG21	2:B:212:ILE:HD11	1.93	0.50
1:A:141:VAL:HG22	1:A:166:LEU:HB3	1.93	0.50
1:A:154:ARG:HH12	1:A:173:ASN:ND2	2.09	0.50
1:A:154:ARG:HH22	1:A:173:ASN:HD21	1.60	0.50
2:D:178:ALA:O	2:D:372:GLY:HA3	2.11	0.50
2:B:11:LEU:HG	2:B:124:LEU:HD21	1.94	0.49
2:D:143:VAL:CG1	2:D:173:ILE:CD1	2.90	0.49
1:A:175:VAL:O	1:A:214:MSE:HE1	2.12	0.49
1:A:364:THR:OG1	1:A:368:GLN:NE2	2.43	0.49
2:B:261:ARG:HD3	2:B:261:ARG:O	2.12	0.49
1:A:292:MSE:HB2	1:A:295:VAL:CG1	2.42	0.49
1:A:117:GLN:O	1:A:121:MSE:HG3	2.13	0.49
1:C:71:ILE:HG22	1:C:74:LEU:HD12	1.94	0.49
2:D:143:VAL:CG1	2:D:173:ILE:HD12	2.42	0.48
1:C:451:LEU:HD22	1:C:455:THR:HG21	1.95	0.48
1:C:124:ASP:OD2	1:C:558:LEU:HD21	2.14	0.48
2:B:342:ARG:NH2	2:B:366:ASP:OD2	2.43	0.48
1:C:18:VAL:HG13	1:C:20:ARG:HG2	1.94	0.48
2:D:49:ARG:HD3	2:D:51:ILE:HD11	1.96	0.48
1:A:409:GLN:NE2	1:A:436:THR:H	2.11	0.47
1:A:458:GLN:NE2	1:A:460:ALA:O	2.47	0.47
1:C:485:ASP:HB2	1:C:486:PRO:HD2	1.94	0.47
1:A:311:LYS:HB3	1:A:312:PRO:HD3	1.96	0.47
1:C:485:ASP:CB	1:C:486:PRO:CD	2.93	0.47
1:C:255:ILE:HG21	1:C:295:VAL:HG11	1.97	0.47
1:C:435:ARG:HG2	1:C:439:PHE:CD1	2.49	0.47
2:D:116:PRO:HA	2:D:119:ILE:HD11	1.97	0.47
1:C:532:ASP:OD2	1:C:532:ASP:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:HG13	1:A:398:HIS:N	2.29	0.47
2:B:197:ILE:N	2:B:197:ILE:HD12	2.28	0.47
1:A:182:TYR:CE1	1:A:186:LYS:HE3	2.50	0.47
1:C:604:MSE:HE1	1:C:630:GLU:HB3	1.96	0.47
1:A:172:VAL:HG21	1:A:379:ILE:HD13	1.96	0.47
1:A:299:SER:OG	1:A:300:GLN:N	2.47	0.47
1:C:364:THR:HG22	1:C:364:THR:O	2.14	0.47
1:A:11:ASN:ND2	1:A:70:ARG:HG2	2.30	0.47
1:A:24:ILE:HD11	1:A:374:LYS:HG2	1.97	0.46
1:A:604:MSE:HB3	1:A:604:MSE:HE2	1.72	0.46
1:A:571:LYS:HB2	1:A:624:TYR:CD1	2.51	0.46
1:A:580:THR:O	1:A:584:LYS:HG3	2.14	0.46
2:B:315:GLU:HB2	2:B:316:PRO:HD3	1.96	0.46
1:C:49:LEU:HB3	1:C:125:LYS:HG3	1.98	0.46
1:A:36:THR:HG21	6:A:2104:HOH:O	2.15	0.46
1:C:311:LYS:HB3	1:C:312:PRO:HD3	1.96	0.46
1:A:74:LEU:O	1:A:100:THR:HG23	2.15	0.46
1:C:150:THR:HG22	1:C:152:GLU:N	2.31	0.46
1:A:282:THR:HG23	6:A:2123:HOH:O	2.15	0.46
2:D:63:PRO:HG2	2:D:64:GLN:NE2	2.31	0.46
1:C:54:LYS:HE3	1:C:57:GLN:OE1	2.16	0.45
1:A:181:SER:HA	1:A:184:ILE:HG12	1.97	0.45
1:C:44:PRO:O	1:C:107:ALA:HA	2.17	0.45
2:B:246:LYS:HA	2:B:251:LYS:O	2.16	0.45
2:D:345:LYS:HE2	2:D:349:LEU:HG	1.98	0.45
1:C:11:ASN:ND2	1:C:70:ARG:HG2	2.31	0.45
1:A:81:PHE:HE1	1:A:100:THR:HG21	1.82	0.44
1:A:74:LEU:HB3	1:A:100:THR:HG23	1.98	0.44
1:A:650:LYS:HA	1:A:653:ILE:HD12	2.00	0.44
1:A:221:LEU:C	1:A:221:LEU:HD12	2.37	0.44
1:C:154:ARG:NH1	1:C:173:ASN:HD21	2.16	0.44
1:C:76:TYR:HD1	1:C:100:THR:HB	1.83	0.44
1:C:214:MSE:HG2	1:C:223:VAL:HB	1.99	0.43
2:D:303:GLU:HB3	2:D:345:LYS:HD2	1.99	0.43
2:B:211:THR:HB	2:B:220:LYS:HD3	2.00	0.43
1:A:341:ILE:HA	1:A:368:GLN:HB3	2.00	0.43
2:B:26:VAL:HG11	2:B:371:TYR:HA	1.99	0.43
1:C:333:GLU:CD	1:C:333:GLU:H	2.21	0.43
2:D:16:SER:HB2	2:D:127:MSE:CE	2.41	0.43
1:C:42:PHE:CD1	1:C:104:VAL:HG11	2.54	0.43
2:D:181:ILE:HD11	2:D:375:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:HA	1:A:4:PRO:HD3	1.91	0.43
2:B:22:GLN:NE2	2:B:134:TYR:OH	2.46	0.42
2:B:77:LYS:O	2:B:80:ASP:HB2	2.19	0.42
2:D:42:VAL:HG13	2:D:51:ILE:HD13	2.00	0.42
2:D:327:ASP:OD2	2:D:328:LYS:N	2.51	0.42
1:A:31:VAL:O	1:A:31:VAL:HG23	2.19	0.42
1:A:202:VAL:HG11	1:A:354:ILE:HD13	2.01	0.42
1:A:448:ILE:HD13	1:A:457:GLU:HA	2.02	0.42
1:C:150:THR:HG22	1:C:153:GLN:H	1.84	0.42
1:C:611:TRP:NE1	1:C:615:GLU:HB3	2.34	0.42
2:D:175:GLU:N	2:D:176:PRO:HD2	2.35	0.42
2:D:181:ILE:HD11	2:D:375:VAL:HG12	2.00	0.42
2:B:146:VAL:HB	2:B:150:PHE:CD1	2.54	0.42
2:B:159:LYS:O	2:B:163:VAL:HG23	2.19	0.42
1:C:411:GLU:HG3	1:C:433:LEU:HD22	2.02	0.42
1:A:344:THR:HG23	1:A:347:ILE:HD12	2.02	0.42
1:C:29:ASN:ND2	1:C:33:ASN:H	2.16	0.42
2:B:151:ASN:H	2:B:154:GLN:NE2	2.13	0.42
1:C:442:ALA:HA	1:C:461:ASN:HA	2.02	0.42
2:D:310:PHE:CD2	2:D:345:LYS:HG2	2.54	0.42
1:C:604:MSE:CE	1:C:630:GLU:HB3	2.49	0.42
2:B:363:ILE:O	2:B:364:ASN:C	2.58	0.42
1:C:26:ILE:HG13	1:C:370:GLU:CD	2.40	0.42
1:A:49:LEU:CB	1:A:125:LYS:HG3	2.47	0.41
1:C:154:ARG:NH2	1:C:173:ASN:HD21	2.16	0.41
1:C:3:THR:HA	1:C:4:PRO:HD3	1.96	0.41
1:A:44:PRO:O	1:A:107:ALA:HA	2.20	0.41
1:C:39:VAL:HG21	1:C:54:LYS:HG2	2.02	0.41
1:A:18:VAL:HG13	1:A:20:ARG:HG3	2.03	0.41
2:D:102:LYS:HD3	2:D:115:TYR:CE2	2.56	0.41
1:A:134:THR:O	1:A:135:LYS:HB2	2.20	0.41
1:C:266:ARG:NH1	1:C:291:VAL:O	2.52	0.41
2:B:234:ASP:O	2:B:238:VAL:HG23	2.21	0.41
1:A:154:ARG:HH12	1:A:173:ASN:HD21	1.67	0.41
2:B:195:VAL:HG13	2:B:333:ASP:HB2	2.01	0.41
1:C:158:ALA:HB2	1:C:171:ILE:CD1	2.51	0.41
1:C:347:ILE:HA	1:C:348:PRO:HD3	1.93	0.41
2:B:39:PRO:HD3	6:B:393:HOH:O	2.21	0.41
1:C:12:ASN:HB2	1:C:206:HIS:CG	2.56	0.41
1:C:448:ILE:HD13	1:C:457:GLU:HA	2.03	0.41
1:A:47:ARG:HD3	1:A:557:MSE:CE	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:ASP:O	2:B:227:HIS:N	2.53	0.40
1:C:18:VAL:CG1	1:C:20:ARG:HG2	2.51	0.40
2:D:363:ILE:O	2:D:364:ASN:C	2.59	0.40
1:A:442:ALA:HA	1:A:461:ASN:HA	2.03	0.40
1:C:259:GLU:HA	1:C:259:GLU:OE1	2.19	0.40
2:D:75:GLY:HA3	2:D:154:GLN:HA	2.02	0.40
2:D:22:GLN:NE2	2:D:134:TYR:OH	2.54	0.40
2:D:78:PHE:O	2:D:99:ASP:OD1	2.40	0.40
1:A:425:PHE:HB2	1:A:426:PRO:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	626/675 (93%)	601 (96%)	23 (4%)	2 (0%)	44	53
1	C	623/675 (92%)	590 (95%)	32 (5%)	1 (0%)	51	61
2	B	377/382 (99%)	366 (97%)	10 (3%)	1 (0%)	44	53
2	D	377/382 (99%)	355 (94%)	19 (5%)	3 (1%)	22	24
All	All	2003/2114 (95%)	1912 (96%)	84 (4%)	7 (0%)	44	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	226	THR
2	D	250	LYS
1	A	499	GLU
1	C	471	GLU
2	D	98	GLY
2	D	81	PRO

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Mol	Chain	Res	Type
1	A	653	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	510/565 (90%)	454 (89%)	56 (11%)	7	7
1	C	508/565 (90%)	460 (91%)	48 (9%)	10	10
2	B	297/310 (96%)	288 (97%)	9 (3%)	46	58
2	D	283/310 (91%)	259 (92%)	24 (8%)	12	13
All	All	1598/1750 (91%)	1461 (91%)	137 (9%)	12	12

All (137) 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	ILE
1	A	29	ASN
1	A	31	VAL
1	A	36	THR
1	A	54	LYS
1	A	58	THR
1	A	60	ASN
1	A	65	VAL
1	A	69	LYS
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	105	ARG
1	A	126	VAL
1	A	132	GLN
1	A	135	LYS
1	A	138	ILE
1	A	141	VAL
1	A	149	TYR
1	A	150	THR
1	A	169	VAL
1	A	175	VAL
1	A	185	PHE
1	A	197	ARG
1	A	209	TYR
1	A	223	VAL
1	A	224	LEU
1	A	251	THR
1	A	254	LYS
1	A	268	LEU
1	A	282	THR
1	A	283	ASN
1	A	291	VAL
1	A	294	ASP
1	A	311	LYS
1	A	330	LEU
1	A	340	ILE
1	A	432	THR
1	A	435	ARG
1	A	451	LEU
1	A	458	GLN
1	A	532	ASP
1	A	543	ASP
1	A	552	GLU
1	A	567	THR
1	A	571	LYS
1	A	604	MSE
1	A	631	LEU
2	B	11	LEU
2	B	13	THR
2	B	61	LEU
2	B	105	VAL
2	B	211	THR
2	B	276	SER

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Mol	Chain	Res	Type
2	B	279	GLN
2	B	336	LEU
2	B	381	MSE
1	C	3	THR
1	C	7	LEU
1	C	13	ASN
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	82	GLU
1	C	89	THR
1	C	92	LEU
1	C	100	THR
1	C	105	ARG
1	C	149	TYR
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	282	THR
1	C	283	ASN
1	C	290	SER
1	C	298	SER
1	C	333	GLU
1	C	352	GLN
1	C	364	THR
1	C	389	VAL
1	C	393	LYS
1	C	432	THR
1	C	435	ARG

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Mol	Chain	Res	Type
1	C	451	LEU
1	C	497	THR
1	C	531	ASP
1	C	532	ASP
1	C	567	THR
1	C	588	GLU
1	C	599	THR
1	C	631	LEU
1	C	647	GLU
2	D	11	LEU
2	D	13	THR
2	D	47	THR
2	D	58	GLN
2	D	61	LEU
2	D	64	GLN
2	D	80	ASP
2	D	93	GLN
2	D	99	ASP
2	D	119	ILE
2	D	156	GLN
2	D	173	ILE
2	D	181	ILE
2	D	204	THR
2	D	249	HIS
2	D	268	GLU
2	D	269	ARG
2	D	279	GLN
2	D	282	LEU
2	D	285	ASP
2	D	289	GLU
2	D	292	ASP
2	D	345	LYS
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	57	GLN

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Mol	Chain	Res	Type
1	A	173	ASN
1	A	368	GLN
1	A	409	GLN
1	A	454	ASN
1	A	458	GLN
1	A	461	ASN
1	A	548	ASN
1	A	555	ASN
1	A	602	GLN
2	B	22	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	117	GLN
1	C	156	ASN
1	C	173	ASN
1	C	458	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	156	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 ⓘ

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 5 ligands modelled in this entry, 2 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	$\# Z > 2$
4	ATP	A	1001	3	27,33,33	1.27	3 (11%)	25,52,52	1.72	2 (8%)
5	GOL	A	2002	-	5,5,5	0.58	0	5,5,5	0.76	0
4	ATP	C	1001	3	27,33,33	1.03	1 (3%)	25,52,52	1.81	4 (16%)

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
4	ATP	A	1001	3	-	0/18/38/38	0/3/3/3
5	GOL	A	2002	-	-	0/4/4/4	0/0/0/0
4	ATP	C	1001	3	-	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)
4	A	1001	ATP	O4'-C1'	2.66	1.44	1.41
4	A	1001	ATP	PG-O3B	2.83	1.64	1.60
4	C	1001	ATP	C5-C4	3.18	1.47	1.40
4	A	1001	ATP	C5-C4	3.34	1.48	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	ATP	N3-C2-N1	-6.47	123.22	128.86
4	A	1001	ATP	N3-C2-N1	-6.26	123.40	128.86
4	C	1001	ATP	C4-C5-N7	-2.88	106.63	109.41
4	A	1001	ATP	C4-C5-N7	-2.44	107.06	109.41
4	C	1001	ATP	C4'-O4'-C1'	-2.01	107.63	109.77
4	C	1001	ATP	C2-N1-C6	2.22	122.65	118.77

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	622/675 (92%)	0.64	68 (10%) 6 10	26, 34, 45, 57	0
1	C	620/675 (91%)	0.79	83 (13%) 4 6	27, 35, 45, 64	0
2	B	375/382 (98%)	0.78	46 (12%) 5 8	27, 34, 45, 70	0
2	D	375/382 (98%)	0.81	49 (13%) 4 6	28, 35, 43, 59	0
All	All	1992/2114 (94%)	0.75	246 (12%) 5 8	26, 35, 45, 70	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	527	THR	9.7
1	C	527	THR	8.1
1	C	410	VAL	7.8
1	C	470	PRO	7.5
1	C	653	ILE	7.0
1	C	475	SER	6.8
1	C	498	ILE	6.5
1	C	474	ASP	6.5
1	C	528	VAL	6.2
2	B	226	THR	6.1
1	A	525	THR	6.0
1	A	653	ILE	6.0
2	B	288	PHE	6.0
1	C	476	VAL	5.7
1	A	473	GLN	5.5
1	C	530	LYS	5.3
1	C	473	GLN	5.3
2	D	226	THR	5.3
2	D	382	GLY	5.3
2	D	261	ARG	5.3
2	B	249	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	430	LEU	5.2
1	C	469	LEU	5.2
2	D	255	GLN	5.1
2	B	291	ILE	5.1
1	A	470	PRO	5.0
1	C	472	GLY	5.0
1	C	185	PHE	4.8
2	B	227	HIS	4.8
2	B	287	LEU	4.8
1	C	468	GLN	4.7
1	C	436	THR	4.7
2	B	260	VAL	4.7
1	A	526	LYS	4.7
1	C	467	VAL	4.6
2	B	18	VAL	4.6
2	B	245	PHE	4.6
2	B	382	GLY	4.6
2	B	255	GLN	4.4
1	C	496	TYR	4.4
2	B	256	ASN	4.4
2	D	229	GLY	4.4
2	D	227	HIS	4.3
1	A	500	ASP	4.3
1	A	142	CYS	4.3
1	C	471	GLU	4.2
2	B	286	SER	4.1
2	D	249	HIS	4.1
1	A	385	PRO	4.1
1	C	647	GLU	4.1
1	A	468	GLN	4.1
1	C	477	PRO	4.0
1	A	469	LEU	4.0
2	B	285	ASP	4.0
1	C	437	GLY	4.0
2	B	7	ILE	3.9
1	C	407	ASP	3.9
1	C	654	ARG	3.9
2	D	230	GLY	3.9
1	C	466	GLY	3.9
2	B	228	LEU	3.9
1	C	650	LYS	3.8
2	B	229	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	196	LEU	3.8
2	B	9	ILE	3.8
2	B	67	VAL	3.8
2	B	196	LEU	3.8
1	A	386	THR	3.7
1	C	412	ASP	3.7
2	D	290	GLY	3.7
2	D	288	PHE	3.7
2	B	109	GLY	3.7
2	D	258	ARG	3.7
2	D	197	ILE	3.6
1	A	387	LEU	3.6
1	C	497	THR	3.6
2	B	197	ILE	3.6
1	A	530	LYS	3.5
2	B	248	LYS	3.5
1	A	241	ILE	3.5
1	C	413	GLU	3.5
1	C	526	LYS	3.4
2	B	8	GLY	3.4
1	C	533	LEU	3.4
2	D	4	ALA	3.4
1	C	648	GLU	3.4
1	A	472	GLY	3.4
2	D	203	GLY	3.3
2	D	256	ASN	3.3
2	D	291	ILE	3.3
2	B	292	ASP	3.3
1	A	204	ILE	3.3
1	C	532	ASP	3.3
1	A	437	GLY	3.3
1	A	68	LEU	3.2
1	C	68	LEU	3.2
1	A	652	ALA	3.2
1	A	531	ASP	3.2
2	B	258	ARG	3.2
2	D	250	LYS	3.2
2	D	9	ILE	3.1
2	D	123	VAL	3.1
1	C	193	GLU	3.1
1	C	465	THR	3.1
2	D	47	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	248	LYS	3.1
1	A	202	VAL	3.1
1	C	529	LYS	3.1
1	A	7	LEU	3.1
1	C	408	LYS	3.1
1	C	414	ASP	3.0
2	B	98	GLY	3.0
2	D	289	GLU	3.0
2	D	15	TYR	2.9
2	D	110	GLU	2.9
1	C	534	THR	2.9
2	B	290	GLY	2.9
1	A	201	PHE	2.9
1	A	376	ALA	2.9
1	C	241	ILE	2.8
2	B	250	LYS	2.8
2	D	356	GLY	2.8
1	A	39	VAL	2.8
1	A	377	ALA	2.8
1	C	613	TYR	2.8
1	A	499	GLU	2.8
2	D	111	THR	2.8
1	A	141	VAL	2.8
1	A	234	GLY	2.8
1	A	344	THR	2.7
1	A	373	ALA	2.7
1	A	388	ARG	2.7
1	C	391	PRO	2.7
2	B	70	ALA	2.7
2	D	254	SER	2.7
2	D	67	VAL	2.7
1	C	40	VAL	2.7
1	C	386	THR	2.7
2	D	18	VAL	2.7
2	D	23	HIS	2.7
1	A	118	LEU	2.7
1	A	6	GLY	2.7
1	C	633	SER	2.6
2	B	254	SER	2.6
1	C	409	GLN	2.6
1	A	5	PHE	2.6
1	A	22	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	218	LYS	2.6
1	C	400	TYR	2.6
1	C	448	ILE	2.6
1	C	406	TRP	2.6
2	B	17	CYS	2.6
1	A	42	PHE	2.6
1	C	617	PHE	2.6
1	C	450	GLN	2.6
1	C	434	ASN	2.6
1	A	471	GLU	2.5
1	A	119	ALA	2.5
2	D	70	ALA	2.5
1	C	22	ARG	2.5
1	A	271	ALA	2.5
1	C	428	THR	2.5
1	C	531	ASP	2.5
2	B	79	GLY	2.5
2	D	207	VAL	2.5
1	C	187	THR	2.5
1	C	2	SER	2.5
2	D	294	TYR	2.5
1	A	177	ALA	2.4
2	D	198	PHE	2.4
1	A	209	TYR	2.4
1	C	191	GLU	2.4
1	A	528	VAL	2.4
1	C	337	PHE	2.4
2	B	42	VAL	2.4
1	A	205	GLY	2.4
2	D	164	ILE	2.4
1	A	122	PHE	2.4
2	B	191	GLY	2.4
2	D	292	ASP	2.4
1	C	118	LEU	2.4
1	C	23	GLY	2.4
2	B	289	GLU	2.4
2	B	374	ALA	2.4
2	D	195	VAL	2.4
2	D	269	ARG	2.4
1	C	120	ALA	2.4
2	B	252	ASP	2.4
1	A	193	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	61	LEU	2.4
1	A	17	ALA	2.4
1	A	40	VAL	2.4
2	D	120	SER	2.3
2	D	109	GLY	2.3
1	A	654	ARG	2.3
2	B	60	ALA	2.3
1	A	384	SER	2.3
1	A	648	GLU	2.3
1	A	126	VAL	2.3
1	C	291	VAL	2.3
2	D	335	VAL	2.3
2	D	191	GLY	2.3
1	A	212	SER	2.3
2	D	100	LYS	2.3
1	A	175	VAL	2.3
2	B	262	ARG	2.3
1	C	649	LYS	2.3
1	C	652	ALA	2.3
1	A	211	CYS	2.3
2	B	234	ASP	2.3
1	C	142	CYS	2.2
2	B	257	LYS	2.2
2	D	260	VAL	2.2
1	A	120	ALA	2.2
2	B	370	ALA	2.2
2	B	327	ASP	2.2
1	C	655	SER	2.2
1	C	478	VAL	2.1
1	C	432	THR	2.1
1	A	143	ILE	2.1
1	A	379	ILE	2.1
1	A	21	ASN	2.1
1	A	65	VAL	2.1
1	C	202	VAL	2.1
1	C	194	GLU	2.1
1	C	385	PRO	2.1
1	C	452	PRO	2.1
2	D	336	LEU	2.1
1	C	535	ILE	2.1
1	A	237	PHE	2.1
1	C	71	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	474	ASP	2.1
1	C	610	GLU	2.1
1	A	137	ASN	2.1
1	C	454	ASN	2.1
1	A	490	HIS	2.0
1	C	189	LEU	2.0
2	D	262	ARG	2.0
2	D	245	PHE	2.0
1	A	71	ILE	2.0
1	A	123	ILE	2.0
1	C	495	ALA	2.0
2	B	247	ARG	2.0
1	A	185	PHE	2.0
1	C	411	GLU	2.0
2	D	202	GLY	2.0

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

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	2001	1/1	0.95	0.21	-0.37	33,33,33,33	0
4	ATP	A	1001	31/31	0.98	0.17	-0.79	28,31,36,36	0
4	ATP	C	1001	31/31	0.98	0.15	-0.81	29,33,35,35	0
5	GOL	A	2002	6/6	0.90	0.15	-0.89	45,46,48,49	0
3	MG	C	2001	1/1	0.97	0.06	-2.99	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.