



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2017 – 08:03 PM EDT

PDB ID : 3M0E
Title : Crystal structure of the ATP-bound state of Walker B mutant of NtrC1 ATPase domain
Authors : Chen, B.; Sysoeva, T.A.; Chowdhury, S.; Rusu, M.; Birmanms, S.; Guo, L.; Hanson, J.; Yang, H.; Nixon, B.T.
Deposited on : unknown
Resolution : 2.63 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

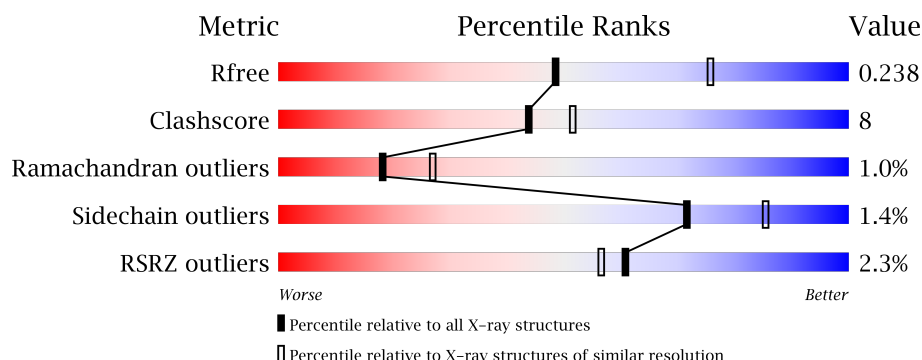
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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	266	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>7%</div> </div> </div>
1	B	266	<div> <div></div> <div> <div>76%</div> <div>17%</div> <div>7%</div> </div> </div>
1	C	266	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>7%</div> </div> </div>
1	D	266	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>7%</div> </div> </div>
1	E	266	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>7%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	266	<div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div>
1	G	266	<div> <div></div> <div>77%</div> <div>15%</div> <div>7%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14440 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 Transcriptional regulator (NtrC family).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1975	1276	333	362	4			
1	B	247	Total	C	N	O	S	0	0	0
			1975	1276	333	362	4			
1	C	247	Total	C	N	O	S	0	0	0
			1975	1276	333	362	4			
1	D	247	Total	C	N	O	S	0	0	0
			1975	1276	333	362	4			
1	E	247	Total	C	N	O	S	0	0	0
			1975	1276	333	362	4			
1	F	247	Total	C	N	O	S	0	0	0
			1975	1276	333	362	4			
1	G	247	Total	C	N	O	S	0	0	0
			1975	1276	333	362	4			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	ALA	GLU	ENGINEERED	UNP O67198
B	239	ALA	GLU	ENGINEERED	UNP O67198
C	239	ALA	GLU	ENGINEERED	UNP O67198
D	239	ALA	GLU	ENGINEERED	UNP O67198
E	239	ALA	GLU	ENGINEERED	UNP O67198
F	239	ALA	GLU	ENGINEERED	UNP O67198
G	239	ALA	GLU	ENGINEERED	UNP O67198

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

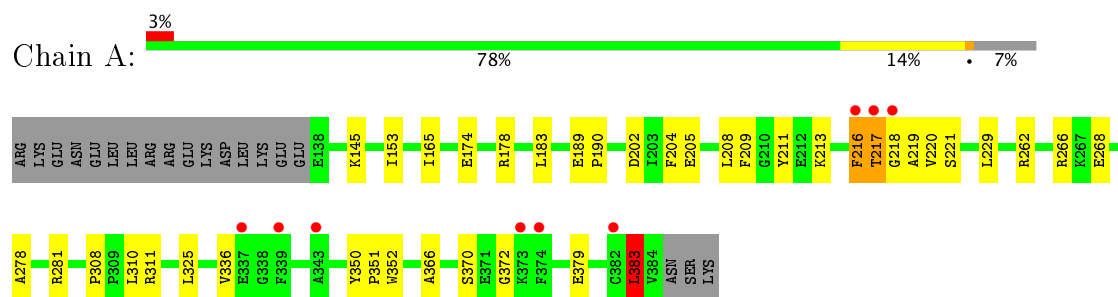
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	62	Total 62	O 62	0	0
4	C	43	Total 43	O 43	0	0
4	D	50	Total 50	O 50	0	0
4	E	46	Total 46	O 46	0	0
4	F	71	Total 71	O 71	0	0
4	G	69	Total 69	O 69	0	0

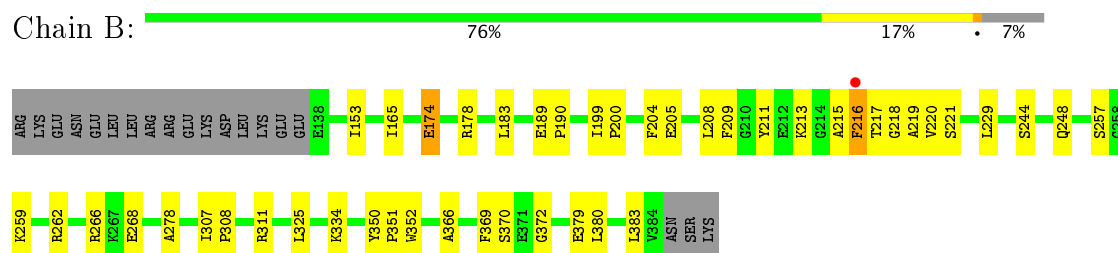
3 Residue-property plots [i](#)

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

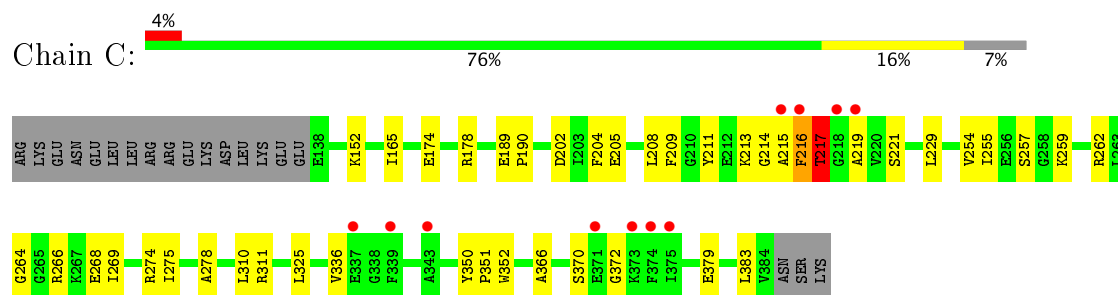
- Molecule 1: Transcriptional regulator (NtrC family)



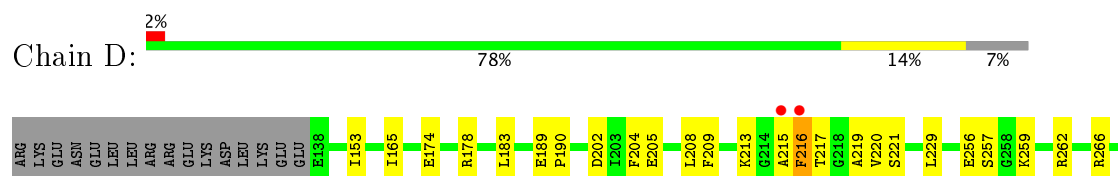
- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)

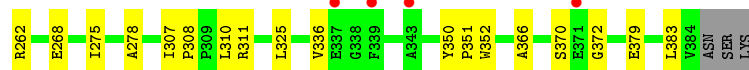
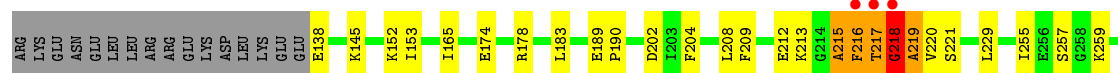
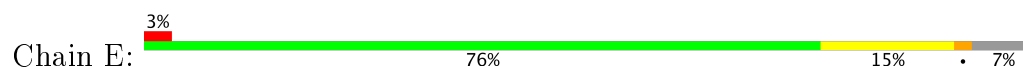


- Molecule 1: Transcriptional regulator (NtrC family)

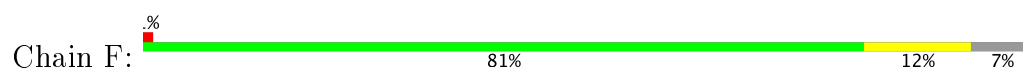




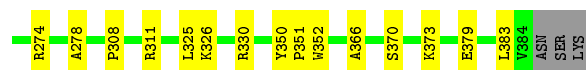
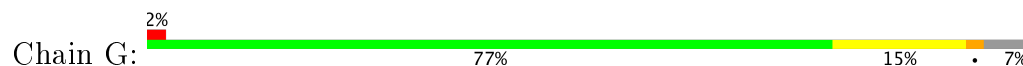
- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	251.21Å 242.59Å 40.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 2.63 47.64 – 2.63	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.64-2.63) 100.0 (47.64-2.63)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.61Å)	Xtriage
Refinement program	ELVES, PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.205 , 0.241 0.204 , 0.238	Depositor DCC
R_{free} test set	7581 reflections (11.09%)	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14440	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/2009	0.63	2/2695 (0.1%)
1	B	0.49	0/2009	0.62	1/2695 (0.0%)
1	C	0.50	0/2009	0.83	3/2695 (0.1%)
1	D	0.48	0/2009	0.63	2/2695 (0.1%)
1	E	0.51	0/2009	0.62	1/2695 (0.0%)
1	F	0.48	0/2009	0.61	0/2695
1	G	0.50	0/2009	0.66	3/2695 (0.1%)
All	All	0.49	0/14063	0.66	12/18865 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	ARG	NE-CZ-NH1	-21.29	109.66	120.30
1	C	311	ARG	NE-CZ-NH2	18.46	129.53	120.30
1	C	311	ARG	CD-NE-CZ	8.68	135.76	123.60
1	G	219	ALA	N-CA-C	8.28	133.35	111.00
1	G	218	GLY	C-N-CA	-7.43	103.11	121.70
1	D	311	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	311	ARG	NE-CZ-NH2	-5.96	117.32	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	311	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	G	311	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	383	LEU	CB-CG-CD1	5.22	119.87	111.00
1	A	311	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	311	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	THR	Peptide
1	E	218	GLY	Peptide

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	1975	0	2039	36	0
1	B	1975	0	2039	37	0
1	C	1975	0	2039	42	0
1	D	1975	0	2039	37	0
1	E	1975	0	2039	31	0
1	F	1975	0	2039	28	0
1	G	1975	0	2039	36	0
2	A	31	0	12	0	0
2	B	31	0	12	3	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	1	0
2	G	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
4	A	50	0	0	1	0
4	B	62	0	0	1	0
4	C	43	0	0	3	0
4	D	50	0	0	1	0
4	E	46	0	0	1	0
4	F	71	0	0	4	0
4	G	69	0	0	3	0
All	All	14440	0	14357	216	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 (216) 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:C:219:ALA:HB2	1:D:215:ALA:CB	1.86	1.04
1:C:214:GLY:O	1:C:217:THR:HB	1.57	1.04
1:C:219:ALA:HB2	1:D:215:ALA:HB2	1.47	0.93
1:F:219:ALA:HB2	1:G:216:PHE:CE2	2.06	0.89
1:C:211:TYR:OH	1:D:215:ALA:HB3	1.75	0.87
1:C:254:VAL:HG23	4:C:416:HOH:O	1.74	0.87
1:C:219:ALA:HB2	1:D:215:ALA:HB1	1.60	0.81
1:G:214:GLY:O	1:G:216:PHE:N	2.15	0.79
1:A:216:PHE:O	1:A:218:GLY:N	2.15	0.78
1:B:217:THR:HG23	1:B:218:GLY:H	1.46	0.78
1:C:219:ALA:CB	1:D:215:ALA:HB2	2.16	0.76
1:E:216:PHE:O	1:E:218:GLY:N	2.19	0.76
2:B:400:ATP:H5'1	2:B:400:ATP:H8	1.52	0.75
2:B:400:ATP:H5'1	2:B:400:ATP:C8	2.22	0.74
1:A:218:GLY:O	1:A:219:ALA:HB3	1.90	0.70
1:D:216:PHE:HZ	1:D:266:ARG:HH22	1.39	0.70
1:E:218:GLY:O	1:E:219:ALA:HB3	1.92	0.68
1:F:219:ALA:CB	1:G:216:PHE:CE2	2.76	0.68
1:B:216:PHE:CD1	1:B:216:PHE:N	2.62	0.67
1:C:229:LEU:CD1	1:D:266:ARG:HB3	2.24	0.67
1:C:229:LEU:HD12	1:D:266:ARG:HB3	1.76	0.66
1:G:218:GLY:O	1:G:219:ALA:HB2	1.93	0.66
1:A:229:LEU:HD12	1:B:266:ARG:HB3	1.78	0.66
1:E:229:LEU:HD12	1:F:266:ARG:HB3	1.76	0.65
1:E:138:GLU:HA	4:E:419:HOH:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:THR:O	1:E:219:ALA:N	2.30	0.65
1:E:229:LEU:CD1	1:F:266:ARG:HB3	2.27	0.63
1:A:229:LEU:CD1	1:B:266:ARG:HB3	2.31	0.60
1:A:216:PHE:C	1:A:218:GLY:N	2.55	0.59
1:C:211:TYR:CZ	1:D:215:ALA:HB3	2.36	0.59
1:C:211:TYR:HE2	1:D:216:PHE:CE1	2.23	0.56
1:F:274:ARG:HD3	4:F:398:HOH:O	2.06	0.56
1:G:217:THR:C	1:G:219:ALA:N	2.57	0.55
1:B:216:PHE:HD1	1:B:216:PHE:N	2.04	0.54
1:G:217:THR:OG1	1:G:218:GLY:N	2.38	0.54
1:C:216:PHE:CD2	1:C:264:GLY:HA2	2.43	0.54
1:G:217:THR:C	1:G:219:ALA:H	2.10	0.54
1:B:219:ALA:HB2	1:C:215:ALA:HB2	1.91	0.52
1:F:366:ALA:O	1:F:370:SER:HB3	2.09	0.52
1:G:366:ALA:O	1:G:370:SER:HB3	2.09	0.52
1:C:219:ALA:CB	1:D:215:ALA:CB	2.73	0.52
1:F:219:ALA:HB2	1:G:216:PHE:CD2	2.45	0.52
1:F:379:GLU:O	1:F:383:LEU:HG	2.10	0.52
1:B:217:THR:HG23	1:B:218:GLY:N	2.21	0.51
1:G:209:PHE:O	1:G:262:ARG:HG2	2.10	0.51
1:A:281:ARG:NH1	4:A:410:HOH:O	2.44	0.51
1:E:174:GLU:O	1:E:178:ARG:HG3	2.11	0.51
1:D:256:GLU:HB2	4:D:426:HOH:O	2.10	0.50
1:E:212:GLU:O	1:E:215:ALA:HB3	2.12	0.50
1:C:189:GLU:HB3	1:C:190:PRO:CD	2.41	0.50
1:E:379:GLU:O	1:E:383:LEU:HG	2.12	0.50
1:E:366:ALA:O	1:E:370:SER:HB3	2.12	0.50
1:B:366:ALA:O	1:B:370:SER:HB3	2.12	0.50
1:A:366:ALA:O	1:A:370:SER:HB3	2.12	0.50
1:A:216:PHE:O	1:A:217:THR:C	2.49	0.50
1:A:217:THR:O	1:A:219:ALA:N	2.45	0.49
1:D:366:ALA:O	1:D:370:SER:HB3	2.13	0.49
1:G:189:GLU:HB3	1:G:190:PRO:CD	2.42	0.49
1:B:209:PHE:O	1:B:262:ARG:HG2	2.12	0.49
1:C:379:GLU:O	1:C:383:LEU:HG	2.12	0.49
1:D:379:GLU:O	1:D:383:LEU:HG	2.13	0.49
1:G:325:LEU:C	1:G:325:LEU:HD23	2.33	0.49
1:E:189:GLU:HB3	1:E:190:PRO:CD	2.42	0.49
1:A:216:PHE:C	1:A:218:GLY:H	2.16	0.49
1:G:379:GLU:O	1:G:383:LEU:HG	2.13	0.48
1:A:209:PHE:O	1:A:262:ARG:HG2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:HB3	1:A:190:PRO:CD	2.42	0.48
1:D:209:PHE:O	1:D:262:ARG:HG2	2.14	0.48
1:E:325:LEU:HD23	1:E:325:LEU:C	2.34	0.48
1:B:189:GLU:HB3	1:B:190:PRO:CD	2.44	0.48
1:D:189:GLU:HB3	1:D:190:PRO:CD	2.43	0.48
1:F:189:GLU:HB3	1:F:190:PRO:CD	2.44	0.48
1:A:217:THR:O	1:A:217:THR:HG22	2.13	0.48
1:B:213:LYS:HB3	1:B:221:SER:HA	1.96	0.48
1:A:217:THR:H	1:G:218:GLY:CA	2.27	0.48
1:G:256:GLU:HB2	4:G:398:HOH:O	2.13	0.48
1:F:334:LYS:HE2	4:F:429:HOH:O	2.13	0.48
1:B:379:GLU:O	1:B:383:LEU:HG	2.13	0.47
1:A:211:TYR:OH	1:B:215:ALA:HB3	2.13	0.47
1:G:213:LYS:HB2	1:G:220:VAL:O	2.15	0.47
1:D:325:LEU:HD23	1:D:325:LEU:C	2.35	0.47
1:B:174:GLU:O	1:B:178:ARG:HG3	2.14	0.47
1:C:229:LEU:HD11	1:D:266:ARG:HB3	1.97	0.47
1:G:213:LYS:HB3	1:G:221:SER:HA	1.97	0.47
1:G:274:ARG:HD3	4:G:39:HOH:O	2.15	0.47
1:A:218:GLY:O	1:A:219:ALA:C	2.50	0.47
1:F:165:ILE:O	1:F:278:ALA:HA	2.15	0.47
1:G:174:GLU:O	1:G:178:ARG:HG3	2.15	0.47
1:C:209:PHE:O	1:C:262:ARG:HG2	2.15	0.46
1:A:229:LEU:HD11	1:B:266:ARG:O	2.15	0.46
1:E:209:PHE:O	1:E:262:ARG:HG2	2.15	0.46
1:F:213:LYS:HB3	1:F:221:SER:HA	1.98	0.46
1:F:325:LEU:HD23	1:F:325:LEU:C	2.36	0.46
1:D:165:ILE:O	1:D:278:ALA:HA	2.16	0.46
1:A:266:ARG:HB3	1:G:229:LEU:HD12	1.98	0.46
1:C:213:LYS:HB3	1:C:221:SER:HA	1.98	0.46
1:A:325:LEU:HD23	1:A:325:LEU:C	2.35	0.46
1:B:325:LEU:C	1:B:325:LEU:HD23	2.35	0.46
1:D:213:LYS:HB3	1:D:221:SER:HA	1.97	0.46
1:F:219:ALA:HA	1:G:216:PHE:CE1	2.51	0.46
1:A:211:TYR:OH	1:B:215:ALA:CB	2.64	0.46
1:F:219:ALA:CB	1:G:216:PHE:CZ	3.00	0.45
1:A:217:THR:C	1:A:219:ALA:N	2.70	0.45
1:A:213:LYS:HB3	1:A:221:SER:HA	1.99	0.45
1:B:217:THR:CG2	1:B:218:GLY:H	2.17	0.45
2:B:400:ATP:H8	2:B:400:ATP:C5'	2.26	0.45
1:G:373:LYS:NZ	4:G:397:HOH:O	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LEU:HD23	1:C:325:LEU:C	2.37	0.45
1:E:219:ALA:HB2	4:F:440:HOH:O	2.17	0.45
1:E:213:LYS:HB3	1:E:221:SER:HA	1.98	0.45
1:E:350:TYR:HA	1:E:351:PRO:HD3	1.81	0.45
1:C:174:GLU:O	1:C:178:ARG:HG3	2.16	0.45
1:G:204:PHE:CE2	1:G:208:LEU:HD22	2.52	0.45
1:F:202:ASP:N	1:F:202:ASP:OD1	2.50	0.45
1:C:350:TYR:HA	1:C:351:PRO:HD3	1.81	0.45
1:E:229:LEU:HD11	1:F:266:ARG:O	2.16	0.45
1:B:350:TYR:HA	1:B:351:PRO:HD3	1.79	0.44
1:G:257:SER:O	1:G:259:LYS:HG3	2.17	0.44
1:D:204:PHE:CE2	1:D:208:LEU:HD22	2.53	0.44
1:B:216:PHE:HD1	1:B:216:PHE:H	1.65	0.44
1:C:229:LEU:HD11	1:D:266:ARG:O	2.18	0.44
2:F:400:ATP:H5'1	2:F:400:ATP:H8	1.81	0.44
1:A:174:GLU:O	1:A:178:ARG:HG3	2.17	0.44
1:B:213:LYS:HB2	1:B:220:VAL:O	2.17	0.44
1:C:366:ALA:O	1:C:370:SER:HB3	2.18	0.44
1:D:202:ASP:N	1:D:202:ASP:OD1	2.51	0.44
1:E:213:LYS:HB2	1:E:220:VAL:O	2.18	0.44
1:E:165:ILE:O	1:E:278:ALA:HA	2.18	0.44
1:A:165:ILE:O	1:A:278:ALA:HA	2.18	0.44
1:D:257:SER:O	1:D:259:LYS:HG3	2.17	0.44
1:F:257:SER:O	1:F:259:LYS:HG3	2.18	0.44
1:B:204:PHE:CE2	1:B:208:LEU:HD22	2.52	0.43
1:C:217:THR:OG1	1:C:219:ALA:N	2.42	0.43
1:D:369:PHE:CZ	1:E:152:LYS:HE3	2.53	0.43
1:F:229:LEU:HD12	1:G:266:ARG:HB3	2.00	0.43
1:G:215:ALA:O	1:G:216:PHE:HB2	2.18	0.43
1:D:325:LEU:HD23	1:D:325:LEU:O	2.18	0.43
1:A:350:TYR:HD2	1:A:352:TRP:CD2	2.36	0.43
1:B:334:LYS:HE2	4:B:421:HOH:O	2.18	0.43
1:F:204:PHE:CE2	1:F:208:LEU:HD22	2.53	0.43
1:G:350:TYR:HD2	1:G:352:TRP:CD2	2.37	0.43
1:C:204:PHE:CE2	1:C:208:LEU:HD22	2.54	0.43
1:C:325:LEU:HD23	1:C:325:LEU:O	2.19	0.43
1:E:325:LEU:HD23	1:E:325:LEU:O	2.19	0.43
1:A:189:GLU:HB3	1:A:190:PRO:HD2	2.01	0.43
1:B:165:ILE:O	1:B:278:ALA:HA	2.18	0.43
1:D:213:LYS:HB2	1:D:220:VAL:O	2.18	0.43
1:E:189:GLU:HB3	1:E:190:PRO:HD2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:LYS:HB2	1:F:220:VAL:O	2.19	0.43
1:A:379:GLU:O	1:A:383:LEU:HD22	2.18	0.43
1:C:262:ARG:HG3	1:C:269:ILE:HD12	2.01	0.43
1:B:153:ILE:HG22	1:B:183:LEU:HD12	2.00	0.43
1:C:202:ASP:OD1	1:C:202:ASP:N	2.52	0.43
1:C:350:TYR:HD2	1:C:352:TRP:CD2	2.37	0.43
1:C:165:ILE:O	1:C:278:ALA:HA	2.19	0.42
1:D:216:PHE:HD1	1:D:216:PHE:H	1.66	0.42
1:D:216:PHE:HZ	1:D:266:ARG:NH2	2.12	0.42
1:A:145:LYS:HD3	1:A:308:PRO:HG2	2.01	0.42
1:B:229:LEU:HD23	1:B:229:LEU:O	2.19	0.42
1:C:215:ALA:O	1:C:217:THR:N	2.52	0.42
1:C:254:VAL:CG2	4:C:416:HOH:O	2.48	0.42
1:C:310:LEU:HA	1:C:310:LEU:HD12	1.82	0.42
1:B:211:TYR:OH	1:C:215:ALA:HB3	2.20	0.42
1:E:204:PHE:CE2	1:E:208:LEU:HD22	2.55	0.42
1:F:174:GLU:O	1:F:178:ARG:HG3	2.19	0.42
1:F:334:LYS:NZ	4:F:435:HOH:O	2.20	0.42
1:A:204:PHE:CE2	1:A:208:LEU:HD22	2.55	0.42
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.84	0.42
1:B:229:LEU:HD12	1:C:266:ARG:HB3	2.02	0.42
1:B:257:SER:O	1:B:259:LYS:HG3	2.19	0.42
1:C:214:GLY:O	1:C:217:THR:CB	2.46	0.42
1:C:255:ILE:HG23	1:C:275:ILE:HD12	2.01	0.42
1:G:326:LYS:HZ3	1:G:330:ARG:HH21	1.68	0.42
1:A:153:ILE:HG22	1:A:183:LEU:HD12	2.01	0.42
1:B:217:THR:OG1	1:B:218:GLY:N	2.53	0.42
1:D:189:GLU:HB3	1:D:190:PRO:HD2	2.02	0.42
1:E:202:ASP:OD1	1:E:202:ASP:N	2.52	0.42
1:A:217:THR:C	1:A:219:ALA:H	2.23	0.42
1:C:257:SER:O	1:C:259:LYS:HG3	2.19	0.42
1:D:350:TYR:HD2	1:D:352:TRP:CD2	2.37	0.42
1:D:307:ILE:HA	1:D:308:PRO:HD3	1.91	0.42
1:F:350:TYR:HD2	1:F:352:TRP:CD2	2.38	0.42
1:G:165:ILE:O	1:G:278:ALA:HA	2.21	0.41
1:A:350:TYR:HA	1:A:351:PRO:HD3	1.81	0.41
1:C:216:PHE:CD2	1:C:264:GLY:CA	3.03	0.41
1:G:325:LEU:HD23	1:G:325:LEU:O	2.20	0.41
1:B:307:ILE:HA	1:B:308:PRO:HD3	1.91	0.41
1:A:266:ARG:HB3	1:G:229:LEU:CD1	2.50	0.41
1:G:145:LYS:HD3	1:G:308:PRO:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:GLU:O	1:D:178:ARG:HG3	2.20	0.41
1:D:153:ILE:HG22	1:D:183:LEU:HD12	2.01	0.41
1:E:255:ILE:HG23	1:E:275:ILE:HD12	2.02	0.41
1:A:202:ASP:N	1:A:202:ASP:OD1	2.50	0.41
1:D:350:TYR:HA	1:D:351:PRO:HD3	1.78	0.41
1:B:189:GLU:HB3	1:B:190:PRO:HD2	2.03	0.41
1:D:229:LEU:O	1:D:229:LEU:HD23	2.20	0.41
1:D:325:LEU:O	1:D:329:SER:HB2	2.21	0.41
1:F:229:LEU:CD1	1:G:266:ARG:HB3	2.50	0.41
1:G:199:ILE:HA	1:G:200:PRO:HD3	1.95	0.41
1:E:310:LEU:HD12	1:E:310:LEU:HA	1.89	0.41
1:F:209:PHE:O	1:F:262:ARG:HG2	2.20	0.41
1:G:350:TYR:HA	1:G:351:PRO:HD3	1.80	0.41
1:B:199:ILE:HA	1:B:200:PRO:HD3	1.97	0.40
1:B:244:SER:O	1:B:248:GLN:HG3	2.21	0.40
1:B:350:TYR:HD2	1:B:352:TRP:CD2	2.40	0.40
1:E:153:ILE:HG22	1:E:183:LEU:HD12	2.02	0.40
1:C:274:ARG:HD3	4:C:95:HOH:O	2.22	0.40
1:F:189:GLU:HB3	1:F:190:PRO:HD2	2.02	0.40
1:A:213:LYS:HB2	1:A:220:VAL:O	2.21	0.40
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.88	0.40
1:B:369:PHE:CZ	1:C:152:LYS:HE3	2.57	0.40
1:E:145:LYS:HD3	1:E:308:PRO:HG2	2.03	0.40
1:E:350:TYR:HD2	1:E:352:TRP:CD2	2.40	0.40
1:E:257:SER:O	1:E:259:LYS:HG3	2.21	0.40
1:E:307:ILE:HA	1:E:308:PRO:HD3	1.91	0.40
1:F:325:LEU:HD23	1:F:325:LEU:O	2.22	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	245/266 (92%)	235 (96%)	7 (3%)	3 (1%)	15	22
1	B	245/266 (92%)	236 (96%)	8 (3%)	1 (0%)	38	54
1	C	245/266 (92%)	239 (98%)	4 (2%)	2 (1%)	22	34
1	D	245/266 (92%)	237 (97%)	6 (2%)	2 (1%)	22	34
1	E	245/266 (92%)	235 (96%)	4 (2%)	6 (2%)	7	9
1	F	245/266 (92%)	236 (96%)	8 (3%)	1 (0%)	38	54
1	G	245/266 (92%)	234 (96%)	9 (4%)	2 (1%)	22	34
All	All	1715/1862 (92%)	1652 (96%)	46 (3%)	17 (1%)	18	27

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	THR
1	D	217	THR
1	E	217	THR
1	F	217	THR
1	G	215	ALA
1	G	216	PHE
1	A	216	PHE
1	D	219	ALA
1	E	218	GLY
1	E	215	ALA
1	E	216	PHE
1	E	219	ALA
1	C	216	PHE
1	B	372	GLY
1	E	372	GLY
1	A	372	GLY
1	C	372	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	211/230 (92%)	207 (98%)	4 (2%)	62	80
1	B	211/230 (92%)	207 (98%)	4 (2%)	62	80
1	C	211/230 (92%)	207 (98%)	4 (2%)	62	80
1	D	211/230 (92%)	209 (99%)	2 (1%)	82	91
1	E	211/230 (92%)	209 (99%)	2 (1%)	82	91
1	F	211/230 (92%)	209 (99%)	2 (1%)	82	91
1	G	211/230 (92%)	209 (99%)	2 (1%)	82	91
All	All	1477/1610 (92%)	1457 (99%)	20 (1%)	71	85

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	GLU
1	A	268	GLU
1	A	336	VAL
1	A	383	LEU
1	B	174	GLU
1	B	205	GLU
1	B	216	PHE
1	B	268	GLU
1	C	205	GLU
1	C	217	THR
1	C	268	GLU
1	C	336	VAL
1	D	205	GLU
1	D	216	PHE
1	E	268	GLU
1	E	336	VAL
1	F	205	GLU
1	F	336	VAL
1	G	205	GLU
1	G	268	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 14 ligands modelled in this entry, 7 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$
2	ATP	A	400	3	27,33,33	1.04	2 (7%)	25,52,52	1.51	4 (16%)
2	ATP	B	400	3	27,33,33	1.12	2 (7%)	25,52,52	1.84	5 (20%)
2	ATP	C	400	3	27,33,33	0.97	2 (7%)	25,52,52	1.62	4 (16%)
2	ATP	D	400	3	27,33,33	0.99	1 (3%)	25,52,52	1.59	3 (12%)
2	ATP	E	400	3	27,33,33	1.06	2 (7%)	25,52,52	1.49	2 (8%)
2	ATP	F	400	3	27,33,33	1.02	2 (7%)	25,52,52	1.72	2 (8%)
2	ATP	G	400	3	27,33,33	0.98	2 (7%)	25,52,52	1.63	2 (8%)

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
2	ATP	A	400	3	-	0/18/38/38	0/3/3/3
2	ATP	B	400	3	-	0/18/38/38	0/3/3/3
2	ATP	C	400	3	-	0/18/38/38	0/3/3/3
2	ATP	D	400	3	-	0/18/38/38	0/3/3/3
2	ATP	E	400	3	-	0/18/38/38	0/3/3/3
2	ATP	F	400	3	-	0/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	G	400	3	-	0/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	ATP	PG-O3B	2.02	1.63	1.60
2	G	400	ATP	PG-O3B	2.08	1.63	1.60
2	E	400	ATP	PG-O3B	2.12	1.63	1.60
2	A	400	ATP	PG-O3B	2.16	1.63	1.60
2	F	400	ATP	PG-O3B	2.28	1.63	1.60
2	B	400	ATP	PG-O3B	2.33	1.63	1.60
2	C	400	ATP	C5-C4	2.64	1.46	1.40
2	G	400	ATP	C5-C4	2.77	1.46	1.40
2	A	400	ATP	C5-C4	3.07	1.47	1.40
2	F	400	ATP	C5-C4	3.08	1.47	1.40
2	D	400	ATP	C5-C4	3.27	1.47	1.40
2	B	400	ATP	C5-C4	3.33	1.48	1.40
2	E	400	ATP	C5-C4	3.42	1.48	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	ATP	N3-C2-N1	-6.62	123.10	128.86
2	B	400	ATP	N3-C2-N1	-6.08	123.56	128.86
2	G	400	ATP	N3-C2-N1	-6.06	123.58	128.86
2	C	400	ATP	N3-C2-N1	-5.79	123.82	128.86
2	D	400	ATP	N3-C2-N1	-5.55	124.03	128.86
2	E	400	ATP	N3-C2-N1	-4.93	124.56	128.86
2	A	400	ATP	N3-C2-N1	-4.78	124.70	128.86
2	D	400	ATP	C4-C5-N7	-2.42	107.08	109.41
2	A	400	ATP	C4-C5-N7	-2.34	107.15	109.41
2	B	400	ATP	C4'-O4'-C1'	-2.15	107.48	109.77
2	B	400	ATP	O3B-PG-O1G	-2.07	98.72	111.44
2	C	400	ATP	O3'-C3'-C4'	-2.01	105.22	111.09
2	E	400	ATP	N6-C6-N1	2.19	123.11	118.77
2	B	400	ATP	C2-N1-C6	2.22	122.65	118.77
2	C	400	ATP	N6-C6-N1	2.24	123.21	118.77
2	D	400	ATP	C2-N1-C6	2.30	122.80	118.77
2	A	400	ATP	N6-C6-N1	2.30	123.33	118.77
2	A	400	ATP	O3G-PG-O2G	2.35	117.08	107.61
2	B	400	ATP	O2A-PA-O5'	2.43	119.63	108.14
2	C	400	ATP	O3G-PG-O2G	2.45	117.49	107.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	G	400	ATP	O3G-PG-O2G	2.50	117.71	107.61
2	F	400	ATP	C2-N1-C6	2.54	123.21	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	ATP	3	0
2	F	400	ATP	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	247/266 (92%)	-0.12	9 (3%) 43 39	29, 50, 85, 135	0
1	B	247/266 (92%)	-0.28	1 (0%) 92 92	31, 48, 82, 151	0
1	C	247/266 (92%)	-0.09	11 (4%) 34 30	31, 51, 86, 156	0
1	D	247/266 (92%)	-0.30	4 (1%) 72 69	31, 50, 82, 139	0
1	E	247/266 (92%)	-0.19	7 (2%) 53 48	32, 50, 85, 155	0
1	F	247/266 (92%)	-0.29	3 (1%) 79 77	31, 49, 82, 163	0
1	G	247/266 (92%)	-0.19	4 (1%) 72 69	30, 47, 83, 161	0
All	All	1729/1862 (92%)	-0.21	39 (2%) 61 56	29, 49, 88, 163	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	218	GLY	8.8
1	D	215	ALA	6.6
1	E	217	THR	6.5
1	F	216	PHE	6.1
1	G	217	THR	6.0
1	A	216	PHE	5.9
1	C	215	ALA	5.6
1	F	217	THR	4.7
1	C	218	GLY	4.6
1	C	216	PHE	4.4
1	G	216	PHE	4.1
1	A	337	GLU	3.8
1	F	218	GLY	3.5
1	D	216	PHE	3.2
1	E	339	PHE	3.0
1	C	374	PHE	3.0
1	C	337	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	381	SER	2.9
1	C	373	LYS	2.8
1	D	382	CYS	2.8
1	A	382	CYS	2.8
1	C	375	ILE	2.7
1	B	216	PHE	2.7
1	A	343	ALA	2.7
1	E	216	PHE	2.6
1	A	339	PHE	2.5
1	A	373	LYS	2.5
1	E	218	GLY	2.5
1	A	217	THR	2.4
1	E	337	GLU	2.4
1	E	371	GLU	2.4
1	C	219	ALA	2.3
1	C	371	GLU	2.2
1	A	218	GLY	2.2
1	C	339	PHE	2.2
1	G	219	ALA	2.2
1	A	374	PHE	2.1
1	E	343	ALA	2.1
1	C	343	ALA	2.1

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(\AA^2)	Q<0.9
2	ATP	E	400	31/31	0.98	0.14	-0.14	30,42,62,71	0
2	ATP	C	400	31/31	0.98	0.15	-0.23	32,44,58,64	0
2	ATP	G	400	31/31	0.98	0.15	-0.26	26,36,51,55	0
2	ATP	B	400	31/31	0.97	0.15	-0.43	23,40,53,64	0
2	ATP	A	400	31/31	0.98	0.14	-0.56	28,44,53,60	0
2	ATP	D	400	31/31	0.98	0.13	-0.70	24,38,52,54	0
2	ATP	F	400	31/31	0.97	0.14	-0.77	20,41,53,65	0
3	MG	A	401	1/1	0.93	0.22	-	46,46,46,46	0
3	MG	C	401	1/1	0.94	0.25	-	54,54,54,54	0
3	MG	F	401	1/1	0.88	0.27	-	51,51,51,51	0
3	MG	B	401	1/1	0.90	0.28	-	54,54,54,54	0
3	MG	G	401	1/1	0.86	0.20	-	50,50,50,50	0
3	MG	D	401	1/1	0.93	0.33	-	55,55,55,55	0
3	MG	E	401	1/1	0.95	0.18	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.