



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:02 AM GMT

PDB ID : 3D2E  
Title : Crystal structure of a complex of Sse1p and Hsp70, Selenomethionine-labeled crystals  
Authors : Polier, S.; Bracher, A.  
Deposited on : 2008-05-08  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

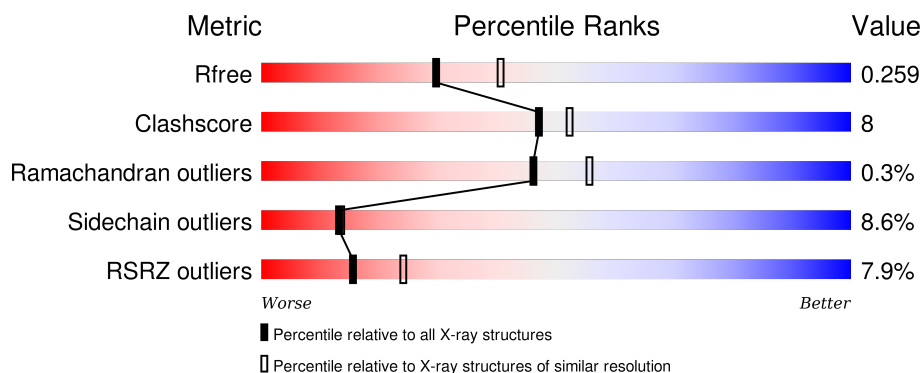
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (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  $\geq 3$ , 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>71% 18% • 7%</div> </div>
1	C	675	<div> <div>8%</div> <div>75% 15% • 7%</div> </div>
2	B	382	<div> <div>9%</div> <div>85% 14% ••</div> </div>
2	D	382	<div> <div>10%</div> <div>81% 15% ••</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

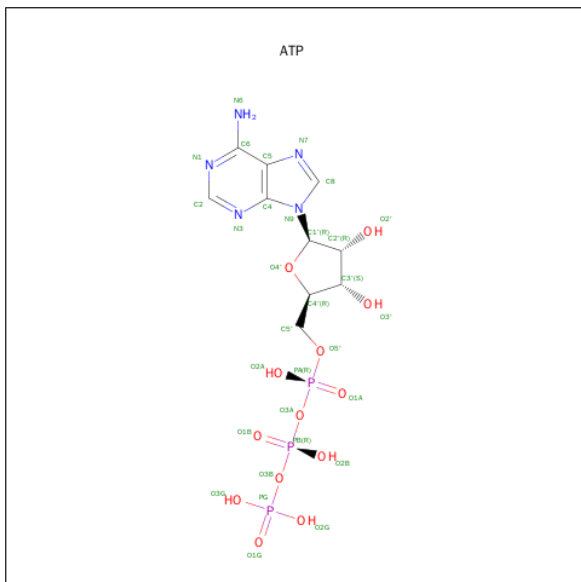
- Molecule 2 is a protein called Heat shock 70 kDa protein 1.

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).

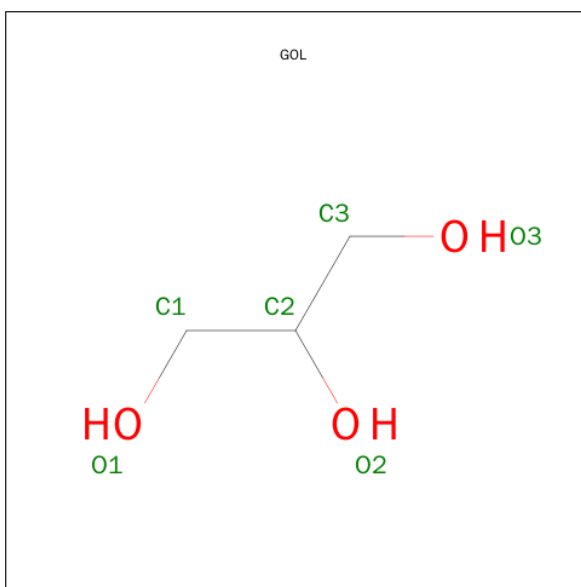
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

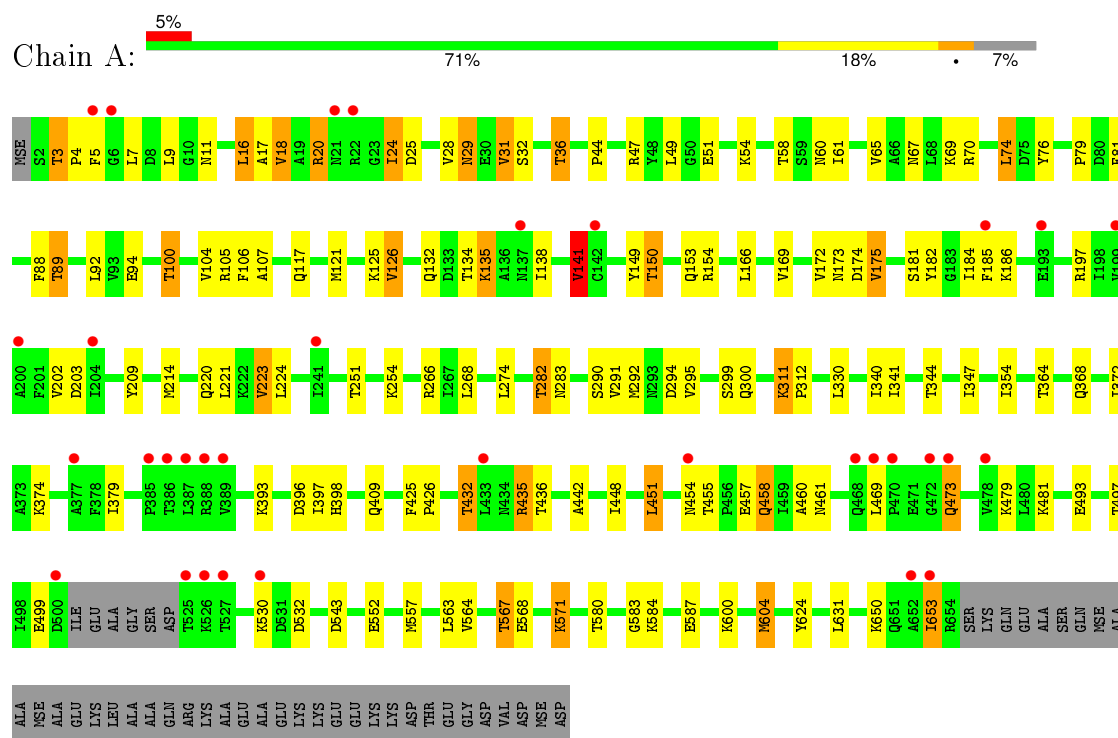
- Molecule 6 is water.

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		

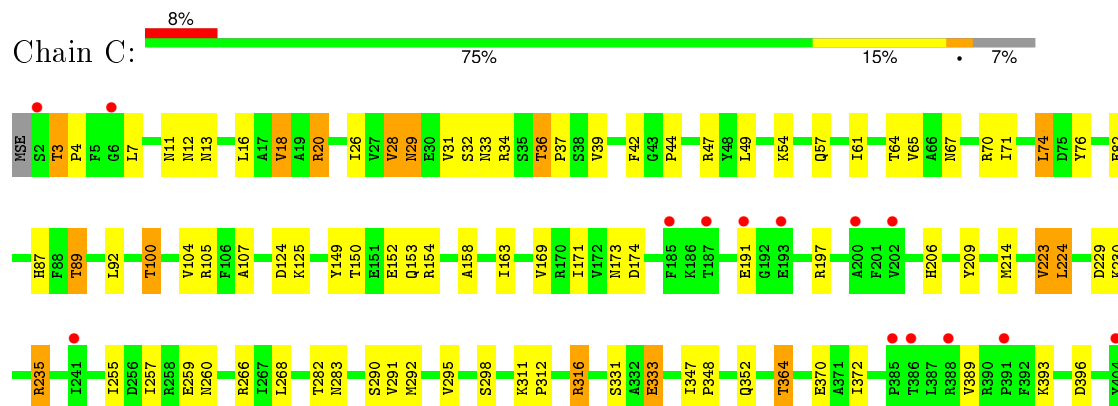
### 3 Residue-property plots [i](#)

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



- Molecule 1: Heat shock protein homolog SSE1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	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 <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 115424 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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
2:D:205:PHE:HB3	2:D:225:ASP:HB3	1.69	0.73
1:C:260:ASN:HB3	1:C:292:MSE:HE2	1.70	0.73
1:A:36:THR:HG22	6:A:2016:HOH:O	1.88	0.73
2:B:235:ASN:HD21	2:B:264:ARG:HH22	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HB2	1:A:125:LYS:HG3	1.71	0.73
1:C:206:HIS:O	1:C:235:ARG:HB2	1.87	0.73
1:C:36:THR:HG22	6:C:2015:HOH:O	1.88	0.72
1:C:11:ASN:HD21	1:C:67:ASN:HA	1.54	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:C:595:ASP:O	1:C:599:THR:HG23	1.96	0.65
1:A:24:ILE:CD1	1:A:374:LYS:HG2	2.26	0.65
1:A:61:ILE:O	1:A:89:THR:CG2	2.44	0.65
1:A:600:LYS:O	1:A:604:MSE:HG2	1.97	0.64
1:A:442:ALA:HB1	1:A:458:GLN:HE22	1.61	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
2:D:364:ASN:C	2:D:364:ASN:HD22	2.05	0.60
1:C:485:ASP:HB2	1:C:486:PRO:CD	2.31	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:568:GLU:HB3	2:D:279:GLN:NE2	2.18	0.59
1:C:28:VAL:HG13	1:C:32:SER:HA	1.85	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
1:C:34:ARG:NH1	1:C:370:GLU:OE2	2.38	0.57
2:B:12:GLY:HA3	2:B:15:TYR:O	2.04	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:C:174:ASP:HB2	1:C:372:ILE:HD13	1.86	0.56
1:A:266:ARG:NH2	1:A:290:SER:O	2.39	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
2:D:100:LYS:HE2	2:D:115:TYR:HE2	1.71	0.55
1:A:564:VAL:O	1:A:568:GLU:HG3	2.07	0.55
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
1:A:16:LEU:HD11	1:A:126:VAL:HG22	1.89	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:D:143:VAL:CG1	2:D:173:ILE:CD1	2.90	0.49
2:B:11:LEU:HG	2:B:124:LEU:HD21	1.94	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:C:71:ILE:HG22	1:C:74:LEU:HD12	1.94	0.49
1:A:117:GLN:O	1:A:121:MSE:HG3	2.13	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:D:49:ARG:HD3	2:D:51:ILE:HD11	1.96	0.48
1:C:18:VAL:HG13	1:C:20:ARG:HG2	1.94	0.48
2:B:342:ARG:NH2	2:B:366:ASP:OD2	2.43	0.48
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:409:GLN:NE2	1:A:436:THR:H	2.11	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
2:D:116:PRO:HA	2:D:119:ILE:HD11	1.97	0.47
1:C:435:ARG:HG2	1:C:439:PHE:CD1	2.49	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:C:364:THR:HG22	1:C:364:THR:O	2.14	0.47
1:A:299:SER:OG	1:A:300:GLN:N	2.47	0.47
1:A:172:VAL:HG21	1:A:379:ILE:HD13	1.96	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:C:150:THR:HG22	1:C:152:GLU:N	2.31	0.46
1:A:74:LEU:O	1:A:100:THR:HG23	2.15	0.46
2:D:63:PRO:HG2	2:D:64:GLN:NE2	2.31	0.46
1:A:282:THR:HG23	6:A:2123:HOH:O	2.15	0.46
1:C:54:LYS:HE3	1:C:57:GLN:OE1	2.16	0.45
1:C:44:PRO:O	1:C:107:ALA:HA	2.17	0.45
1:A:181:SER:HA	1:A:184:ILE:HG12	1.97	0.45
2:D:345:LYS:HE2	2:D:349:LEU:HG	1.98	0.45
2:B:246:LYS:HA	2:B:251:LYS:O	2.16	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
2:D:181:ILE:HD11	2:D:375:VAL:CG1	2.48	0.43
1:C:42:PHE:CD1	1:C:104:VAL:HG11	2.54	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:D:42:VAL:HG13	2:D:51:ILE:HD13	2.00	0.42
2:B:77:LYS:O	2:B:80:ASP:HB2	2.19	0.42
2:B:22:GLN:NE2	2:B:134:TYR:OH	2.46	0.42
2:D:327:ASP:OD2	2:D:328:LYS:N	2.51	0.42
1:A:31:VAL:HG23	1:A:31:VAL:O	2.19	0.42
1:C:150:THR:HG22	1:C:153:GLN:H	1.84	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
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:611:TRP:NE1	1:C:615:GLU:HB3	2.34	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:C:29:ASN:ND2	1:C:33:ASN:H	2.16	0.42
1:A:344:THR:HG23	1:A:347:ILE:HD12	2.02	0.42
2:B:151:ASN:H	2:B:154:GLN:NE2	2.13	0.42
2:D:310:PHE:CD2	2:D:345:LYS:HG2	2.54	0.42
1:C:442:ALA:HA	1:C:461:ASN:HA	2.02	0.42
1:C:604:MSE:CE	1:C:630:GLU:HB3	2.49	0.42
1:C:26:ILE:HG13	1:C:370:GLU:CD	2.40	0.42
2:B:363:ILE:O	2:B:364:ASN:C	2.58	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:C:39:VAL:HG21	1:C:54:LYS:HG2	2.02	0.41
1:A:44:PRO:O	1:A:107:ALA:HA	2.20	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:C:266:ARG:NH1	1:C:291:VAL:O	2.52	0.41
1:A:134:THR:O	1:A:135:LYS:HB2	2.20	0.41
2:B:234:ASP:O	2:B:238:VAL:HG23	2.21	0.41
2:B:195:VAL:HG13	2:B:333:ASP:HB2	2.01	0.41
1:A:154:ARG:HH12	1:A:173:ASN:HD21	1.67	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
1:C:12:ASN:HB2	1:C:206:HIS:CG	2.56	0.41
2:B:39:PRO:HD3	6:B:393:HOH:O	2.21	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:D:363:ILE:O	2:D:364:ASN:C	2.59	0.40
1:C:18:VAL:CG1	1:C:20:ARG:HG2	2.51	0.40
2:B:225:ASP:O	2:B:227:HIS:N	2.53	0.40
1:A:442:ALA:HA	1:A:461:ASN:HA	2.03	0.40
2:D:75:GLY:HA3	2:D:154:GLN:HA	2.02	0.40
1:C:259:GLU:HA	1:C:259:GLU:OE1	2.19	0.40
2:D:78:PHE:O	2:D:99:ASP:OD1	2.40	0.40
2:D:22:GLN:NE2	2:D:134:TYR:OH	2.54	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%)	46	55
1	C	623/675 (92%)	590 (95%)	32 (5%)	1 (0%)	52	63
2	B	377/382 (99%)	366 (97%)	10 (3%)	1 (0%)	46	55
2	D	377/382 (99%)	355 (94%)	19 (5%)	3 (1%)	24	26
All	All	2003/2114 (95%)	1912 (96%)	84 (4%)	7 (0%)	46	55

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%)	8	7
1	C	508/565 (90%)	460 (91%)	48 (9%)	11	10
2	B	297/310 (96%)	288 (97%)	9 (3%)	48	62
2	D	283/310 (91%)	259 (92%)	24 (8%)	13	14
All	All	1598/1750 (91%)	1461 (91%)	137 (9%)	13	13

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 [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 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	24,33,33	1.19	2 (8%)	31,52,52	1.85	5 (16%)
5	GOL	A	2002	-	5,5,5	0.57	0	5,5,5	0.78	0
4	ATP	C	1001	3	24,33,33	1.00	1 (4%)	31,52,52	1.93	5 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	ATP	O4'-C1'	2.96	1.44	1.41
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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	ATP	N3-C2-N1	-7.41	123.22	128.89
4	A	1001	ATP	N3-C2-N1	-7.17	123.40	128.89
4	C	1001	ATP	C4-C5-N7	-3.10	106.63	109.48
4	A	1001	ATP	C2'-C1'-N9	-2.69	110.17	114.29
4	A	1001	ATP	C4-C5-N7	-2.63	107.06	109.48
4	C	1001	ATP	C1'-N9-C4	-2.34	123.41	126.94
4	C	1001	ATP	C2-N1-C6	2.17	122.65	118.77
4	A	1001	ATP	O3G-PG-O1G	2.29	117.95	110.58
4	A	1001	ATP	O4'-C1'-N9	2.48	113.28	108.10
4	C	1001	ATP	O4'-C1'-N9	2.59	113.53	108.10

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	622/675 (92%)	0.19	33 (5%)	30	45	26, 34, 45, 57	0
1	C	620/675 (91%)	0.37	51 (8%)	14	23	27, 35, 45, 64	0
2	B	375/382 (98%)	0.40	35 (9%)	11	18	27, 34, 45, 70	0
2	D	375/382 (98%)	0.45	39 (10%)	8	14	28, 35, 43, 59	0
All	All	1992/2114 (94%)	0.33	158 (7%)	15	24	26, 35, 45, 70	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	THR	7.8
1	A	653	ILE	7.1
1	A	527	THR	6.9
1	A	525	THR	6.5
1	C	410	VAL	6.5
1	C	653	ILE	6.4
2	D	382	GLY	5.8
2	B	227	HIS	5.8
2	D	227	HIS	5.6
1	A	385	PRO	5.5
1	C	527	THR	5.5
1	A	473	GLN	5.5
2	D	196	LEU	5.4
1	A	386	THR	5.3
1	C	474	ASP	5.3
2	D	226	THR	5.3
2	D	229	GLY	5.2
2	B	382	GLY	5.1
1	C	528	VAL	5.0
1	C	473	GLN	4.8
2	D	197	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	436	THR	4.7
2	B	228	LEU	4.6
1	C	654	ARG	4.6
1	C	185	PHE	4.6
2	B	7	ILE	4.5
2	B	196	LEU	4.2
2	D	261	ARG	4.1
1	A	526	LYS	4.1
1	C	498	ILE	4.0
2	B	229	GLY	3.9
1	A	652	ALA	3.8
2	B	18	VAL	3.8
1	C	475	SER	3.7
2	B	197	ILE	3.7
2	B	288	PHE	3.7
1	A	387	LEU	3.7
1	A	500	ASP	3.6
1	A	472	GLY	3.6
1	C	530	LYS	3.6
1	C	412	ASP	3.6
2	B	249	HIS	3.6
1	C	650	LYS	3.5
1	C	470	PRO	3.5
2	D	255	GLN	3.5
2	D	67	VAL	3.4
2	D	198	PHE	3.4
1	C	647	GLU	3.4
1	A	468	GLN	3.4
2	D	356	GLY	3.3
1	A	470	PRO	3.3
1	C	466	GLY	3.2
1	C	202	VAL	3.2
1	C	469	LEU	3.2
2	D	203	GLY	3.2
2	D	202	GLY	3.1
2	D	23	HIS	3.1
2	D	4	ALA	3.1
1	A	388	ARG	3.1
1	C	430	LEU	3.0
2	D	123	VAL	3.0
2	B	256	ASN	3.0
1	A	530	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	230	GLY	3.0
2	D	47	THR	3.0
1	A	478	VAL	2.9
2	B	67	VAL	2.9
1	C	471	GLU	2.9
2	D	207	VAL	2.9
2	B	245	PHE	2.9
1	C	193	GLU	2.9
1	C	472	GLY	2.9
2	B	8	GLY	2.9
2	D	7	ILE	2.9
1	C	468	GLN	2.8
2	B	109	GLY	2.8
1	A	22	ARG	2.8
1	A	454	ASN	2.8
1	C	617	PHE	2.8
2	B	9	ILE	2.8
2	B	191	GLY	2.8
1	C	534	THR	2.8
2	D	291	ILE	2.7
2	D	250	LYS	2.7
1	A	21	ASN	2.7
2	D	256	ASN	2.7
2	D	15	TYR	2.7
1	C	648	GLU	2.7
1	C	613	TYR	2.7
1	C	533	LEU	2.7
2	D	119	ILE	2.7
1	A	142	CYS	2.7
2	D	73	LEU	2.6
2	B	291	ILE	2.6
2	D	249	HIS	2.6
1	C	480	LEU	2.6
1	C	414	ASP	2.6
1	C	478	VAL	2.6
2	D	195	VAL	2.6
1	A	193	GLU	2.6
2	D	18	VAL	2.6
2	B	23	HIS	2.6
1	C	413	GLU	2.5
1	C	450	GLN	2.5
1	C	391	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	260	VAL	2.5
2	B	253	ILE	2.5
1	A	469	LEU	2.5
2	D	269	ARG	2.4
1	A	204	ILE	2.4
1	C	439	PHE	2.4
1	C	651	GLN	2.4
2	D	164	ILE	2.4
1	C	200	ALA	2.4
2	D	110	GLU	2.4
1	C	388	ARG	2.4
1	A	433	LEU	2.4
1	A	241	ILE	2.4
1	C	2	SER	2.4
1	C	633	SER	2.3
1	C	464	ILE	2.3
1	C	652	ALA	2.3
1	A	137	ASN	2.3
1	C	404	TYR	2.3
2	B	6	ALA	2.3
1	C	191	GLU	2.3
2	B	286	SER	2.3
2	B	73	LEU	2.3
1	A	199	VAL	2.2
2	D	258	ARG	2.2
1	A	6	GLY	2.2
2	D	9	ILE	2.2
2	B	198	PHE	2.2
2	D	248	LYS	2.2
1	A	377	ALA	2.2
1	C	241	ILE	2.2
2	D	8	GLY	2.2
2	B	263	LEU	2.2
2	D	143	VAL	2.1
2	B	202	GLY	2.1
1	A	185	PHE	2.1
2	B	287	LEU	2.1
2	B	98	GLY	2.1
1	C	386	THR	2.1
2	D	111	THR	2.1
1	C	6	GLY	2.1
1	C	385	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	389	VAL	2.1
2	B	255	GLN	2.1
2	B	248	LYS	2.1
1	A	5	PHE	2.1
1	C	532	ASP	2.1
2	B	42	VAL	2.1
2	B	19	GLY	2.0
1	A	200	ALA	2.0
2	B	15	TYR	2.0
2	D	191	GLY	2.0
1	C	187	THR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GOL	A	2002	6/6	0.90	0.15	1.98	45,46,48,49	0
3	MG	A	2001	1/1	0.99	0.12	-0.70	33,33,33,33	0
4	ATP	A	1001	31/31	0.99	0.09	-1.06	28,31,36,36	0
4	ATP	C	1001	31/31	0.99	0.09	-1.23	29,33,35,35	0
3	MG	C	2001	1/1	0.99	0.03	-3.62	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.