



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:45 PM UTC

PDB ID : 3D2E / pdb_00003d2e
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

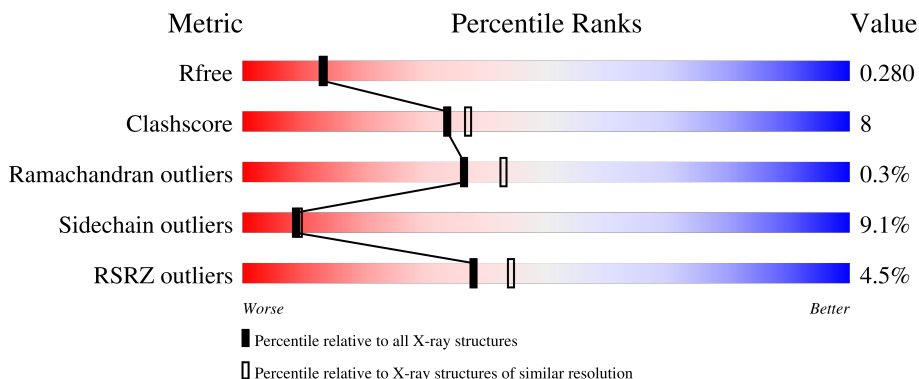
1 Overall quality at a glance i

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
1	C	675	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
2	B	382	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div>
2	D	382	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div>

2 Entry composition [i](#)

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
			Total	C	N	O	S	Se			
1	A	629	4835	3056	813	954	5	7	0	1	0
1	C	627	4812	3040	808	952	5	7	0	0	0

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.

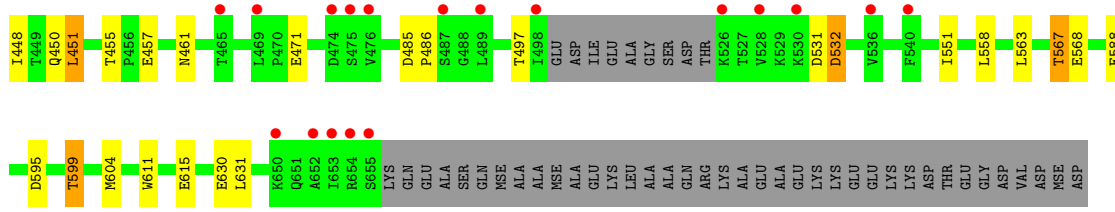
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	379	2869	1811	497	554	3	4	0	0	0
2	D	379	2820	1775	486	552	3	4	0	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

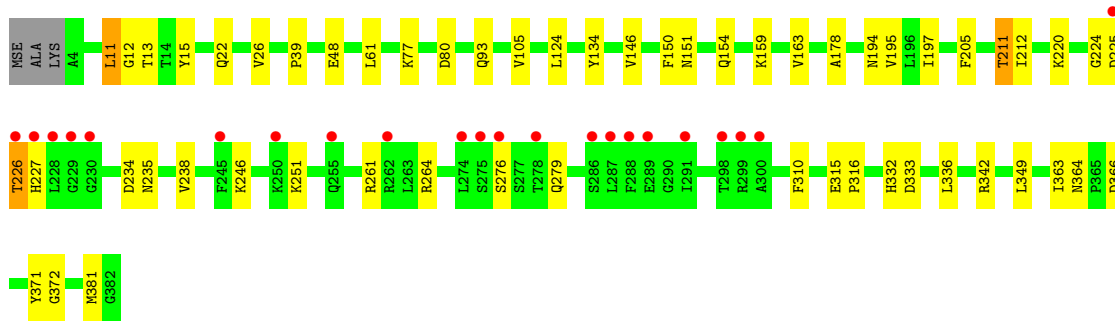
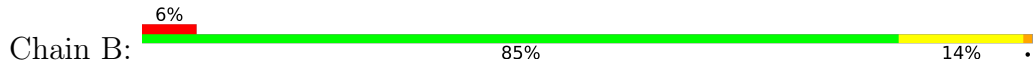
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 6 is water.

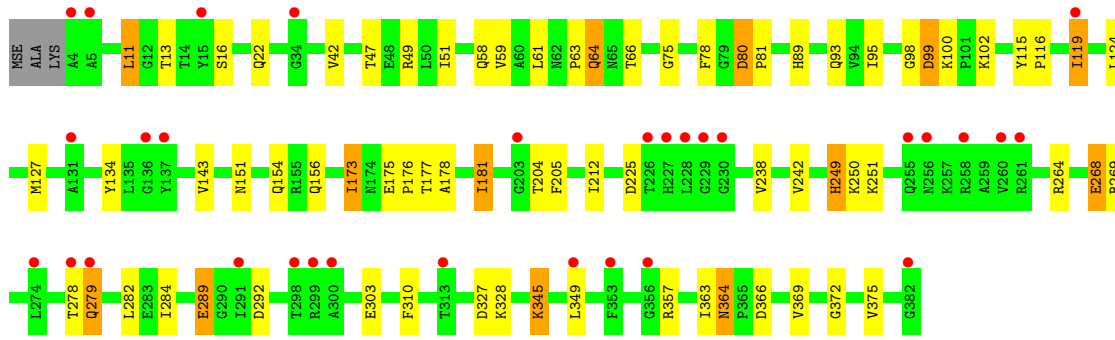
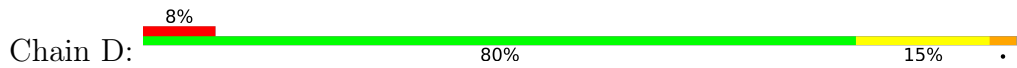
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	161	Total 161	O 161	0	0
6	B	65	Total 65	O 65	0	0
6	C	144	Total 144	O 144	0	0
6	D	58	Total 58	O 58	0	0



● 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) 99.6 (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)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.262 (Not available) , 0.280	Depositor DCC
R_{free} test set	5797 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15834	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage'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, ATP, MG

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	0.77	3/4918 (0.1%)	1.03	14/6663 (0.2%)
1	C	0.70	1/4894 (0.0%)	1.01	8/6630 (0.1%)
2	B	0.72	0/2913	0.90	1/3944 (0.0%)
2	D	0.76	2/2862 (0.1%)	0.94	2/3882 (0.1%)
All	All	0.74	6/15587 (0.0%)	0.99	25/21119 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	289	GLU	CD-OE1	15.00	1.53	1.25
2	D	289	GLU	CD-OE2	9.29	1.43	1.25
1	A	473	GLN	CD-OE1	6.80	1.36	1.23
1	A	473	GLN	CD-NE2	6.17	1.46	1.33
1	C	65	VAL	CA-CB	5.61	1.60	1.54
1	A	65	VAL	CA-CB	5.39	1.60	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	80	ASP	CA-C-N	7.61	129.35	119.84
2	D	80	ASP	C-N-CA	7.61	129.35	119.84
1	A	89	THR	N-CA-C	-7.23	104.71	113.97
1	C	43	GLY	CA-C-N	7.11	126.81	119.56
1	C	43	GLY	C-N-CA	7.11	126.81	119.56
1	A	141	VAL	CB-CA-C	-6.99	99.50	110.69
1	C	100	THR	N-CA-C	5.86	118.50	109.07
1	C	260	ASN	CA-C-N	5.80	125.94	119.32
1	C	260	ASN	C-N-CA	5.80	125.94	119.32
1	A	223	VAL	N-CA-CB	5.73	116.78	110.53
1	C	65	VAL	CB-CA-C	5.71	119.34	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	VAL	CB-CA-C	5.68	118.54	111.15
1	A	69	LYS	CB-CA-C	-5.49	101.35	110.68
1	A	24	ILE	CB-CA-C	5.38	118.18	110.33
1	A	89	THR	CB-CA-C	5.32	118.00	109.07
1	A	295	VAL	N-CA-C	5.26	115.16	107.37
1	A	89	THR	N-CA-CB	-5.25	103.38	110.67
1	C	89	THR	N-CA-C	-5.17	107.35	113.97
1	A	68	LEU	CA-C-N	5.17	127.46	120.38
1	A	68	LEU	C-N-CA	5.17	127.46	120.38
1	A	65	VAL	CB-CA-C	5.15	118.04	110.98
2	B	48	GLU	N-CA-C	5.10	116.56	108.96
1	A	150	THR	N-CA-CB	-5.06	102.76	110.45
1	C	126	VAL	CB-CA-C	5.05	119.19	112.22
1	A	452	PRO	O-C-N	5.02	123.62	121.31

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	86	0
1	C	4812	0	4667	77	0
2	B	2869	0	2813	29	0
2	D	2820	0	2700	44	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	234	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 (234) 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
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:HD13	1:A:24:ILE:C	2.20	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
2:D:364:ASN:HD22	2:D:364:ASN:C	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:67:ASN:HB2	1:A:88:PHE:CZ	2.33	0.63
1:A:150:THR:HG23	6:A:2159:HOH:O	1.97	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:A:29:ASN:C	1:A:29:ASN:HD22	2.07	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: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: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
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: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:76:TYR:CD2	1:A:94:GLU:HB2	2.40	0.56
1:A:481:LYS:HE3	1:A:493:GLU:OE1	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:29:ASN:C	1:C:29:ASN:HD22	2.14	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:221:LEU:HD12	1:A:221:LEU:C	2.37	0.48
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:333:GLU:CD	1:C:333:GLU:H	2.21	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
1:A:182:TYR:CE1	1:A:186:LYS:HE3	2.50	0.47
1:A:397:ILE:HG13	1:A:398:HIS:N	2.29	0.47
2:B:197:ILE:HD12	2:B:197:ILE:N	2.28	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:O	1:C:364:THR:HG22	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
2:B:363:ILE:O	2:B:364:ASN:C	2.58	0.46
1:A:604:MSE:HE2	1:A:604:MSE:HB3	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:C:248:GLU:OE1	1:C:299:SER:OG	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:ILE:HG13	1:C:370:GLU:CD	2.40	0.45
1:C:44:PRO:O	1:C:107:ALA:HA	2.17	0.45
2:D:363:ILE:O	2:D:364:ASN:C	2.59	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: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:C:221:LEU:C	1:C:221:LEU:HD12	2.43	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
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
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:B:224:GLY:C	2:B:226:THR:H	2.25	0.42
2:D:42:VAL:HG13	2:D:51:ILE:HD13	2.00	0.42
2:D:364:ASN:C	2:D:364:ASN:ND2	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:24:ILE:C	1:A:24:ILE:CD1	2.92	0.42
1:A:49:LEU:CB	1:A:125:LYS:HG3	2.47	0.41
1:C:3:THR:HA	1:C:4:PRO:HD3	1.96	0.41
1:C:154:ARG:NH2	1:C:173:ASN:HD21	2.16	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
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
1:A:209:TYR:C	1:A:209:TYR:CD2	2.99	0.40
1:A:442:ALA:HA	1:A:461:ASN:HA	2.03	0.40
1:C:259:GLU:OE1	1:C:259:GLU:HA	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%)	36	43
1	C	623/675 (92%)	590 (95%)	32 (5%)	1 (0%)	43	52
2	B	377/382 (99%)	366 (97%)	10 (3%)	1 (0%)	36	43
2	D	377/382 (99%)	355 (94%)	19 (5%)	3 (1%)	16	17
All	All	2003/2114 (95%)	1912 (96%)	84 (4%)	7 (0%)	36	43

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
1	A	653	ILE

5.3.2 Protein sidechains [i](#)

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%)	451 (88%)	59 (12%)	5	5
1	C	508/565 (90%)	456 (90%)	52 (10%)	7	6
2	B	297/310 (96%)	288 (97%)	9 (3%)	36	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	283/310 (91%)	258 (91%)	25 (9%)	9 10
All	All	1598/1750 (91%)	1453 (91%)	145 (9%)	9 9

All (145) 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	28	VAL
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
1	A	105	ARG
1	A	125	LYS
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	221	LEU

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Mol	Chain	Res	Type
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	291	VAL
1	A	294	ASP
1	A	311	LYS
1	A	330	LEU
1	A	340	ILE
1	A	397	ILE
1	A	432	THR
1	A	435	ARG
1	A	451	LEU
1	A	458	GLN
1	A	497	THR
1	A	532	ASP
1	A	543	ASP
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
2	B	279	GLN
2	B	336	LEU
2	B	381	MSE
1	C	3	THR
1	C	7	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

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Mol	Chain	Res	Type
1	C	54	LYS
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	104	VAL
1	C	105	ARG
1	C	125	LYS
1	C	126	VAL
1	C	149	TYR
1	C	150	THR
1	C	169	VAL
1	C	171	ILE
1	C	191	GLU
1	C	197	ARG
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	291	VAL
1	C	298	SER
1	C	333	GLU
1	C	352	GLN
1	C	364	THR
1	C	389	VAL
1	C	397	ILE
1	C	432	THR
1	C	435	ARG
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

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Mol	Chain	Res	Type
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	212	ILE
2	D	249	HIS
2	D	268	GLU
2	D	269	ARG
2	D	279	GLN
2	D	282	LEU
2	D	284	ILE
2	D	289	GLU
2	D	292	ASP
2	D	345	LYS
2	D	364	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	21	ASN
1	A	29	ASN
1	A	46	ASN
1	A	57	GLN
1	A	60	ASN
1	A	156	ASN
1	A	173	ASN
1	A	368	GLN
1	A	409	GLN
1	A	454	ASN
1	A	458	GLN
1	A	548	ASN

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Mol	Chain	Res	Type
1	A	555	ASN
1	A	602	GLN
2	B	22	GLN
2	B	93	GLN
2	B	154	GLN
2	B	235	ASN
2	B	240	HIS
2	B	279	GLN
2	B	332	HIS
1	C	11	ASN
1	C	13	ASN
1	C	29	ASN
1	C	46	ASN
1	C	60	ASN
1	C	83	GLN
1	C	117	GLN
1	C	156	ASN
1	C	173	ASN
1	C	352	GLN
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	89	HIS
2	D	141	ASN
2	D	154	GLN
2	D	156	GLN
2	D	168	ASN
2	D	194	ASN
2	D	279	GLN
2	D	364	ASN
2	D	376	GLN

5.3.3 RNA [i](#)

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 oligosaccharides 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	32,33,33	1.71	4 (12%)	48,52,52	1.85	10 (20%)
4	ATP	C	1001	3	32,33,33	1.52	4 (12%)	48,52,52	1.91	14 (29%)
5	GOL	A	2002	-	5,5,5	0.62	0	5,5,5	0.83	0

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	-	1/22/38/38	0/3/3/3
4	ATP	C	1001	3	-	2/22/38/38	0/3/3/3
5	GOL	A	2002	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	ATP	PB-O3B	5.13	1.65	1.59
4	A	1001	ATP	C5-C4	5.01	1.48	1.39
4	C	1001	ATP	C5-C4	4.81	1.47	1.39
4	C	1001	ATP	PB-O3B	4.20	1.64	1.59
4	A	1001	ATP	C5-C6	2.99	1.49	1.41
4	C	1001	ATP	C5-C6	2.54	1.48	1.41
4	A	1001	ATP	PB-O3A	2.32	1.62	1.59
4	C	1001	ATP	C8-N7	2.29	1.36	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	ATP	C5-C4-N3	-5.36	119.33	126.72
4	C	1001	ATP	C5-C4-N3	-5.31	119.41	126.72
4	A	1001	ATP	N3-C4-N9	4.96	135.60	127.17
4	C	1001	ATP	N3-C4-N9	4.63	135.04	127.17
4	A	1001	ATP	C4-N9-C8	3.63	109.55	105.74
4	C	1001	ATP	N3-C2-N1	-3.54	123.22	128.58
4	A	1001	ATP	C2-N3-C4	3.54	120.47	111.83
4	C	1001	ATP	C4-C5-N7	-3.46	106.63	110.58
4	A	1001	ATP	N3-C2-N1	-3.42	123.40	128.58
4	C	1001	ATP	C2-N3-C4	3.41	120.16	111.83
4	C	1001	ATP	C4-N9-C8	3.39	109.29	105.74
4	A	1001	ATP	C4-C5-N7	-3.08	107.06	110.58
4	C	1001	ATP	C5-N7-C8	2.99	108.14	103.45
4	C	1001	ATP	O4'-C1'-N9	2.83	113.53	108.09
4	A	1001	ATP	O4'-C1'-N9	2.70	113.28	108.09
4	C	1001	ATP	N9-C8-N7	-2.51	110.38	113.94
4	C	1001	ATP	O2B-PB-O3B	2.47	113.94	107.27
4	A	1001	ATP	C5-N7-C8	2.45	107.30	103.45
4	C	1001	ATP	C2-N1-C6	2.39	122.65	118.73
4	C	1001	ATP	O3A-PB-O1B	-2.35	103.63	110.70
4	C	1001	ATP	O2A-PA-O1A	2.18	122.58	112.44
4	C	1001	ATP	C6-C5-N7	2.14	136.22	132.09
4	A	1001	ATP	N9-C8-N7	-2.05	111.02	113.94
4	A	1001	ATP	C2-N1-C6	2.03	122.06	118.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

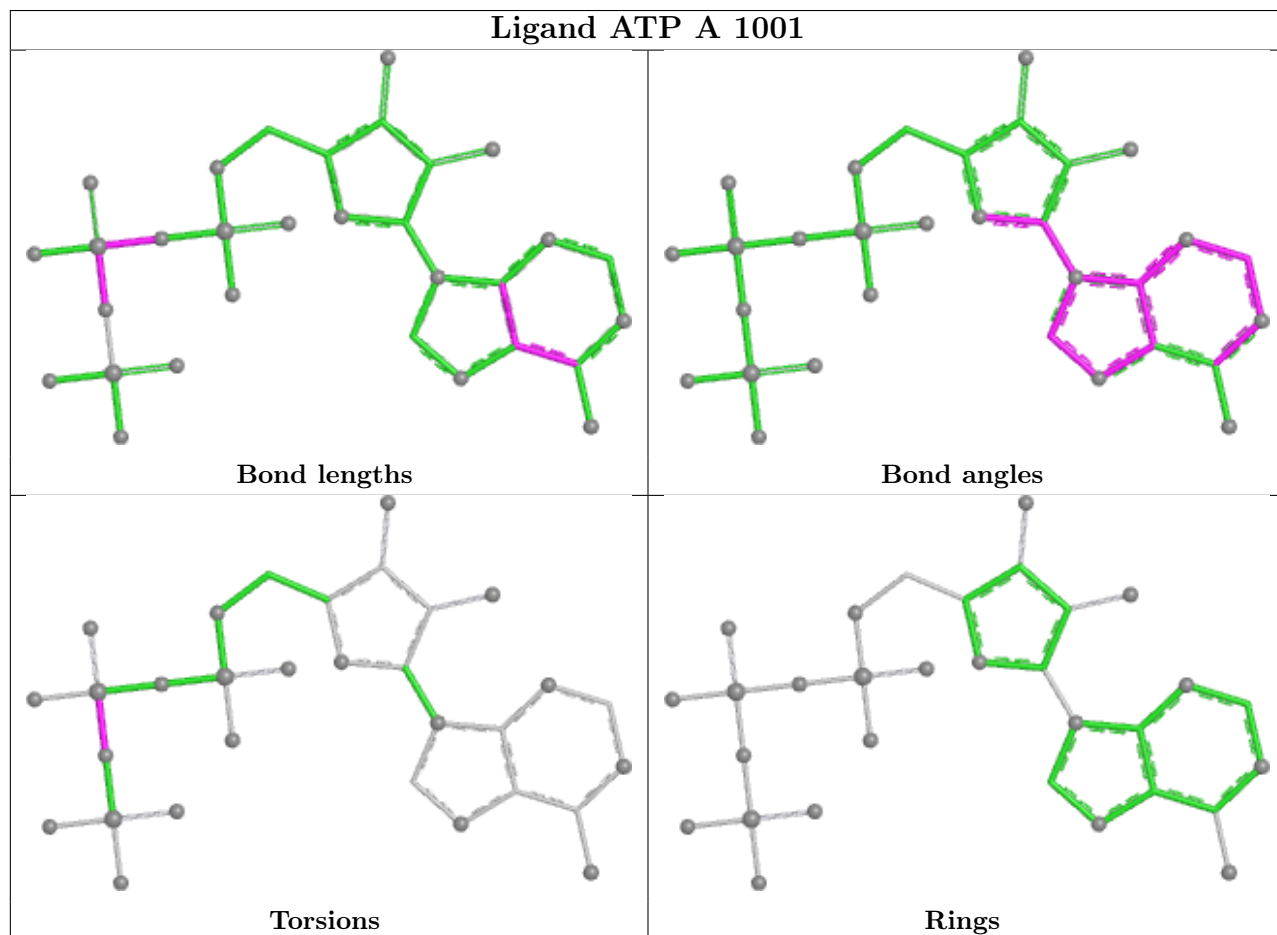
Mol	Chain	Res	Type	Atoms
5	A	2002	GOL	O2-C2-C3-O3
5	A	2002	GOL	C1-C2-C3-O3
4	A	1001	ATP	PG-O3B-PB-O2B
4	C	1001	ATP	PG-O3B-PB-O2B
4	C	1001	ATP	PG-O3B-PB-O1B

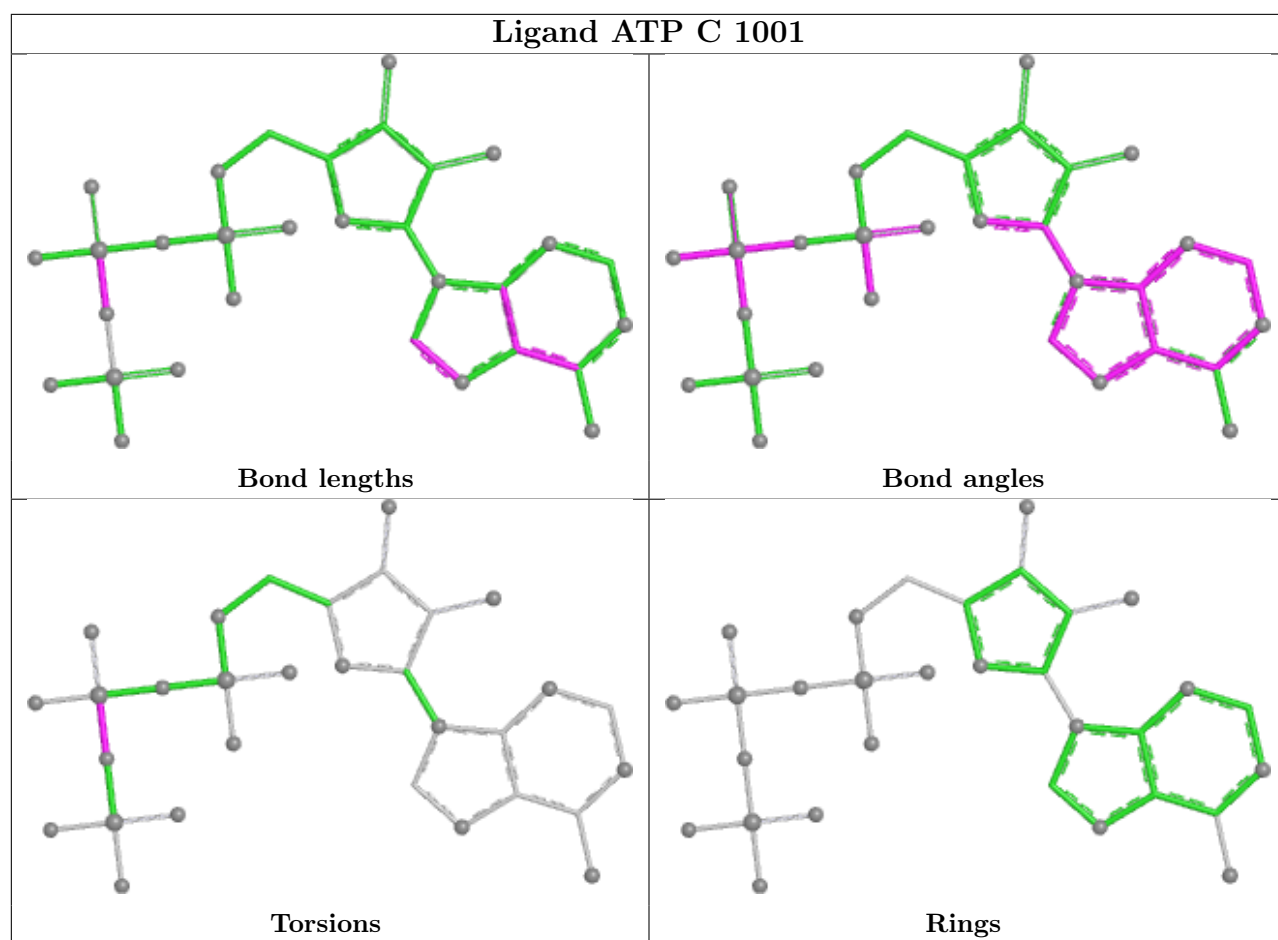
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.08	14 (2%) 61 66	16, 34, 45, 57	1 (0%)
1	C	620/675 (91%)	0.28	22 (3%) 47 53	27, 35, 45, 64	0
2	B	375/382 (98%)	0.24	22 (5%) 28 32	27, 34, 45, 70	0
2	D	375/382 (98%)	0.67	31 (8%) 17 19	28, 35, 43, 59	0
All	All	1992/2114 (94%)	0.28	89 (4%) 38 44	16, 35, 45, 70	1 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	230	GLY	5.7
1	A	527	THR	5.4
2	D	229	GLY	4.4
1	C	489	LEU	4.1
1	A	654	ARG	4.0
2	B	226	THR	3.8
2	D	300	ALA	3.7
2	D	260	VAL	3.6
1	C	655	SER	3.6
1	A	525	THR	3.6
2	D	278	THR	3.6
1	A	450[A]	GLN	3.5
2	D	255	GLN	3.5
2	D	227	HIS	3.5
2	D	256	ASN	3.5
2	D	291	ILE	3.4
1	C	185	PHE	3.4
2	B	245	PHE	3.3
2	B	229	GLY	3.3
2	D	226	THR	3.3
1	A	472	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	536	VAL	3.2
1	A	473	GLN	3.1
2	B	288	PHE	3.1
2	B	275	SER	3.0
1	A	477	PRO	3.0
2	D	258	ARG	3.0
2	B	228	LEU	2.9
2	B	276	SER	2.8
2	D	4	ALA	2.8
1	C	487	SER	2.7
2	B	227	HIS	2.7
2	D	228	LEU	2.6
2	B	300	ALA	2.6
2	D	5	ALA	2.6
1	A	185	PHE	2.6
1	C	137	ASN	2.6
2	B	278	THR	2.6
2	D	230	GLY	2.6
2	D	279	GLN	2.6
2	D	34	GLY	2.5
2	D	15	TYR	2.5
1	C	654	ARG	2.5
2	D	313	THR	2.5
2	D	274	LEU	2.5
1	C	436	THR	2.4
1	C	653	ILE	2.4
2	B	255	GLN	2.4
2	D	203	GLY	2.4
1	C	650	LYS	2.4
1	A	653	ILE	2.4
1	A	468	GLN	2.3
2	B	286	SER	2.3
2	D	299	ARG	2.3
1	C	498	ILE	2.3
2	B	287	LEU	2.2
1	C	475	SER	2.2
1	C	476	VAL	2.2
1	C	526	LYS	2.2
2	B	291	ILE	2.2
1	A	500	ASP	2.2
2	D	261	ARG	2.2
1	C	652	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	469	LEU	2.2
1	C	474	ASP	2.2
2	D	382	GLY	2.2
2	D	298	THR	2.2
1	A	499	GLU	2.1
2	B	262	ARG	2.1
2	B	299	ARG	2.1
2	B	274	LEU	2.1
1	A	293	ASN	2.1
1	C	465	THR	2.1
2	D	356	GLY	2.1
2	B	298	THR	2.1
1	C	530	LYS	2.1
2	B	250	LYS	2.1
2	D	131	ALA	2.1
2	B	289	GLU	2.1
2	B	225	ASP	2.1
1	C	528	VAL	2.1
1	C	540	PHE	2.1
2	D	349	LEU	2.0
1	A	340	ILE	2.0
2	D	119	ILE	2.0
2	D	137	TYR	2.0
2	D	136	GLY	2.0
2	D	353	PHE	2.0
1	C	190	PRO	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 [\(i\)](#)

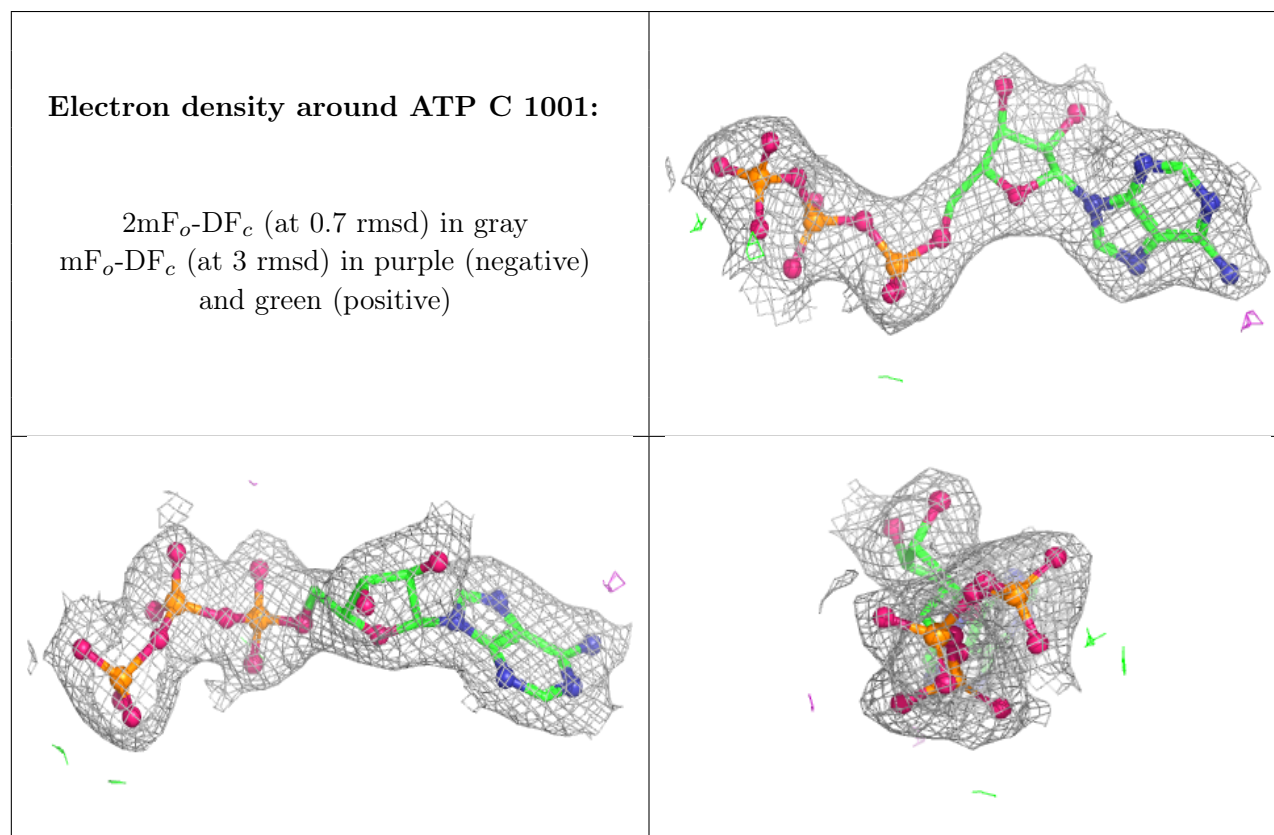
There are no oligosaccharides in this entry.

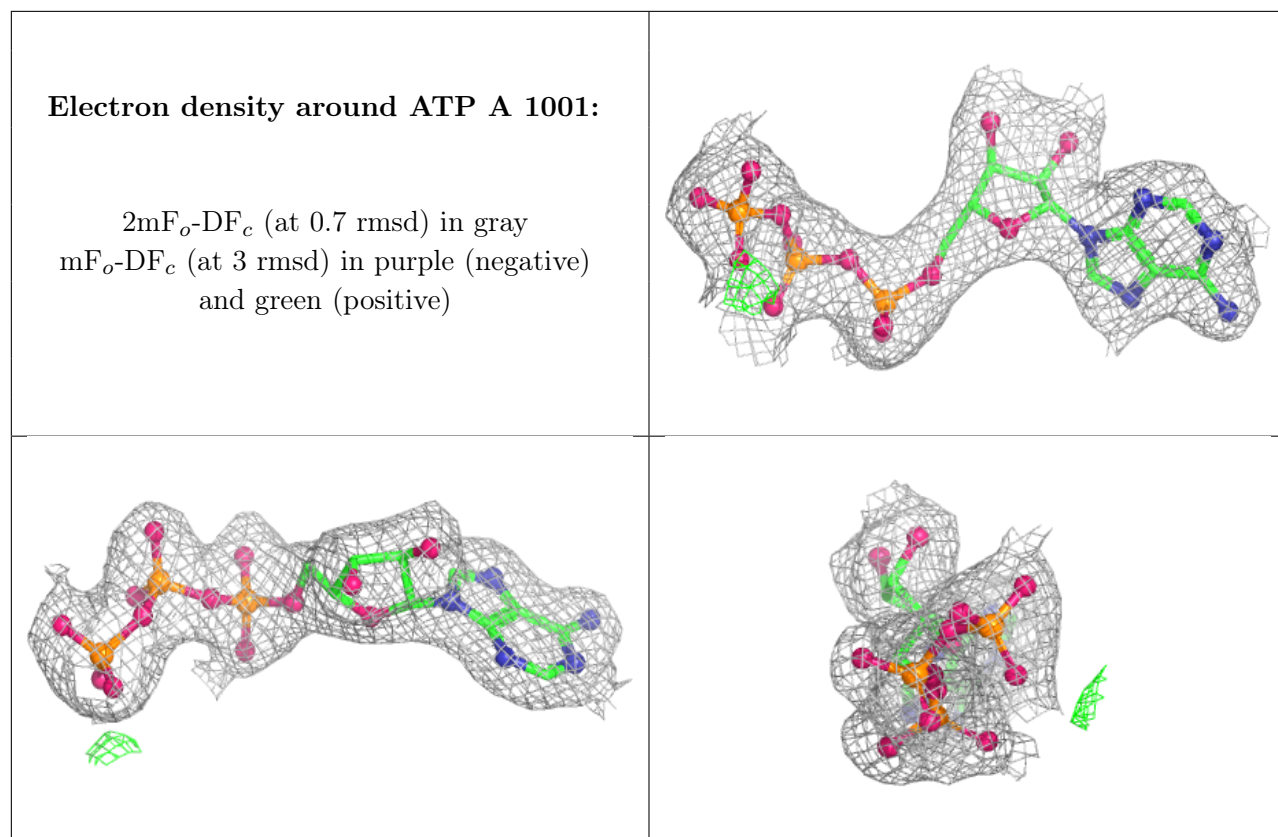
6.4 Ligands [\(i\)](#)

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
5	GOL	A	2002	6/6	0.81	0.14	45,46,48,49	0
4	ATP	C	1001	31/31	0.98	0.05	29,33,35,35	0
4	ATP	A	1001	31/31	0.98	0.05	28,31,36,36	0
3	MG	C	2001	1/1	0.99	0.03	28,28,28,28	0
3	MG	A	2001	1/1	0.99	0.04	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.