



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:18 AM GMT

PDB ID : 2CK3
Title : Azide inhibited bovine F1-ATPase
Authors : Bowler, M.W.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2006-04-10
Resolution : 1.95 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 (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

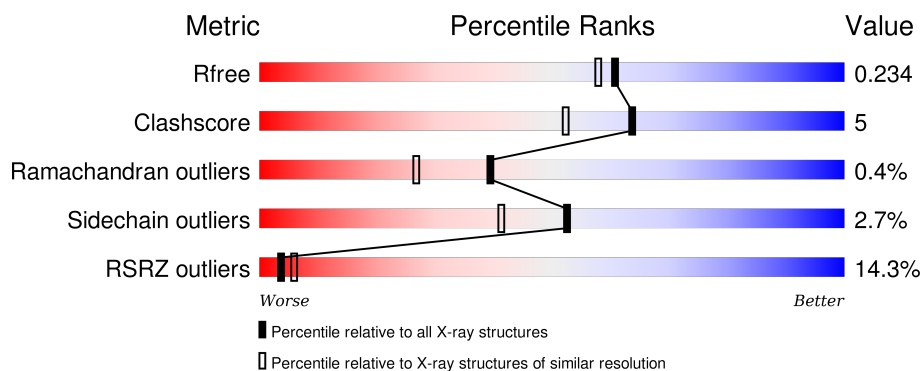
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	510	<div> <div>13%</div> <div>83%</div> <div>11% • 5%</div> </div>
1	B	510	<div> <div>15%</div> <div>87%</div> <div>6% • 6%</div> </div>
1	C	510	<div> <div>6%</div> <div>85%</div> <div>11% • •</div> </div>
2	D	482	<div> <div>6%</div> <div>87%</div> <div>9% • •</div> </div>
2	E	482	<div> <div>18%</div> <div>86%</div> <div>8% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	482	
3	G	272	
4	H	146	
5	I	50	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PO4	E	602	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26509 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	4	0
			3738	2359	658	709	12			
1	B	480	Total	C	N	O	S	0	1	0
			3667	2310	649	696	12			
1	C	490	Total	C	N	O	S	0	0	0
			3735	2353	659	711	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	CLONING ARTIFACT	UNP P19483
B	481	GLY	SER	CLONING ARTIFACT	UNP P19483
C	481	GLY	SER	CLONING ARTIFACT	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	2	0
			3550	2252	602	685	11			
2	E	458	Total	C	N	O	S	0	2	0
			3486	2209	596	671	10			
2	F	466	Total	C	N	O	S	0	3	0
			3541	2248	600	682	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	182	Total	C	N	O	S	0	0	1
			1397	881	250	260	6			

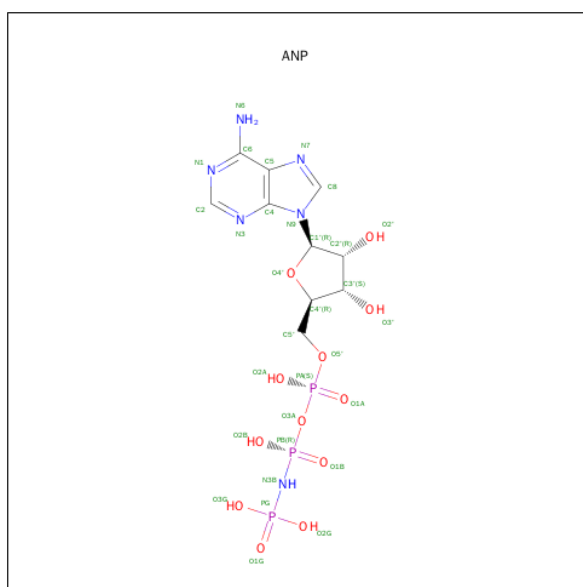
- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	83	Total	C	N	O	S	0	0	0
			620	391	102	126	1			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	25	Total	C	N	O	S	0	0	0
			203	130	38	34	1			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

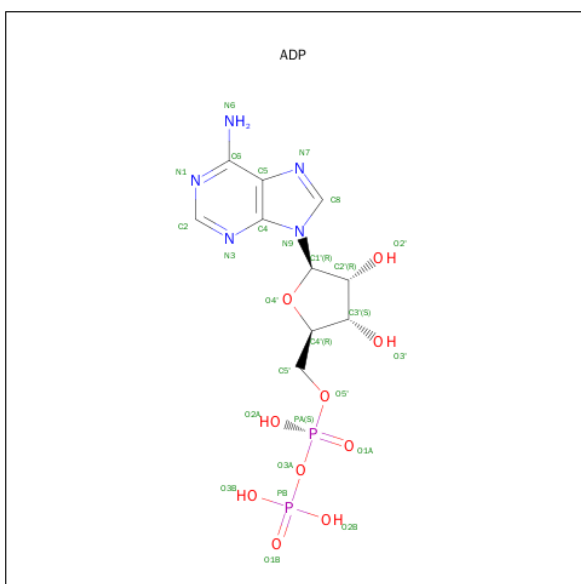
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		

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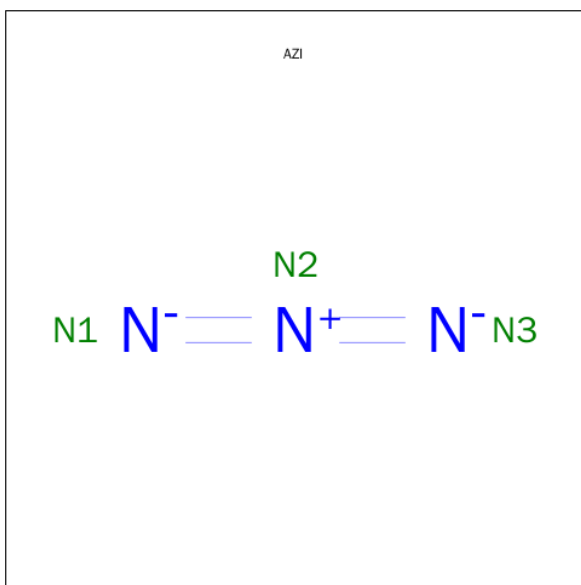
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



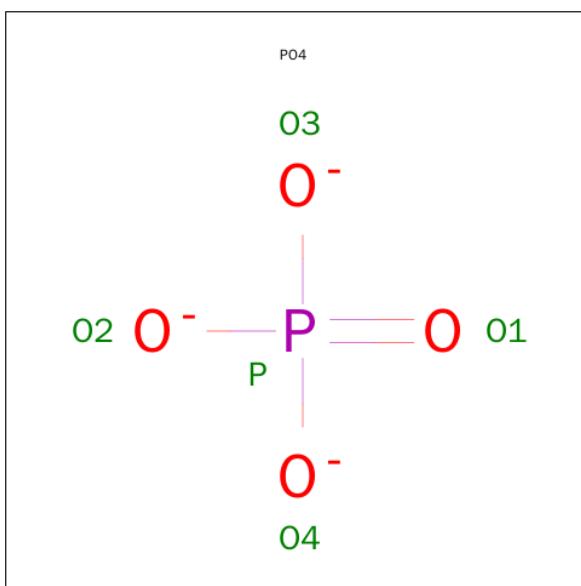
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total N 3 3	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	1	Total O P 5 4 1	0	0

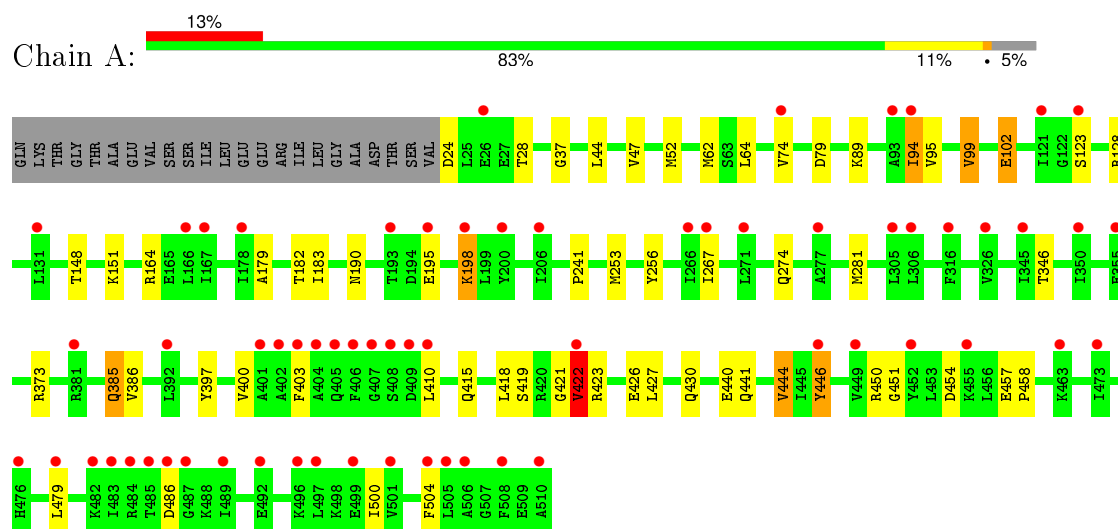
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	380	Total 380	O 380	0	0
11	B	409	Total 409	O 409	0	0
11	C	378	Total 378	O 378	0	0
11	D	383	Total 383	O 383	0	0
11	E	246	Total 246	O 246	0	0
11	F	484	Total 484	O 484	0	0
11	G	113	Total 113	O 113	0	0
11	H	8	Total 8	O 8	0	0
11	I	7	Total 7	O 7	0	0

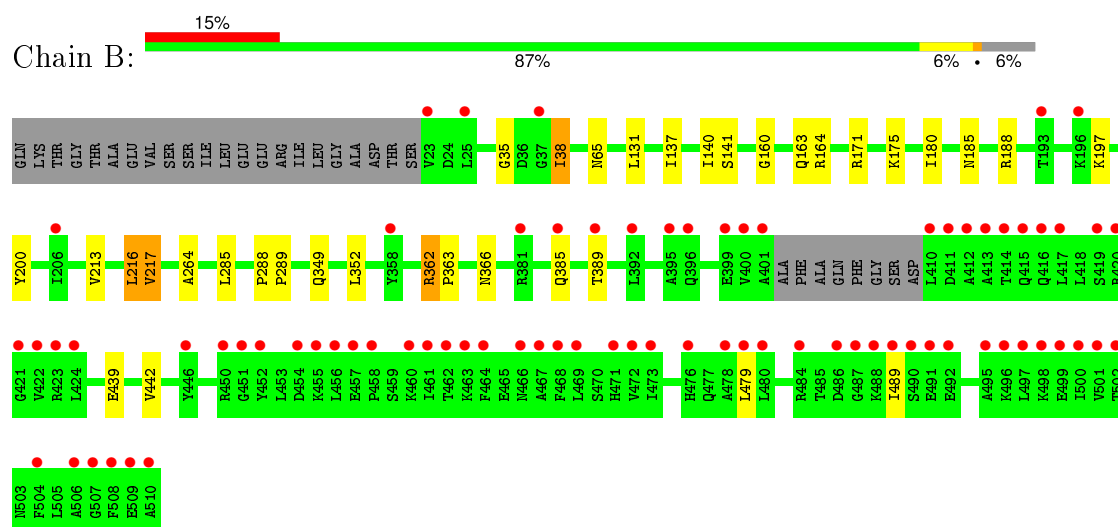
3 Residue-property plots

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

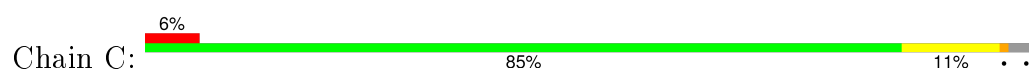
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

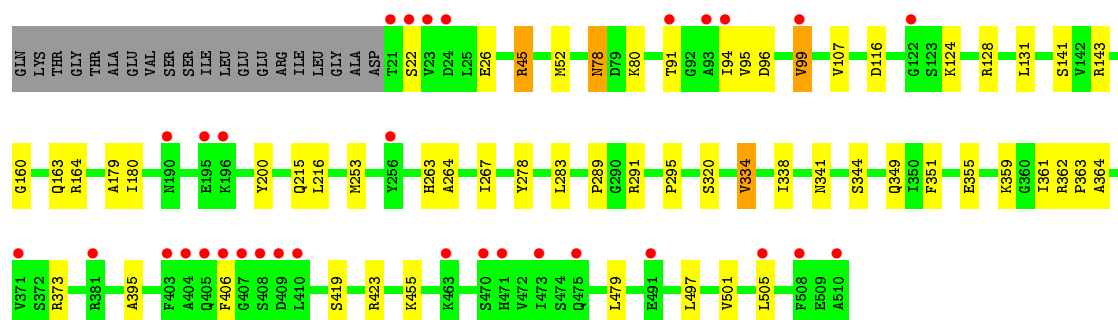


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

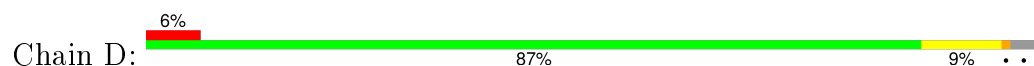


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

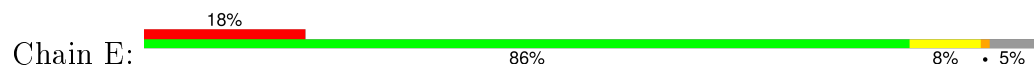




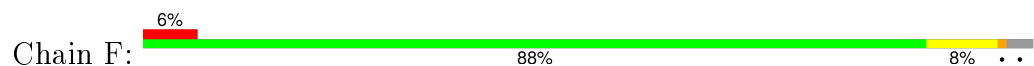
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

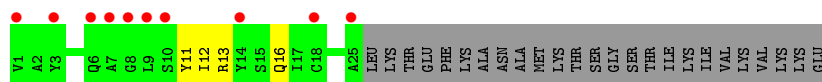


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	261.16Å 105.22Å 122.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 43.53 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-1.95) 98.4 (43.53-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.226 0.207 , 0.234	Depositor DCC
R_{free} test set	12041 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 242015 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26509	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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, 0.375 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: AZI, MG, ANP, PO4, ADP

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	0.39	2/3798 (0.1%)	0.55	0/5123
1	B	0.38	0/3719	0.52	0/5016
1	C	0.35	0/3786	0.51	0/5108
2	D	0.36	0/3611	0.55	0/4901
2	E	0.35	0/3547	0.52	0/4811
2	F	0.39	0/3607	0.54	0/4895
3	G	0.38	0/1406	0.47	0/1880
4	H	0.39	0/623	0.62	0/840
5	I	0.41	0/207	0.59	0/279
All	All	0.37	2/24304 (0.0%)	0.53	0/32853

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422[A]	VAL	CA-CB	5.47	1.66	1.54
1	A	422[B]	VAL	CA-CB	5.47	1.66	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3738	0	3850	43	0
1	B	3667	0	3776	22	0
1	C	3735	0	3835	32	0
2	D	3550	0	3608	43	0
2	E	3486	0	3542	44	0
2	F	3541	0	3609	31	0
3	G	1397	0	1481	16	0
4	H	620	0	614	27	0
5	I	203	0	205	3	0
6	A	31	0	13	0	0
6	B	31	0	13	0	0
6	C	31	0	13	0	0
6	F	31	0	13	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	D	27	0	12	1	0
9	D	3	0	0	1	0
10	E	5	0	0	0	0
11	A	380	0	0	3	0
11	B	409	0	0	4	0
11	C	378	0	0	6	0
11	D	383	0	0	2	0
11	E	246	0	0	3	0
11	F	484	0	0	6	0
11	G	113	0	0	3	0
11	H	8	0	0	0	0
11	I	7	0	0	0	0
All	All	26509	0	24584	253	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 5.

All (253) 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)
4:H:122:ALA:HA	4:H:123:ALA:CB	1.74	1.18
3:G:68:ILE:HB	3:G:69:ILE:HA	1.30	1.13
2:D:89:GLU:HG3	2:D:110:THR:HB	1.29	1.09
2:E:256:ASP:HA	2:E:257[B]:ASN:HB3	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:104:ASP:HA	4:H:105:LEU:HB2	1.31	1.09
2:D:228:ALA:O	2:D:232[A]:VAL:HG13	1.52	1.09
4:H:121:GLY:HA3	4:H:122:ALA:HB3	1.40	1.03
4:H:122:ALA:HA	4:H:123:ALA:HB2	1.38	1.01
4:H:99:THR:HA	4:H:100:LEU:HB2	1.46	0.95
2:D:97:VAL:HA	2:D:232[B]:VAL:HG23	1.49	0.94
2:F:282:GLN:H	2:F:282:GLN:HE21	1.06	0.93
2:E:282:GLN:H	2:E:282:GLN:HE21	1.14	0.91
4:H:104:ASP:CA	4:H:105:LEU:HB2	2.01	0.91
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.53	0.90
3:G:20:THR:HG22	3:G:232:MET:HE3	1.53	0.90
2:D:282:GLN:H	2:D:282:GLN:HE21	0.94	0.89
1:A:74[B]:VAL:CG1	1:A:241:PRO:HG3	2.02	0.89
2:E:63:MET:SD	11:E:2044:HOH:O	2.30	0.88
4:H:122:ALA:HA	4:H:123:ALA:HB3	1.56	0.83
4:H:104:ASP:HA	4:H:105:LEU:CB	2.07	0.83
1:A:79:ASP:HB3	11:A:2059:HOH:O	1.80	0.82
4:H:122:ALA:CA	4:H:123:ALA:CB	2.58	0.81
4:H:122:ALA:CA	4:H:123:ALA:HB2	2.10	0.81
1:B:197:LYS:HG3	11:B:2225:HOH:O	1.81	0.80
2:F:97[B]:VAL:HG23	11:F:2278:HOH:O	1.79	0.80
1:A:74[B]:VAL:HG12	1:A:241:PRO:HG3	1.60	0.79
1:A:151:LYS:H	1:A:430:GLN:HE22	1.30	0.79
2:E:257[B]:ASN:HB2	2:E:309:ALA:O	1.83	0.78
1:C:291:ARG:HD2	11:C:2226:HOH:O	1.85	0.77
2:E:293:GLN:HE22	2:E:308:GLN:HE22	1.32	0.77
1:A:195:GLU:HA	1:A:198[B]:LYS:HD3	1.66	0.76
2:F:97[A]:VAL:HG12	2:F:232:VAL:HB	1.66	0.76
4:H:99:THR:CA	4:H:100:LEU:HB2	2.16	0.75
2:E:256:ASP:OD1	2:E:257[B]:ASN:ND2	2.19	0.75
2:D:282:GLN:H	2:D:282:GLN:NE2	1.78	0.75
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.71	0.73
2:D:85:PRO:HB3	2:D:110:THR:HG21	1.69	0.73
2:D:97:VAL:HA	2:D:232[B]:VAL:CG2	2.19	0.72
3:G:2:THR:HB	11:G:2006:HOH:O	1.89	0.72
2:E:256:ASP:HA	2:E:257[B]:ASN:CB	2.07	0.72
2:D:282:GLN:N	2:D:282:GLN:HE21	1.79	0.71
2:F:223:ASN:H	2:F:223:ASN:HD22	1.36	0.70
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.74	0.70
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.72	0.70
1:A:418:LEU:O	1:A:422[B]:VAL:HG12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41[B]:ARG:HG2	2:E:42:GLU:N	2.05	0.69
1:B:171:ARG:HD3	11:E:2224:HOH:O	1.94	0.68
2:D:97:VAL:CA	2:D:232[B]:VAL:HG23	2.23	0.67
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.77	0.66
2:F:97[A]:VAL:CG1	2:F:232:VAL:HB	2.25	0.66
2:D:89:GLU:CG	2:D:110:THR:HB	2.19	0.66
1:A:37:GLY:HA2	11:A:2059:HOH:O	1.96	0.65
2:D:89:GLU:HG3	2:D:110:THR:CB	2.17	0.65
4:H:121:GLY:HA3	4:H:122:ALA:CB	2.18	0.65
4:H:127:THR:N	4:H:128:ARG:HB2	2.12	0.64
1:A:102:GLU:HG3	1:A:123:SER:HA	1.80	0.64
1:A:419:SER:O	1:A:423:ARG:HD3	1.99	0.63
3:G:68:ILE:CB	3:G:69:ILE:HA	2.12	0.63
2:D:96:ASN:C	2:D:96:ASN:HD22	2.02	0.63
4:H:127:THR:H	4:H:128:ARG:HB2	1.64	0.62
4:H:127:THR:H	4:H:128:ARG:CB	2.13	0.62
1:C:160:GLY:H	1:C:163:GLN:NE2	1.98	0.61
2:F:97[A]:VAL:HG12	2:F:232:VAL:CB	2.31	0.60
1:C:128:ARG:HD2	1:C:131:LEU:HG	1.83	0.60
4:H:103:LEU:HB3	4:H:105:LEU:HD13	1.83	0.60
2:F:96:ASN:HD22	2:F:96:ASN:C	2.05	0.60
2:F:282:GLN:N	2:F:282:GLN:HE21	1.88	0.59
1:A:74[B]:VAL:HG12	1:A:241:PRO:CG	2.30	0.59
4:H:99:THR:HB	4:H:101:ASP:H	1.68	0.59
2:E:257[A]:ASN:OD1	2:E:260:ARG:HG3	2.03	0.58
3:G:260:LYS:HD2	11:G:2048:HOH:O	2.02	0.58
4:H:99:THR:HA	4:H:100:LEU:CB	2.26	0.58
2:D:85:PRO:HB3	2:D:110:THR:CG2	2.32	0.58
1:A:190:ASN:HA	1:A:198[A]:LYS:HG2	1.86	0.57
1:B:38:ILE:HD12	1:B:285:LEU:HD21	1.86	0.57
2:D:188:GLU:O	2:D:221:GLN:HB3	2.02	0.57
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.86	0.57
1:B:366:ASN:ND2	11:B:2359:HOH:O	2.32	0.57
1:B:137:ILE:HG13	2:F:103:ASP:HA	1.86	0.57
1:C:78:ASN:ND2	11:C:2058:HOH:O	2.35	0.57
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.86	0.57
4:H:127:THR:CA	4:H:128:ARG:HB2	2.34	0.57
2:E:63:MET:HE3	2:E:97:VAL:HG21	1.87	0.57
2:D:186:VAL:HG13	2:D:232[A]:VAL:CG2	2.35	0.56
2:E:412:ARG:HG2	2:E:458:TYR:HB2	1.86	0.56
1:B:160:GLY:H	1:B:163:GLN:NE2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.41	0.56
2:F:282:GLN:H	2:F:282:GLN:NE2	1.90	0.56
1:A:440:GLU:O	1:A:444:VAL:HG12	2.05	0.56
4:H:58:LEU:N	5:I:11:TYR:HH	2.04	0.55
2:D:366:GLU:O	2:D:370:VAL:HG23	2.06	0.55
1:C:344:SER:HA	9:D:1092:AZI:N3	2.22	0.55
1:B:175:LYS:HG2	1:B:352:LEU:HD12	1.89	0.55
1:A:410:LEU:HD12	1:A:415:GLN:HG3	1.89	0.55
1:B:160:GLY:H	1:B:163:GLN:HE21	1.55	0.55
1:B:385:GLN:HE22	1:B:489:ILE:HB	1.71	0.54
2:F:223:ASN:N	2:F:223:ASN:HD22	2.02	0.54
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.89	0.54
4:H:127:THR:HB	4:H:128:ARG:HB2	1.88	0.54
1:A:44:LEU:O	1:A:47:VAL:HG22	2.07	0.54
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.89	0.53
1:B:439:GLU:O	1:B:442:VAL:HG12	2.08	0.53
1:A:427:LEU:HD22	1:A:444:VAL:HG23	1.91	0.53
2:F:188:GLU:O	2:F:221:GLN:HB3	2.09	0.52
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.90	0.52
2:E:223:ASN:H	2:E:223:ASN:HD22	1.56	0.52
1:C:215:GLN:HB3	2:F:356:ARG:HH22	1.75	0.52
2:D:220:GLY:HA3	2:D:232[A]:VAL:HG11	1.92	0.52
3:G:73:SER:HA	3:G:131:VAL:HG23	1.92	0.52
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.91	0.52
1:C:497:LEU:O	1:C:501:VAL:HG22	2.09	0.52
1:C:94:ILE:HG22	1:C:95:VAL:H	1.75	0.52
2:E:41[B]:ARG:HD3	2:E:43:THR:O	2.08	0.51
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.37	0.51
2:E:223:ASN:N	2:E:223:ASN:HD22	2.09	0.51
1:C:355:GLU:HG2	1:C:359:LYS:HE2	1.93	0.51
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.46	0.50
2:E:452:LEU:HB3	2:E:453:PRO:HD2	1.94	0.50
4:H:99:THR:HB	4:H:101:ASP:N	2.26	0.50
2:D:221:GLN:HA	2:D:221:GLN:HE21	1.75	0.50
2:E:229:ARG:HH22	2:E:267:GLU:CD	2.13	0.50
2:E:41[B]:ARG:CG	2:E:42:GLU:N	2.70	0.50
1:A:148:THR:HA	1:A:182:THR:HG23	1.94	0.50
1:C:338:ILE:HD12	11:C:2266:HOH:O	2.11	0.50
1:C:160:GLY:H	1:C:163:GLN:HE21	1.60	0.50
2:E:345:TYR:HA	2:E:346:PRO:C	2.30	0.50
2:E:257[B]:ASN:HB3	2:E:309:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.40	0.50
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.74	0.49
1:A:183:ILE:HD11	1:A:267:ILE:HD13	1.93	0.49
5:I:13:ARG:HH11	5:I:16:GLN:NE2	2.11	0.49
2:F:287:THR:O	2:F:291:THR:HG23	2.13	0.49
1:A:74[A]:VAL:HG22	1:A:241:PRO:HG3	1.93	0.49
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.48	0.49
4:H:127:THR:CB	4:H:128:ARG:HB2	2.43	0.49
3:G:13:ILE:HG22	3:G:243:ILE:HG13	1.95	0.48
1:C:355:GLU:HB2	11:C:2274:HOH:O	2.14	0.48
1:A:74[A]:VAL:HG21	1:A:281:MET:HG2	1.96	0.48
2:E:257[B]:ASN:ND2	11:E:2167:HOH:O	2.45	0.48
3:G:260:LYS:HG3	11:G:2100:HOH:O	2.13	0.48
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.79	0.48
2:E:449:TYR:HD2	2:E:452:LEU:HD12	1.78	0.48
1:B:217:VAL:HG11	2:E:123:PHE:HZ	1.78	0.48
1:A:446:TYR:CE1	1:A:450:ARG:HD2	2.48	0.48
2:F:97[B]:VAL:HG22	2:F:232:VAL:HB	1.95	0.48
2:E:257[A]:ASN:OD1	2:E:259:PHE:HB3	2.13	0.47
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.50	0.47
1:C:141:SER:HB2	1:C:143:ARG:HH21	1.79	0.47
1:B:288:PRO:HB3	2:F:276:PRO:HG3	1.96	0.47
2:F:139:VAL:HG22	11:F:2444:HOH:O	2.14	0.47
1:B:140:ILE:HG13	11:F:2264:HOH:O	2.15	0.47
2:E:257[A]:ASN:OD1	2:E:260:ARG:N	2.47	0.47
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.50	0.47
1:C:78:ASN:HD22	1:C:80:LYS:H	1.63	0.46
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.50	0.46
2:F:26:ASP:HB2	11:F:2003:HOH:O	2.15	0.46
1:A:419:SER:O	1:A:422[B]:VAL:HG13	2.16	0.46
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.45	0.46
1:C:395:ALA:HB2	11:C:2302:HOH:O	2.15	0.46
1:C:362:ARG:HA	1:C:363:PRO:C	2.36	0.46
2:D:130:GLN:HE22	2:D:356:ARG:HD2	1.81	0.46
2:D:287:THR:O	2:D:291:THR:HG23	2.16	0.46
4:H:121:GLY:CA	4:H:122:ALA:HB3	2.29	0.46
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.80	0.46
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.96	0.46
1:A:198[B]:LYS:HB2	11:A:2216:HOH:O	2.15	0.46
1:A:446:TYR:HE1	1:A:450:ARG:HD2	1.80	0.46
1:B:213:VAL:O	1:B:217:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:69:ILE:HG23	3:G:107:GLY:H	1.81	0.46
4:H:122:ALA:N	4:H:123:ALA:HB2	2.31	0.45
1:A:385:GLN:HG3	1:A:386:VAL:HG13	1.97	0.45
2:E:330:ASP:HA	2:E:356:ARG:HD2	1.97	0.45
2:F:391:LEU:HB3	2:F:395:GLU:HG3	1.99	0.45
2:D:370:VAL:HG21	2:D:442:GLN:HG3	1.99	0.45
3:G:206:GLU:O	5:I:12:ILE:HD11	2.16	0.45
1:A:500:ILE:O	1:A:504:PHE:HB2	2.17	0.45
1:A:457:GLU:HA	1:A:458:PRO:HD2	1.75	0.45
1:A:62:MET:CE	1:A:64:LEU:HD21	2.47	0.45
1:A:99:VAL:HG13	1:A:256:TYR:HB2	1.99	0.45
2:D:225:PRO:HB2	11:D:2042:HOH:O	2.16	0.45
2:D:167:MET:HE1	11:D:2170:HOH:O	2.17	0.45
1:C:107:VAL:HB	1:C:116:ASP:HB3	1.99	0.45
2:E:256:ASP:CA	2:E:257[B]:ASN:CB	2.89	0.45
1:A:151:LYS:H	1:A:430:GLN:NE2	2.07	0.45
4:H:112:LEU:HG	4:H:138:ASN:HB3	1.99	0.45
3:G:68:ILE:HB	3:G:69:ILE:CA	2.23	0.44
2:D:97:VAL:HG13	2:D:232[B]:VAL:HG23	1.99	0.44
2:D:25:PHE:O	2:D:56:SER:HB3	2.18	0.44
1:A:400:VAL:HG13	1:A:403:PHE:CE1	2.52	0.44
2:E:412:ARG:HH11	2:E:455:GLN:HE22	1.64	0.44
1:A:441:GLN:O	1:A:444:VAL:HG13	2.17	0.44
1:B:362:ARG:HA	1:B:363:PRO:C	2.37	0.44
2:F:139:VAL:HG13	2:F:414:LEU:HB3	2.00	0.44
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.33	0.44
1:B:141:SER:HB3	11:F:2259:HOH:O	2.17	0.44
1:A:346:THR:O	1:A:373:ARG:NH2	2.51	0.44
2:E:181:SER:HB2	2:E:215:VAL:HG13	1.99	0.44
1:A:99:VAL:HG22	1:A:253:MET:HA	1.99	0.44
2:D:96:ASN:C	2:D:96:ASN:ND2	2.71	0.43
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.33	0.43
2:E:63:MET:HE3	2:E:97:VAL:CG2	2.48	0.43
1:C:362:ARG:NH1	11:C:2278:HOH:O	2.50	0.43
2:D:9:THR:HG21	2:D:28:GLY:HA3	2.00	0.43
1:C:179:ALA:HB1	1:C:267:ILE:HD13	2.00	0.43
2:F:142:LEU:HD12	2:F:438:ILE:HD13	2.01	0.43
1:B:289:PRO:HD3	11:B:2292:HOH:O	2.18	0.43
2:F:70:VAL:H	2:F:73:GLN:HE21	1.68	0.42
3:G:68:ILE:HB	3:G:69:ILE:HD13	2.00	0.42
2:D:97:VAL:HG22	2:D:232[A]:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:ASP:O	2:D:363:VAL:HG22	2.20	0.42
1:C:419:SER:O	1:C:423:ARG:HD2	2.20	0.42
3:G:138:PHE:HE1	3:G:211:ASN:HD22	1.68	0.42
1:C:99:VAL:HG22	1:C:253:MET:HA	2.02	0.42
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.02	0.42
1:B:288:PRO:HA	1:B:289:PRO:HD3	1.92	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB3	2.02	0.42
2:F:198:HIS:HD2	11:F:2134:HOH:O	2.01	0.42
1:B:349:GLN:NE2	11:B:2348:HOH:O	2.35	0.42
4:H:79:SER:O	4:H:94:ALA:HA	2.20	0.41
2:D:412:ARG:HE	2:D:455:GLN:NE2	2.18	0.41
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.55	0.41
2:E:257[B]:ASN:CB	2:E:309:ALA:HB3	2.50	0.41
1:A:24:ASP:O	1:A:28:THR:OG1	2.37	0.41
2:D:256:ASP:HA	2:D:257:ASN:HA	1.81	0.41
1:C:361:ILE:O	1:C:364:ALA:HA	2.20	0.41
1:B:200:TYR:O	1:B:264:ALA:HA	2.21	0.41
2:D:188:GLU:H	2:D:221:GLN:NE2	2.19	0.41
1:A:28:THR:HG22	1:A:89:LYS:HG2	2.02	0.41
1:C:406:PHE:CE1	2:D:393:MET:HB2	2.55	0.41
2:F:97[B]:VAL:HG21	2:F:228:ALA:HB1	2.03	0.41
2:D:163:THR:O	2:D:166:ILE:HG22	2.20	0.41
2:E:282:GLN:H	2:E:282:GLN:NE2	1.96	0.41
2:F:9:THR:HB	2:F:10:THR:H	1.62	0.41
2:D:73:GLN:HE21	2:D:73:GLN:HB2	1.71	0.41
1:C:52:MET:O	1:C:91:THR:HB	2.21	0.41
2:E:30:PRO:HA	2:E:31:PRO:HD2	1.96	0.41
2:F:13:ILE:HD12	2:F:73:GLN:HB3	2.02	0.41
2:E:139:VAL:HG12	2:E:414:LEU:HD22	2.01	0.41
2:F:367:HIS:CE1	2:F:434:LEU:HD11	2.56	0.41
2:E:257[A]:ASN:ND2	2:E:259:PHE:H	2.19	0.40
2:F:233:ALA:O	2:F:237:LEU:HD13	2.21	0.40
1:C:263:HIS:HD2	1:C:320:SER:OG	2.04	0.40
2:D:32:ILE:O	2:D:33:LEU:HB2	2.21	0.40
1:A:74[B]:VAL:HG11	1:A:241:PRO:HG3	1.97	0.40
2:D:275[B]:ILE:HG22	3:G:269:ALA:HA	2.04	0.40
3:G:136:PRO:CD	3:G:221:THR:HG21	2.49	0.40
2:D:70:VAL:H	2:D:73:GLN:HE21	1.70	0.40
1:C:200:TYR:O	1:C:264:ALA:HA	2.20	0.40
1:C:373:ARG:HA	8:D:600:ADP:O3'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	489/510 (96%)	468 (96%)	16 (3%)	5 (1%)	19	8
1	B	477/510 (94%)	466 (98%)	10 (2%)	1 (0%)	52	43
1	C	488/510 (96%)	476 (98%)	12 (2%)	0	100	100
2	D	467/482 (97%)	446 (96%)	21 (4%)	0	100	100
2	E	456/482 (95%)	444 (97%)	11 (2%)	1 (0%)	52	43
2	F	467/482 (97%)	452 (97%)	12 (3%)	3 (1%)	30	16
3	G	170/272 (62%)	161 (95%)	8 (5%)	1 (1%)	30	16
4	H	73/146 (50%)	64 (88%)	6 (8%)	3 (4%)	3	0
5	I	23/50 (46%)	22 (96%)	1 (4%)	0	100	100
All	All	3110/3444 (90%)	2999 (96%)	97 (3%)	14 (0%)	39	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198[A]	LYS
1	A	198[B]	LYS
2	F	383[A]	SER
2	F	383[B]	SER
4	H	123	ALA
4	H	128	ARG
1	A	422[A]	VAL
1	A	422[B]	VAL
4	H	105	LEU
2	E	279	VAL
1	B	35	GLY
3	G	106	ILE
2	F	279	VAL
1	A	451	GLY

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	397/412 (96%)	384 (97%)	13 (3%)	45	32
1	B	390/412 (95%)	381 (98%)	9 (2%)	58	50
1	C	396/412 (96%)	383 (97%)	13 (3%)	45	32
2	D	379/386 (98%)	373 (98%)	6 (2%)	70	66
2	E	372/386 (96%)	364 (98%)	8 (2%)	60	51
2	F	379/386 (98%)	367 (97%)	12 (3%)	46	33
3	G	152/230 (66%)	145 (95%)	7 (5%)	33	17
4	H	66/109 (61%)	64 (97%)	2 (3%)	48	36
5	I	19/41 (46%)	19 (100%)	0	100	100
All	All	2550/2774 (92%)	2480 (97%)	70 (3%)	52	41

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	99	VAL
1	A	102	GLU
1	A	164	ARG
1	A	274	GLN
1	A	385	GLN
1	A	422[A]	VAL
1	A	422[B]	VAL
1	A	444	VAL
1	A	446	TYR
1	A	454	ASP
1	A	479	LEU
1	A	486	ASP
1	B	38	ILE
1	B	65	ASN
1	B	131	LEU
1	B	164	ARG
1	B	216	LEU

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Mol	Chain	Res	Type
1	B	217	VAL
1	B	362	ARG
1	B	389	THR
1	B	479	LEU
1	C	22	SER
1	C	45	ARG
1	C	78	ASN
1	C	96	ASP
1	C	99	VAL
1	C	124	LYS
1	C	164	ARG
1	C	334	VAL
1	C	341	ASN
1	C	349	GLN
1	C	455	LYS
1	C	479	LEU
1	C	505	LEU
2	D	89	GLU
2	D	96	ASN
2	D	97	VAL
2	D	249	GLN
2	D	274	ARG
2	D	282	GLN
2	E	215	VAL
2	E	223	ASN
2	E	282	GLN
2	E	293	GLN
2	E	301	LYS
2	E	412	ARG
2	E	439	LYS
2	E	450	ASP
2	F	27	GLU
2	F	96	ASN
2	F	112	GLN
2	F	139	VAL
2	F	175	LYS
2	F	223	ASN
2	F	274	ARG
2	F	282	GLN
2	F	385	GLN
2	F	387	ILE
2	F	398	GLU

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Mol	Chain	Res	Type
2	F	419	GLN
3	G	33	ARG
3	G	69	ILE
3	G	130	GLU
3	G	166	ARG
3	G	212	ILE
3	G	218	LYS
3	G	262	LEU
4	H	112	LEU
4	H	118	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	A	396	GLN
1	A	430	GLN
1	A	477	GLN
1	B	42	HIS
1	B	48	GLN
1	B	65	ASN
1	B	163	GLN
1	B	208	GLN
1	B	466	ASN
1	B	503	ASN
1	C	78	ASN
1	C	163	GLN
1	C	263	HIS
1	C	341	ASN
1	C	349	GLN
2	D	73	GLN
2	D	96	ASN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	246	GLN
2	D	282	GLN
2	D	361	ASN
2	E	171	ASN
2	E	194	ASN
2	E	198	HIS
2	E	223	ASN

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Mol	Chain	Res	Type
2	E	249	GLN
2	E	282	GLN
2	E	293	GLN
2	E	367	HIS
2	E	419	GLN
2	E	427	HIS
2	E	455	GLN
2	F	51	GLN
2	F	73	GLN
2	F	96	ASN
2	F	112	GLN
2	F	194	ASN
2	F	198	HIS
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	379	GLN
2	F	443	GLN
3	G	211	ASN
3	G	225	GLN
4	H	91	GLN
5	I	16	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 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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
6	ANP	A	600	7	27,33,33	2.02	7 (25%)	30,52,52	2.26	5 (16%)
6	ANP	B	600	7	27,33,33	2.01	5 (18%)	30,52,52	2.11	5 (16%)
6	ANP	C	600	7	27,33,33	1.96	6 (22%)	30,52,52	2.35	6 (20%)
9	AZI	D	1092	-	0,2,2	0.00	-	0,1,1	0.00	-
8	ADP	D	600	7	22,29,29	1.06	2 (9%)	27,45,45	1.84	3 (11%)
10	PO4	E	602	-	4,4,4	0.46	0	6,6,6	0.28	0
6	ANP	F	600	7	27,33,33	2.07	6 (22%)	30,52,52	2.32	6 (20%)

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
6	ANP	A	600	7	-	0/12/38/38	0/3/3/3
6	ANP	B	600	7	-	0/12/38/38	0/3/3/3
6	ANP	C	600	7	-	0/12/38/38	0/3/3/3
9	AZI	D	1092	-	-	0/0/0/0	0/0/0/0
8	ADP	D	600	7	-	0/12/32/32	0/3/3/3
10	PO4	E	602	-	-	0/0/0/0	0/0/0/0
6	ANP	F	600	7	-	1/12/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PB-O2B	-2.19	1.50	1.56
6	A	600	ANP	PG-O2G	-2.16	1.50	1.56
6	C	600	ANP	PB-O2B	-2.09	1.50	1.56
6	F	600	ANP	PG-O2G	-2.03	1.51	1.56
8	D	600	ADP	O4'-C1'	2.11	1.43	1.41
6	C	600	ANP	C5-C4	3.11	1.47	1.40
8	D	600	ADP	C5-C4	3.17	1.47	1.40
6	F	600	ANP	C5-C4	3.18	1.47	1.40
6	A	600	ANP	C5-C4	3.24	1.47	1.40
6	B	600	ANP	C5-C4	3.26	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PB-O1B	3.86	1.50	1.46
6	C	600	ANP	PB-N3B	3.95	1.73	1.63
6	F	600	ANP	PG-N3B	4.00	1.73	1.63
6	A	600	ANP	PG-N3B	4.03	1.74	1.63
6	A	600	ANP	PB-N3B	4.12	1.74	1.63
6	C	600	ANP	PG-N3B	4.12	1.74	1.63
6	F	600	ANP	PB-N3B	4.13	1.74	1.63
6	B	600	ANP	PG-N3B	4.15	1.74	1.63
6	C	600	ANP	PB-O1B	4.20	1.50	1.46
6	B	600	ANP	PB-N3B	4.22	1.74	1.63
6	B	600	ANP	PG-O1G	4.26	1.51	1.46
6	C	600	ANP	PG-O1G	4.26	1.51	1.46
6	B	600	ANP	PB-O1B	4.44	1.51	1.46
6	F	600	ANP	PB-O1B	4.50	1.51	1.46
6	A	600	ANP	PG-O1G	4.79	1.51	1.46
6	F	600	ANP	PG-O1G	5.13	1.52	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	600	ANP	N3-C2-N1	-7.54	123.12	128.89
6	F	600	ANP	O1G-PG-N3B	-7.53	100.36	111.90
6	C	600	ANP	O1G-PG-N3B	-7.45	100.47	111.90
6	A	600	ANP	O1G-PG-N3B	-7.27	100.75	111.90
6	F	600	ANP	N3-C2-N1	-7.17	123.41	128.89
6	A	600	ANP	N3-C2-N1	-7.12	123.44	128.89
6	B	600	ANP	N3-C2-N1	-7.08	123.47	128.89
8	D	600	ADP	N3-C2-N1	-6.95	123.57	128.89
6	B	600	ANP	O1G-PG-N3B	-5.94	102.79	111.90
8	D	600	ADP	C2'-C1'-N9	-3.85	108.41	114.29
6	C	600	ANP	C4-C5-N7	-3.31	106.44	109.48
6	B	600	ANP	C4-C5-N7	-3.25	106.49	109.48
6	F	600	ANP	C2'-C1'-N9	-3.22	109.37	114.29
6	A	600	ANP	C4-C5-N7	-3.19	106.55	109.48
8	D	600	ADP	C4-C5-N7	-2.86	106.84	109.48
6	F	600	ANP	C4-C5-N7	-2.84	106.87	109.48
6	C	600	ANP	PA-O3A-PB	-2.30	124.96	132.67
6	A	600	ANP	PA-O3A-PB	-2.11	125.60	132.67
6	B	600	ANP	PA-O3A-PB	-2.05	125.81	132.67
6	F	600	ANP	O3G-PG-O2G	2.35	114.53	107.58
6	C	600	ANP	O3G-PG-O2G	2.46	114.87	107.58
6	F	600	ANP	O2B-PB-O1B	3.14	116.56	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	600	ANP	O2B-PB-O1B	3.58	117.46	110.00
6	A	600	ANP	O2B-PB-O1B	3.61	117.53	110.00
6	B	600	ANP	O2B-PB-O1B	3.71	117.74	110.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	1092	AZI	1	0
8	D	600	ADP	1	0

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	487/510 (95%)	0.89	64 (13%) 5 8	12, 21, 45, 63	0
1	B	480/510 (94%)	0.88	77 (16%) 3 4	10, 20, 57, 82	0
1	C	490/510 (96%)	0.67	32 (6%) 22 32	12, 21, 38, 75	0
2	D	467/482 (96%)	0.59	29 (6%) 24 34	12, 19, 41, 67	0
2	E	458/482 (95%)	1.11	87 (18%) 2 2	12, 24, 64, 77	0
2	F	466/482 (96%)	0.49	28 (6%) 25 35	13, 19, 41, 62	0
3	G	182/272 (66%)	1.95	71 (39%) 0 0	10, 29, 48, 58	0
4	H	83/146 (56%)	2.82	52 (62%) 0 0	5, 26, 44, 49	0
5	I	25/50 (50%)	2.36	10 (40%) 0 0	8, 17, 43, 46	0
All	All	3138/3444 (91%)	0.91	450 (14%) 4 6	5, 21, 50, 82	0

All (450) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	THR	12.1
3	G	106	ILE	11.9
1	B	510	ALA	10.8
4	H	105	LEU	10.2
2	E	470	ALA	9.9
1	C	406	PHE	9.7
4	H	100	LEU	9.4
1	C	407	GLY	9.4
2	E	384	LEU	8.3
1	B	413	ALA	8.3
1	C	22	SER	8.3
1	B	401	ALA	8.2
2	E	387	ILE	8.2
2	F	473	LEU	8.2
3	G	160	ILE	8.0

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Mol	Chain	Res	Type	RSRZ
2	E	400	ASP	7.9
2	E	407	ALA	7.9
5	I	9	LEU	7.9
2	E	424	PHE	7.8
2	E	423	VAL	7.8
3	G	212	ILE	7.8
2	E	457	PHE	7.5
2	E	428	LEU	7.4
1	A	195	GLU	7.3
3	G	85	VAL	7.3
1	B	508	PHE	7.3
2	E	427	HIS	7.2
2	E	446	ALA	7.2
1	B	410	LEU	7.2
2	E	402	LEU	7.1
2	E	377	ILE	6.8
2	F	9	THR	6.8
1	C	23	VAL	6.7
2	D	9	THR	6.7
2	D	248	GLY	6.6
3	G	43	VAL	6.6
1	B	495	ALA	6.5
2	E	467	VAL	6.4
2	E	345	TYR	6.4
1	B	412	ALA	6.4
5	I	8	GLY	6.4
5	I	7	ALA	6.4
4	H	27	PHE	6.3
4	H	65	VAL	6.3
2	E	449	TYR	6.2
2	E	468	ALA	6.2
3	G	105	ILE	6.0
2	E	456	ALA	6.0
5	I	6	GLN	6.0
1	B	456	LEU	5.9
1	B	417	LEU	5.9
3	G	70	GLY	5.9
3	G	69	ILE	5.9
4	H	92	LEU	5.9
2	E	460	VAL	5.9
1	B	451	GLY	5.8
2	E	474	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
2	F	474	ALA	5.7
2	E	445	LEU	5.7
2	E	401	LYS	5.6
3	G	116	LEU	5.6
1	B	419	SER	5.5
2	E	398	GLU	5.5
2	E	452	LEU	5.5
4	H	62	LEU	5.5
3	G	112	ILE	5.5
2	E	473	LEU	5.5
1	C	94	ILE	5.5
2	E	453	PRO	5.5
4	H	28	PHE	5.4
3	G	148	LEU	5.4
3	G	71	VAL	5.4
1	B	416	GLN	5.4
2	E	451	HIS	5.4
2	F	178	GLY	5.3
2	E	458	TYR	5.3
1	B	455	LYS	5.3
1	C	409	ASP	5.2
1	B	468	PHE	5.2
4	H	18	PHE	5.2
1	B	506	ALA	5.2
2	E	383	SER	5.2
1	B	464	PHE	5.2
4	H	101	ASP	5.1
1	A	483	ILE	5.1
2	E	41[A]	ARG	5.1
1	A	446	TYR	5.0
1	A	510	ALA	4.9
1	B	504	PHE	4.9
1	B	411	ASP	4.9
4	H	107	ALA	4.9
1	A	406	PHE	4.9
1	B	400	VAL	4.8
1	A	404	ALA	4.8
3	G	114	SER	4.8
1	B	414	THR	4.8
1	C	93	ALA	4.8
2	E	379	GLN	4.7
2	F	10	THR	4.7

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Mol	Chain	Res	Type	RSRZ
3	G	46	VAL	4.7
3	G	215	TYR	4.6
5	I	1	VAL	4.6
1	A	489	ILE	4.6
3	G	128	PHE	4.5
3	G	25	MET	4.5
2	E	472	LYS	4.5
4	H	123	ALA	4.5
2	F	472	LYS	4.5
2	E	471	ASP	4.4
2	E	454	GLU	4.4
3	G	169	ILE	4.4
4	H	120	LEU	4.4
1	A	501	VAL	4.4
3	G	115	ILE	4.3
1	B	392	LEU	4.3
1	B	479	LEU	4.3
2	E	462	PRO	4.3
1	B	23	VAL	4.3
2	D	473	LEU	4.3
4	H	20	PHE	4.3
3	G	168	VAL	4.3
4	H	125	GLU	4.3
2	E	425	THR	4.3
1	A	422[A]	VAL	4.3
4	H	119	LEU	4.2
2	F	248	GLY	4.2
1	B	469	LEU	4.2
1	B	499	GLU	4.2
2	E	257[A]	ASN	4.1
1	A	407	GLY	4.1
2	D	232[A]	VAL	4.1
1	A	408	SER	4.1
1	B	476	HIS	4.1
3	G	161	ILE	4.1
2	E	386	ASP	4.1
4	H	104	ASP	4.0
1	A	497	LEU	4.0
4	H	126	ALA	4.0
3	G	80	ALA	4.0
1	C	405	GLN	4.0
4	H	91	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
4	H	58	LEU	3.9
4	H	122	ALA	3.9
4	H	26	VAL	3.9
1	A	402	ALA	3.9
3	G	3	LEU	3.8
2	E	410	ILE	3.8
2	E	439	LYS	3.8
4	H	24	THR	3.8
1	A	485	THR	3.8
2	E	342	LEU	3.8
3	G	172	LYS	3.8
2	D	246	GLN	3.7
1	A	499	GLU	3.7
3	G	165	PHE	3.7
2	E	404	VAL	3.7
4	H	38	VAL	3.7
3	G	145	ALA	3.7
2	E	406	ARG	3.7
3	G	81	ILE	3.6
1	B	492	GLU	3.6
4	H	118	GLU	3.6
3	G	67	LEU	3.6
4	H	121	GLY	3.6
1	A	121	ILE	3.6
3	G	127	THR	3.6
1	A	409	ASP	3.6
2	D	475	GLU	3.6
2	E	381	TYR	3.5
4	H	19	THR	3.5
1	A	381	ARG	3.5
2	E	405	SER	3.5
4	H	64	VAL	3.5
4	H	102	MET	3.5
2	E	370	VAL	3.5
1	A	504	PHE	3.5
2	F	210	ASP	3.5
1	B	458	PRO	3.5
5	I	25	ALA	3.5
2	E	409	LYS	3.4
1	B	473	ILE	3.4
1	B	509	GLU	3.4
1	C	475	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	488	LYS	3.4
1	A	405	GLN	3.4
1	C	508	PHE	3.4
2	E	397	SER	3.4
2	E	399	GLU	3.4
1	A	401	ALA	3.4
1	B	395	ALA	3.3
1	B	415	GLN	3.3
4	H	29	ASN	3.3
3	G	147	GLU	3.3
1	B	463	LYS	3.3
2	E	373	GLY	3.3
1	B	457	GLU	3.3
3	G	113	ARG	3.3
1	B	399	GLU	3.3
1	B	491	GLU	3.3
2	E	447	GLY	3.3
2	E	375	GLN	3.3
3	G	171	TYR	3.2
1	B	467	ALA	3.2
3	G	68	ILE	3.2
2	E	413	PHE	3.2
1	B	454	ASP	3.2
1	B	486	ASP	3.2
2	E	396	LEU	3.2
3	G	129	LYS	3.2
3	G	33	ARG	3.2
2	E	403	THR	3.2
2	F	428	LEU	3.2
1	B	450	ARG	3.1
1	B	500	ILE	3.1
2	D	249	GLN	3.1
2	F	468	ALA	3.1
3	G	2	THR	3.1
1	B	423	ARG	3.1
5	I	10	SER	3.1
1	A	508	PHE	3.1
2	E	455	GLN	3.1
3	G	208	SER	3.1
2	F	426	GLY	3.1
2	E	412	ARG	3.1
1	B	446	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
4	H	93	LEU	3.1
3	G	39	LYS	3.1
3	G	163	ASN	3.1
3	G	221	THR	3.0
3	G	170	SER	3.0
1	A	484	ARG	3.0
2	E	466	ALA	3.0
2	D	26	ASP	3.0
4	H	124	ASP	3.0
1	A	476	HIS	3.0
1	C	195	GLU	3.0
2	D	76	LEU	3.0
2	D	474	ALA	3.0
3	G	162	PHE	3.0
2	D	177	HIS	3.0
1	A	123	SER	3.0
3	G	173	THR	3.0
3	G	133	ARG	3.0
4	H	128	ARG	3.0
1	A	410	LEU	3.0
3	G	144	ILE	3.0
1	B	358	TYR	3.0
1	C	99	VAL	3.0
2	D	209	LYS	3.0
2	F	174	ALA	3.0
4	H	97	ALA	3.0
1	A	305	LEU	3.0
1	A	479	LEU	2.9
1	A	267	ILE	2.9
2	E	426	GLY	2.9
4	H	76	PHE	2.9
1	B	490	SER	2.9
3	G	271	ALA	2.9
1	B	420	ARG	2.9
2	D	242	TYR	2.9
1	A	93	ALA	2.9
1	A	496	LYS	2.9
3	G	83	SER	2.9
1	A	74[A]	VAL	2.9
3	G	36	ARG	2.9
1	B	466	ASN	2.9
2	E	9	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	408	SER	2.9
1	B	422	VAL	2.9
1	B	472	VAL	2.9
2	F	111	LYS	2.9
4	H	98	VAL	2.9
3	G	19	ILE	2.8
4	H	36	VAL	2.8
2	F	383[A]	SER	2.8
1	B	396	GLN	2.8
2	E	344	ILE	2.8
1	C	24	ASP	2.8
2	E	430	LYS	2.8
3	G	1	ALA	2.8
1	B	489	ILE	2.8
4	H	113	GLU	2.8
2	E	111	LYS	2.8
1	A	316	PHE	2.8
2	E	443	GLN	2.8
1	B	461	ILE	2.8
2	D	393	MET	2.8
2	E	420	VAL	2.8
2	E	382	LYS	2.8
3	G	72	SER	2.8
4	H	114	LYS	2.8
2	D	212	THR	2.7
2	E	459	MET	2.7
3	G	5	ASP	2.7
1	B	421	GLY	2.7
2	E	429	GLY	2.7
1	A	455	LYS	2.7
3	G	78	CYS	2.7
1	A	94	ILE	2.7
2	D	210	ASP	2.7
1	A	403	PHE	2.7
3	G	28	ALA	2.7
3	G	108	VAL	2.7
2	F	209	LYS	2.7
3	G	111	LYS	2.7
5	I	18	CYS	2.7
2	E	444	ILE	2.7
1	A	506	ALA	2.7
1	C	122	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
4	H	106	GLY	2.7
2	F	438	ILE	2.6
1	C	256	TYR	2.6
1	A	355[A]	GLU	2.6
2	E	411	GLN	2.6
4	H	127	THR	2.6
1	A	473	ILE	2.6
1	A	487	GLY	2.6
2	E	465	GLU	2.6
4	H	80	GLY	2.6
1	A	306	LEU	2.6
1	C	403	PHE	2.6
1	B	498	LYS	2.6
1	C	463	LYS	2.6
4	H	17	SER	2.6
1	C	190	ASN	2.6
2	E	128	VAL	2.6
2	E	376	LYS	2.5
3	G	9	ARG	2.5
2	E	463	ILE	2.5
1	A	505	LEU	2.5
1	B	480	LEU	2.5
1	B	484	ARG	2.5
2	E	343	GLY	2.5
2	F	249	GLN	2.5
1	A	131	LEU	2.5
1	B	501	VAL	2.5
1	A	482	LYS	2.5
2	D	10	THR	2.5
1	C	371	VAL	2.5
1	A	206	ILE	2.5
1	C	471	HIS	2.4
4	H	109	LYS	2.4
1	C	473	ILE	2.4
2	D	178	GLY	2.4
1	B	460	LYS	2.4
1	B	452	TYR	2.4
1	B	497	LEU	2.4
3	G	240	SER	2.4
2	E	113	PHE	2.4
2	F	186	VAL	2.4
1	A	167	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	178	ILE	2.4
3	G	206	GLU	2.4
1	B	196	LYS	2.4
1	A	492	GLU	2.4
2	E	366	GLU	2.4
3	G	84	SER	2.3
1	A	326	VAL	2.3
4	H	63	VAL	2.3
1	A	350	ILE	2.3
1	C	470	SER	2.3
3	G	166	ARG	2.3
2	F	113	PHE	2.3
2	F	110	THR	2.3
2	E	380	ASP	2.3
2	F	88	PRO	2.3
1	A	452	TYR	2.3
3	G	44	TYR	2.3
2	E	28	GLY	2.3
4	H	137	ALA	2.3
3	G	23	MET	2.3
1	C	196	LYS	2.3
2	D	109	LYS	2.3
1	B	381	ARG	2.3
1	A	193	THR	2.3
4	H	115	ALA	2.3
1	B	471	HIS	2.2
1	C	505	LEU	2.2
4	H	81	SER	2.2
2	E	440	GLY	2.2
1	B	462	THR	2.2
2	D	247	GLU	2.2
1	C	510	ALA	2.2
2	E	408	ARG	2.2
1	A	486	ASP	2.2
2	F	176	ALA	2.2
2	D	390	ILE	2.2
3	G	213	ILE	2.2
2	E	419	GLN	2.2
1	A	392	LEU	2.2
2	D	12	ARG	2.2
1	B	389	THR	2.2
1	C	91	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	464	GLU	2.2
3	G	134	ARG	2.2
3	G	164	ARG	2.2
1	A	463	LYS	2.2
2	F	97[A]	VAL	2.2
4	H	140	ALA	2.1
2	F	455	GLN	2.1
4	H	135	ILE	2.1
1	C	410	LEU	2.1
2	E	450	ASP	2.1
1	C	491	GLU	2.1
2	E	418	PHE	2.1
1	B	502	THR	2.1
2	D	255	ILE	2.1
3	G	229	MET	2.1
5	I	3	TYR	2.1
1	B	25	LEU	2.1
1	B	424	LEU	2.1
2	D	208	LEU	2.1
3	G	38	LEU	2.1
1	B	478	ALA	2.1
2	E	372	ARG	2.1
2	D	213	SER	2.1
1	A	200	TYR	2.1
1	A	271	LEU	2.1
1	C	404	ALA	2.1
2	E	369	ASP	2.1
2	F	386	ASP	2.1
3	G	230	THR	2.1
4	H	40	THR	2.1
1	B	487	GLY	2.1
2	F	296	ILE	2.1
1	B	385	GLN	2.1
4	H	25	GLN	2.1
1	A	198[A]	LYS	2.1
1	A	26	GLU	2.1
1	B	507	GLY	2.1
2	D	112	GLN	2.1
2	F	424	PHE	2.0
5	I	14	TYR	2.0
1	A	449	VAL	2.0
1	B	37	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	193	THR	2.0
1	A	266	ILE	2.0
1	A	345	ILE	2.0
1	B	206	ILE	2.0
2	D	261	PHE	2.0
2	E	362	ILE	2.0
1	A	166	LEU	2.0
1	C	381	ARG	2.0
2	D	97	VAL	2.0
1	B	496	LYS	2.0
1	A	277	ALA	2.0
2	D	174	ALA	2.0
4	H	21	ALA	2.0
3	G	47	GLY	2.0
3	G	110	ASP	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
10	PO4	E	602	5/5	0.89	0.17	2.16	68,69,72,72	0
9	AZI	D	1092	3/3	0.92	0.16	0.86	17,17,19,25	0
6	ANP	A	600	31/31	0.98	0.14	-0.35	11,15,20,23	0
6	ANP	B	600	31/31	0.97	0.10	-0.45	13,19,27,32	0
8	ADP	D	600	27/27	0.98	0.13	-0.71	10,17,21,22	0
6	ANP	C	600	31/31	0.98	0.11	-0.76	12,16,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MG	F	601	1/1	0.98	0.13	-1.22	13,13,13,13	0
6	ANP	F	600	31/31	0.98	0.12	-1.36	12,16,20,22	0
7	MG	D	601	1/1	0.98	0.07	-3.03	16,16,16,16	0
7	MG	B	601	1/1	0.96	0.09	-	19,19,19,19	0
7	MG	A	601	1/1	0.96	0.10	-	14,14,14,14	0
7	MG	C	601	1/1	0.98	0.11	-	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.