Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:24 PM GMT

PDB ID	:	5C18
Title	:	p97-delta709-728 in complex with ATP-gamma-S
Authors	:	Haenzelmann, P.; Schindelin, H.
Deposited on	:	2015-06-13
Resolution	:	3.30 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:

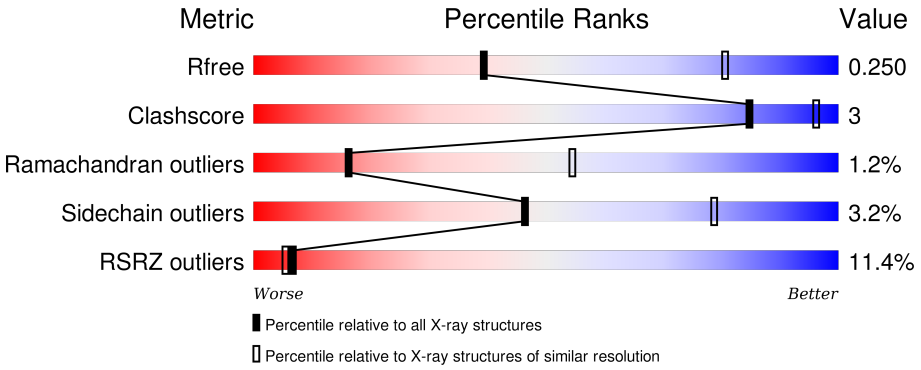
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.30 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.



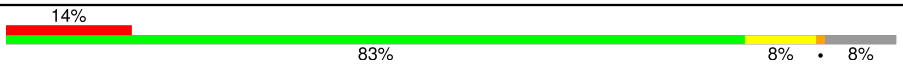
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	785	14% 85% 7% • 8%
1	B	785	5% 82% 9% • 8%
1	C	785	9% 83% 9% • 8%
1	D	785	14% 84% 7% • 8%
1	E	785	6% 81% 10% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	785	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 69089 atoms, of which 34628 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	722	Total	C	H	N	O	S	0	0	0
			11409	3567	5741	1001	1070	30			
1	B	723	Total	C	H	N	O	S	0	0	0
			11420	3570	5746	1002	1072	30			
1	C	724	Total	C	H	N	O	S	0	0	0
			11427	3572	5749	1003	1073	30			
1	D	722	Total	C	H	N	O	S	0	0	0
			11409	3567	5741	1001	1070	30			
1	E	723	Total	C	H	N	O	S	0	0	0
			11418	3570	5745	1002	1071	30			
1	F	724	Total	C	H	N	O	S	0	0	0
			11430	3573	5750	1004	1073	30			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLN	deletion	UNP P55072
A	?	-	THR	deletion	UNP P55072
A	?	-	ASN	deletion	UNP P55072
A	?	-	PRO	deletion	UNP P55072
A	?	-	SER	deletion	UNP P55072
A	?	-	ALA	deletion	UNP P55072
A	?	-	MET	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	VAL	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ASP	deletion	UNP P55072

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P55072
A	?	-	PRO	deletion	UNP P55072
A	?	-	VAL	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLN	deletion	UNP P55072
B	?	-	THR	deletion	UNP P55072
B	?	-	ASN	deletion	UNP P55072
B	?	-	PRO	deletion	UNP P55072
B	?	-	SER	deletion	UNP P55072
B	?	-	ALA	deletion	UNP P55072
B	?	-	MET	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	VAL	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ASP	deletion	UNP P55072
B	?	-	ASP	deletion	UNP P55072
B	?	-	PRO	deletion	UNP P55072
B	?	-	VAL	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLN	deletion	UNP P55072
C	?	-	THR	deletion	UNP P55072
C	?	-	ASN	deletion	UNP P55072
C	?	-	PRO	deletion	UNP P55072
C	?	-	SER	deletion	UNP P55072
C	?	-	ALA	deletion	UNP P55072
C	?	-	MET	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	VAL	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ASP	deletion	UNP P55072
C	?	-	ASP	deletion	UNP P55072
C	?	-	PRO	deletion	UNP P55072

Continued on next page...

Continued from previous page...

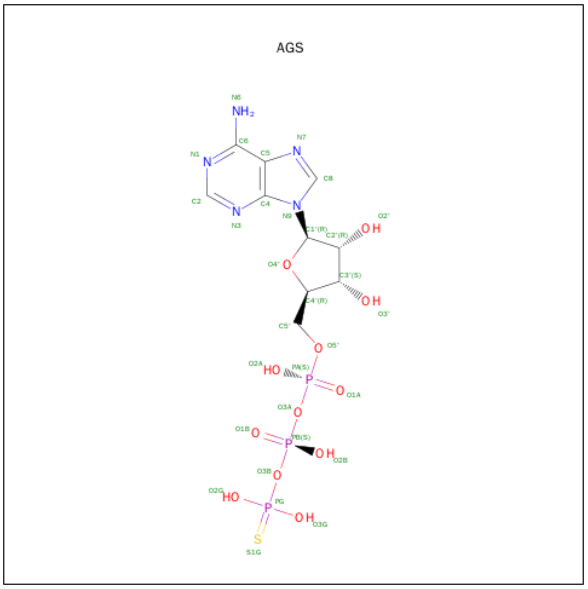
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLN	deletion	UNP P55072
D	?	-	THR	deletion	UNP P55072
D	?	-	ASN	deletion	UNP P55072
D	?	-	PRO	deletion	UNP P55072
D	?	-	SER	deletion	UNP P55072
D	?	-	ALA	deletion	UNP P55072
D	?	-	MET	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	VAL	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ASP	deletion	UNP P55072
D	?	-	ASP	deletion	UNP P55072
D	?	-	PRO	deletion	UNP P55072
D	?	-	VAL	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLN	deletion	UNP P55072
E	?	-	THR	deletion	UNP P55072
E	?	-	ASN	deletion	UNP P55072
E	?	-	PRO	deletion	UNP P55072
E	?	-	SER	deletion	UNP P55072
E	?	-	ALA	deletion	UNP P55072
E	?	-	MET	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	VAL	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ASP	deletion	UNP P55072
E	?	-	ASP	deletion	UNP P55072
E	?	-	PRO	deletion	UNP P55072
E	?	-	VAL	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLU	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072
F	?	-	GLN	deletion	UNP P55072
F	?	-	THR	deletion	UNP P55072
F	?	-	ASN	deletion	UNP P55072
F	?	-	PRO	deletion	UNP P55072
F	?	-	SER	deletion	UNP P55072
F	?	-	ALA	deletion	UNP P55072
F	?	-	MET	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	VAL	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	ASP	deletion	UNP P55072
F	?	-	ASP	deletion	UNP P55072
F	?	-	PRO	deletion	UNP P55072
F	?	-	VAL	deletion	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is water.

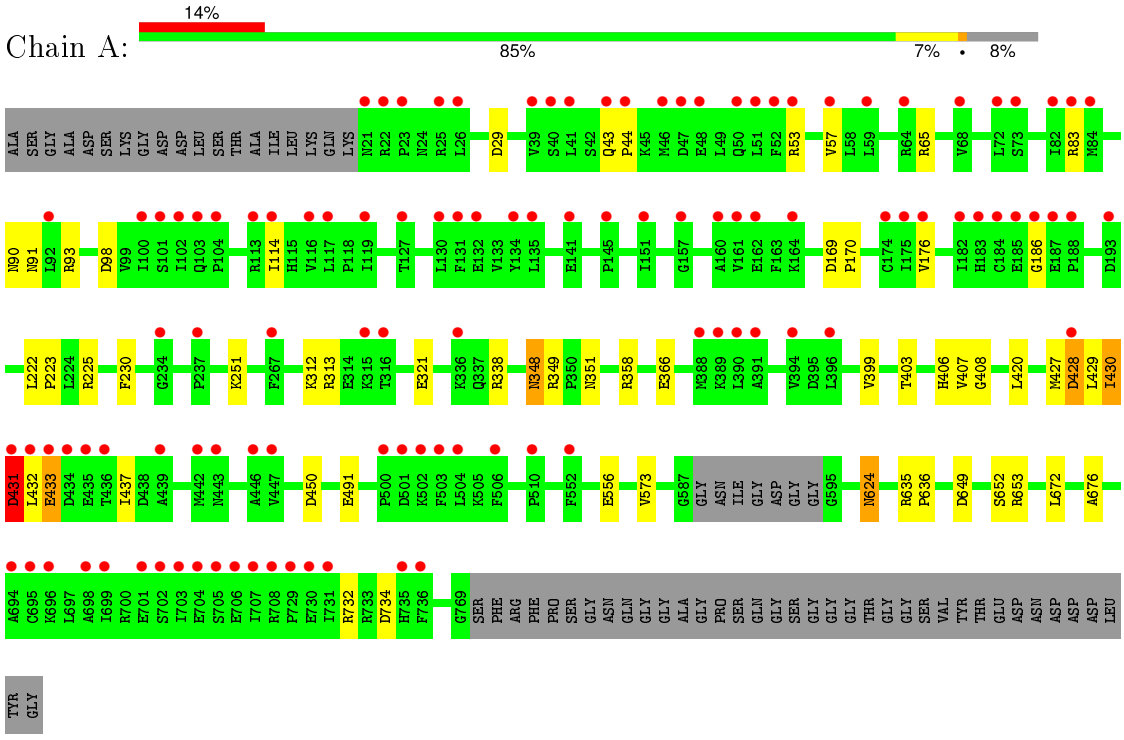
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	5	Total O 5 5	0	0
5	C	5	Total O 5 5	0	0
5	D	5	Total O 5 5	0	0
5	E	5	Total O 5 5	0	0
5	F	5	Total O 5 5	0	0

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 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.

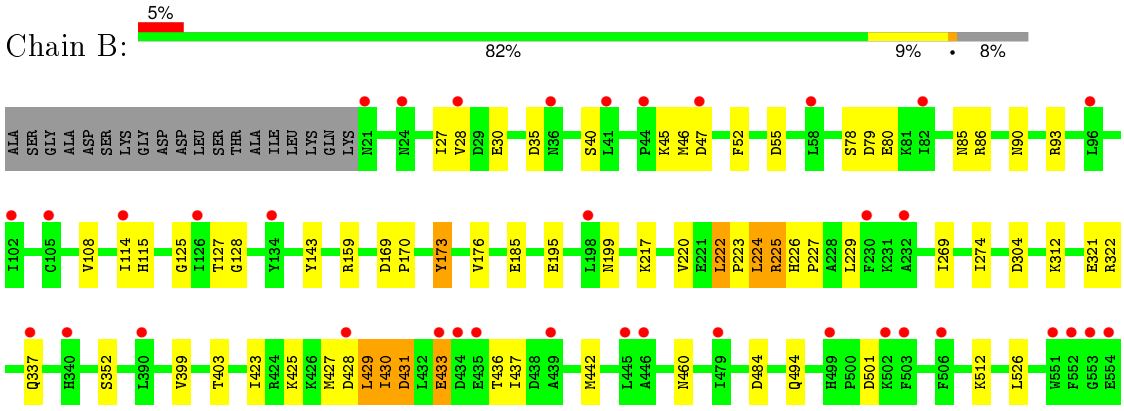
- Molecule 1: Transitional endoplasmic reticulum ATPase

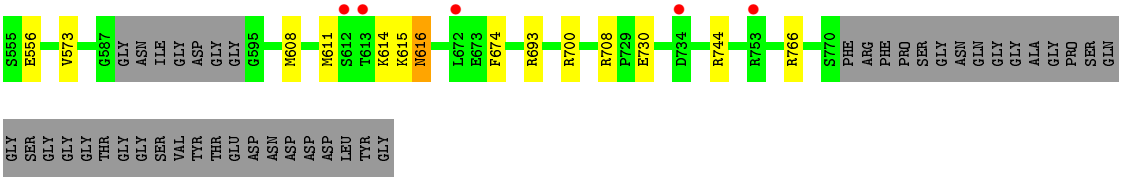
Chain A:



- Molecule 1: Transitional endoplasmic reticulum ATPase

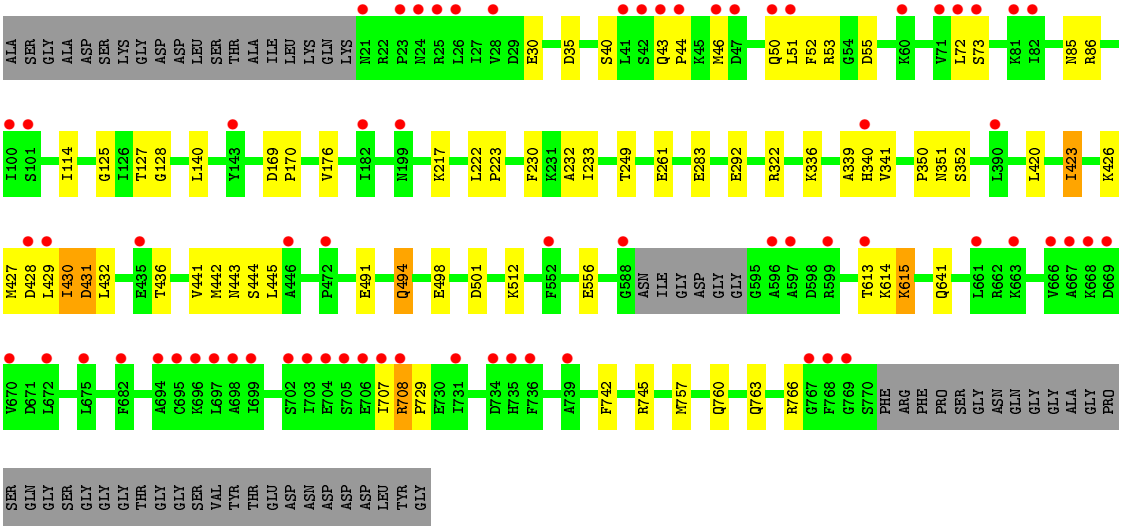
Chain B:





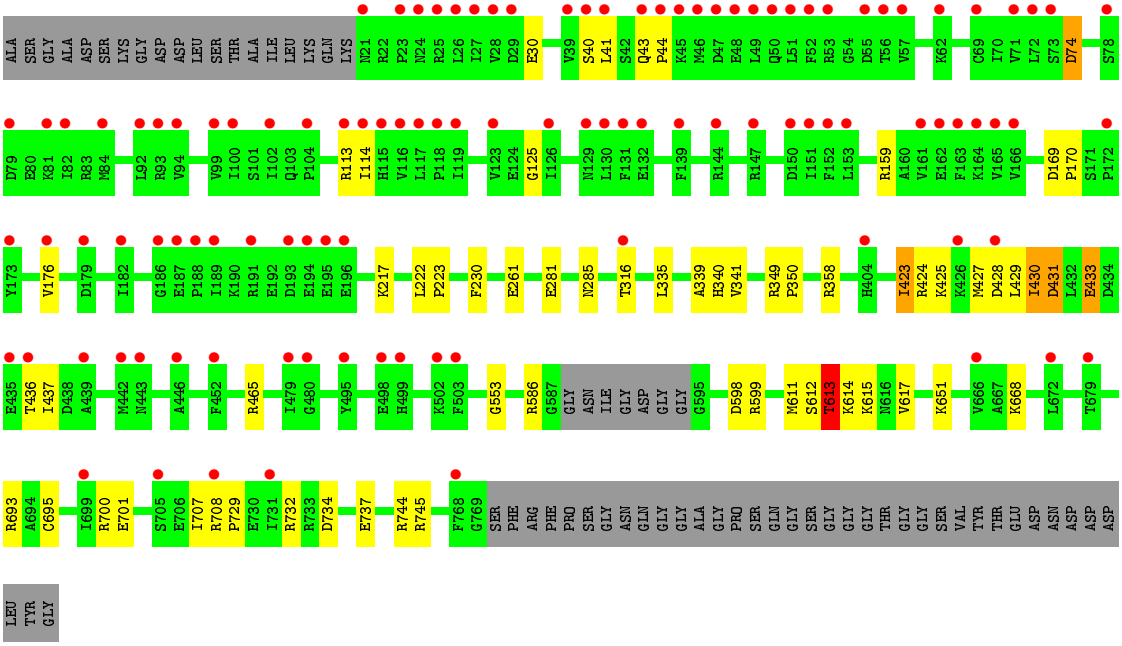
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



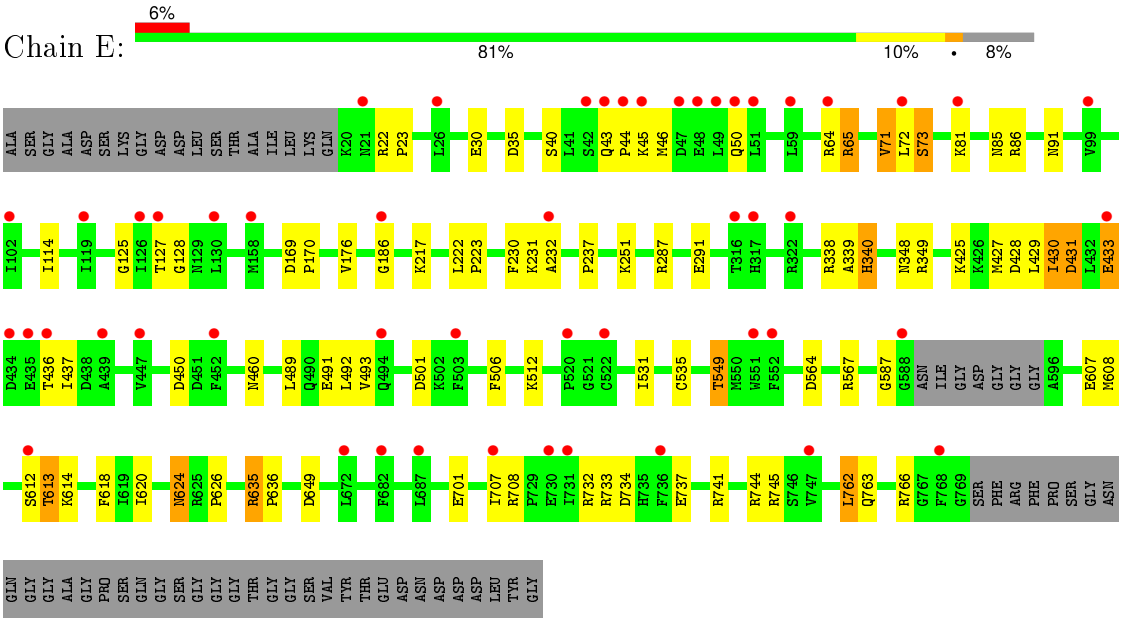
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



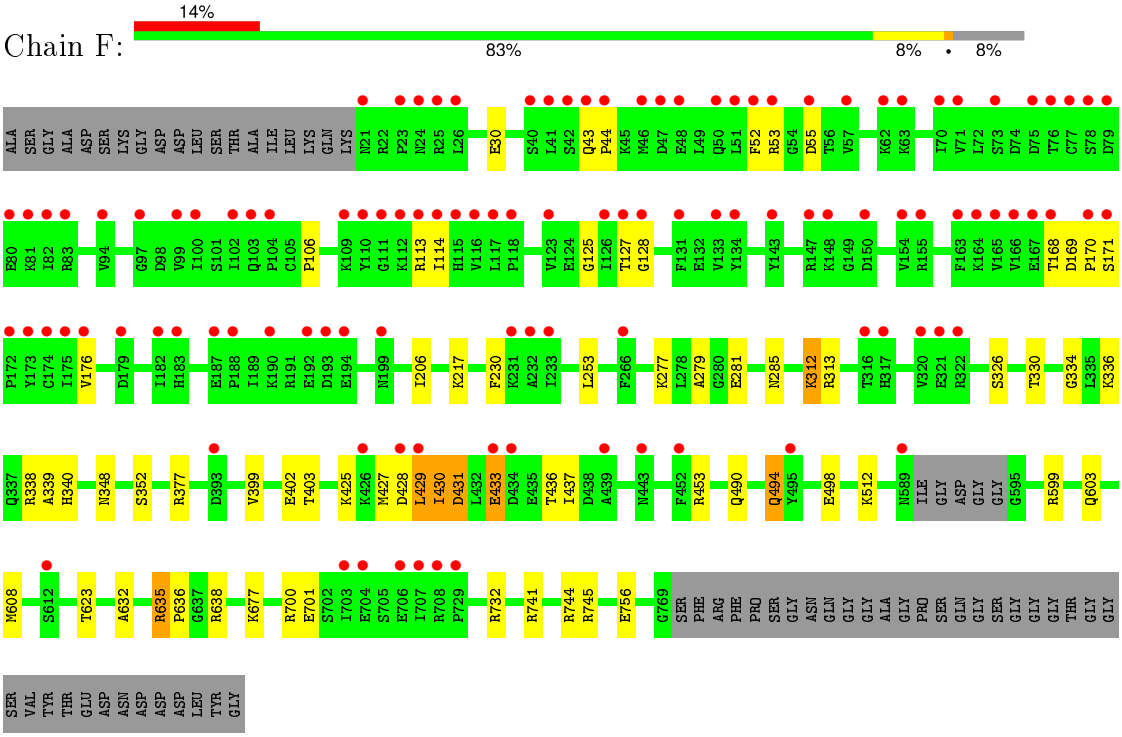
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.33Å 180.06Å 255.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.30 49.18 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-3.30) 100.0 (49.18-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.249 0.222 , 0.250	Depositor DCC
R_{free} test set	4868 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	101.3	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 77.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 97871 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	69089	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, AGS, CL

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	0.22	0/5761	0.40	0/7778
1	B	0.22	0/5767	0.41	0/7786
1	C	0.23	0/5771	0.41	0/7791
1	D	0.22	0/5761	0.40	0/7778
1	E	0.22	0/5766	0.41	0/7785
1	F	0.22	0/5773	0.40	0/7794
All	All	0.22	0/34599	0.40	0/46712

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	339	ALA	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	5668	5741	5741	30	0
1	B	5674	5746	5746	39	0
1	C	5678	5749	5749	34	0
1	D	5668	5741	5741	32	0
1	E	5673	5745	5743	45	0
1	F	5680	5750	5750	32	0
2	A	62	26	24	2	0
2	B	62	26	24	3	0
2	C	62	26	24	0	0
2	D	62	26	24	0	0
2	E	62	26	24	2	0
2	F	62	26	24	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	2	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	1	0
5	F	5	0	0	1	0
All	All	34461	34628	34614	201	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 3.

All (201) 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:B:512:LYS:NZ	1:B:608:MET:O	2.14	0.81
1:F:313:ARG:NH2	1:F:326:SER:OG	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:512:LYS:NZ	1:F:608:MET:O	2.20	0.75
1:A:65:ARG:NH1	1:A:91:ASN:O	2.19	0.75
1:A:653:ARG:NH2	1:A:676:ALA:O	2.20	0.75
1:F:338:ARG:O	1:F:340:HIS:N	2.22	0.73
1:E:701:GLU:OE2	1:E:732:ARG:NH1	2.22	0.72
1:E:30:GLU:OE2	1:E:217:LYS:NZ	2.24	0.71
1:B:304:ASP:OD2	5:B:1001:HOH:O	2.09	0.70
1:E:45:LYS:NZ	1:E:81:LYS:O	2.25	0.69
1:E:427:MET:O	1:E:429:LEU:N	2.26	0.69
1:A:399:VAL:O	1:A:403:THR:OG1	2.09	0.68
1:B:30:GLU:OE2	1:B:217:LYS:NZ	2.23	0.67
1:B:321:GLU:OE1	1:C:322:ARG:NH1	2.27	0.67
1:D:465:ARG:NH1	1:E:607:GLU:OE2	2.28	0.66
1:B:35:ASP:O	1:B:85:ASN:ND2	2.28	0.66
1:E:512:LYS:NZ	1:E:608:MET:O	2.28	0.66
1:A:90:ASN:O	1:A:93:ARG:NH1	2.30	0.65
1:C:339:ALA:O	1:C:341:VAL:N	2.29	0.65
1:B:399:VAL:O	1:B:403:THR:OG1	2.09	0.65
2:A:901:AGS:S1G	1:B:766:ARG:NH2	2.70	0.63
1:D:700:ARG:NH1	1:E:491:GLU:OE2	2.31	0.63
1:C:46:MET:SD	1:C:73:SER:N	2.72	0.63
1:C:35:ASP:O	1:C:85:ASN:ND2	2.32	0.63
1:D:339:ALA:O	1:D:341:VAL:N	2.32	0.63
1:F:281:GLU:O	1:F:285:ASN:ND2	2.32	0.62
2:B:901:AGS:S1G	1:C:766:ARG:NH1	2.71	0.62
1:D:612:SER:O	1:D:614:LYS:N	2.33	0.61
1:F:125:GLY:O	1:F:436:THR:OG1	2.17	0.61
1:E:46:MET:O	1:E:50:GLN:N	2.34	0.61
1:E:624:ASN:OD1	1:E:624:ASN:N	2.34	0.60
1:D:430:ILE:HG23	1:D:431:ASP:H	1.66	0.59
1:D:701:GLU:OE1	1:D:732:ARG:NH1	2.36	0.59
1:B:427:MET:O	1:B:429:LEU:N	2.36	0.59
1:F:399:VAL:O	1:F:403:THR:OG1	2.10	0.59
1:A:358:ARG:NH1	1:A:366:GLU:OE2	2.36	0.59
1:D:465:ARG:NH2	1:E:564:ASP:OD1	2.36	0.58
1:A:430:ILE:HG23	1:A:431:ASP:H	1.69	0.57
1:C:429:LEU:O	1:C:431:ASP:N	2.37	0.57
1:A:431:ASP:O	1:A:433:GLU:N	2.35	0.57
1:F:430:ILE:HG23	1:F:431:ASP:H	1.70	0.57
1:B:431:ASP:O	1:B:433:GLU:N	2.38	0.57
1:C:423:ILE:O	1:C:427:MET:N	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HG23	1:B:431:ASP:H	1.70	0.56
1:A:98:ASP:OD2	1:A:225:ARG:NH2	2.38	0.56
1:B:125:GLY:O	1:B:436:THR:OG1	2.10	0.56
1:A:251:LYS:NZ	2:A:902:AGS:O3G	2.39	0.56
1:F:427:MET:O	1:F:429:LEU:N	2.38	0.56
1:E:251:LYS:NZ	2:E:902:AGS:O1B	2.38	0.56
1:F:336:LYS:O	1:F:338:ARG:NE	2.39	0.56
1:E:35:ASP:O	1:E:85:ASN:ND2	2.39	0.55
1:C:127:THR:OG1	1:C:128:GLY:N	2.39	0.55
1:D:159:ARG:NH2	1:E:232:ALA:O	2.36	0.55
1:D:427:MET:O	1:D:429:LEU:N	2.39	0.55
1:A:491:GLU:OE2	1:F:700:ARG:NH2	2.39	0.54
1:A:427:MET:SD	1:A:430:ILE:HG21	2.48	0.54
1:D:427:MET:O	1:D:430:ILE:N	2.41	0.54
1:F:312:LYS:N	1:F:352:SER:O	2.39	0.54
2:F:902:AGS:O1A	5:F:1001:HOH:O	2.19	0.54
1:E:430:ILE:HG23	1:E:431:ASP:H	1.73	0.54
1:A:624:ASN:N	1:A:624:ASN:OD1	2.40	0.54
1:B:614:LYS:O	1:B:616:ASN:N	2.41	0.54
1:A:732:ARG:NE	1:A:734:ASP:OD1	2.41	0.54
1:C:430:ILE:HG23	1:C:432:LEU:HG	1.91	0.53
1:C:613:THR:O	1:C:615:LYS:N	2.41	0.53
1:F:431:ASP:O	1:F:433:GLU:N	2.38	0.52
2:E:902:AGS:O1A	5:E:1001:HOH:O	2.19	0.52
1:D:431:ASP:O	1:D:433:GLU:N	2.38	0.52
1:C:430:ILE:HG23	1:C:431:ASP:H	1.76	0.51
1:B:700:ARG:NH2	1:C:491:GLU:OE2	2.43	0.51
1:F:632:ALA:O	1:F:638:ARG:NH1	2.43	0.51
1:D:125:GLY:O	1:D:436:THR:OG1	2.23	0.51
1:E:732:ARG:NH2	1:E:734:ASP:OD2	2.44	0.50
1:C:30:GLU:OE2	1:C:217:LYS:NZ	2.32	0.50
1:F:30:GLU:OE2	1:F:217:LYS:NZ	2.25	0.50
1:B:220:VAL:HG12	1:B:224:LEU:HD11	1.94	0.50
1:C:125:GLY:O	1:C:436:THR:OG1	2.18	0.49
1:A:312:LYS:NZ	1:A:351:ASN:O	2.30	0.49
1:E:431:ASP:O	1:E:433:GLU:N	2.42	0.49
1:C:52:PHE:N	1:C:55:ASP:OD2	2.45	0.49
1:C:494:GLN:NE2	1:C:498:GLU:OE2	2.46	0.49
1:E:72:LEU:O	1:E:73:SER:OG	2.28	0.49
1:E:125:GLY:O	1:E:436:THR:OG1	2.17	0.49
1:F:169:ASP:HB3	1:F:170:PRO:HD3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:701:GLU:OE1	1:F:732:ARG:NH2	2.45	0.49
1:C:427:MET:HG3	1:C:430:ILE:HG21	1.95	0.49
1:C:283:GLU:OE1	1:C:283:GLU:N	2.42	0.48
1:F:402:GLU:OE1	1:F:453:ARG:NH1	2.47	0.48
1:A:348:ASN:N	1:A:348:ASN:OD1	2.46	0.48
1:B:127:THR:OG1	1:B:128:GLY:N	2.47	0.48
1:C:708:ARG:N	1:C:729:PRO:HD3	2.28	0.48
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.96	0.48
1:C:140:LEU:O	1:C:140:LEU:HD12	2.13	0.48
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.94	0.47
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.96	0.47
1:D:430:ILE:HD11	1:D:437:ILE:HD12	1.96	0.47
1:E:564:ASP:OD1	1:E:567:ARG:NH1	2.48	0.47
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.96	0.47
1:C:429:LEU:HD12	1:C:430:ILE:N	2.29	0.47
1:C:427:MET:O	1:C:429:LEU:N	2.47	0.47
1:D:423:ILE:O	1:D:425:LYS:N	2.48	0.47
1:A:114:ILE:CD1	1:A:176:VAL:HG22	2.45	0.47
1:B:79:ASP:OD1	1:B:79:ASP:N	2.48	0.47
1:D:350:PRO:O	1:D:358:ARG:NH2	2.45	0.47
1:C:114:ILE:CD1	1:C:176:VAL:HG22	2.44	0.47
1:B:159:ARG:NH2	1:C:232:ALA:O	2.41	0.47
1:E:114:ILE:CD1	1:E:176:VAL:HG22	2.44	0.47
1:B:222:LEU:HB2	1:B:223:PRO:HD3	1.97	0.46
1:A:321:GLU:OE2	1:B:322:ARG:NE	2.48	0.46
1:A:429:LEU:HG	1:A:430:ILE:N	2.30	0.46
1:B:114:ILE:CD1	1:B:176:VAL:HG22	2.46	0.46
1:D:732:ARG:NE	1:D:734:ASP:OD1	2.41	0.46
1:A:635:ARG:NH1	1:A:636:PRO:O	2.49	0.46
1:E:127:THR:OG1	1:E:128:GLY:N	2.48	0.46
1:D:30:GLU:OE2	1:D:217:LYS:NZ	2.34	0.46
1:B:93:ARG:NH2	1:B:195:GLU:OE2	2.46	0.46
1:A:29:ASP:OD2	1:A:83:ARG:NH1	2.49	0.46
1:D:613:THR:O	1:D:615:LYS:N	2.48	0.45
1:D:281:GLU:O	1:D:285:ASN:ND2	2.44	0.45
1:E:493:VAL:HG12	1:E:535:CYS:SG	2.56	0.45
1:B:708:ARG:NH1	1:B:730:GLU:OE1	2.49	0.45
1:D:41:LEU:O	1:D:74:ASP:N	2.47	0.45
1:E:531:ILE:HD11	1:E:620:ILE:CD1	2.47	0.45
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.97	0.45
1:F:277:LYS:NZ	1:F:285:ASN:OD1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:635:ARG:NE	1:E:636:PRO:O	2.48	0.45
1:F:490:GLN:O	1:F:494:GLN:N	2.49	0.45
1:F:635:ARG:NE	1:F:636:PRO:O	2.47	0.45
1:E:46:MET:HE2	1:E:71:VAL:HG12	1.99	0.44
1:C:501:ASP:N	1:C:501:ASP:OD1	2.50	0.44
1:E:493:VAL:HG13	1:E:618:PHE:CD2	2.53	0.44
1:B:484:ASP:OD1	1:B:484:ASP:N	2.49	0.44
1:F:377:ARG:NE	1:F:403:THR:O	2.51	0.44
1:A:430:ILE:HD11	1:A:437:ILE:HD12	1.99	0.44
1:E:493:VAL:HG13	1:E:618:PHE:CE2	2.53	0.44
1:E:237:PRO:HG2	1:E:340:HIS:NE2	2.32	0.44
1:E:287:ARG:NH1	1:E:291:GLU:OE2	2.51	0.44
1:A:321:GLU:OE1	1:B:322:ARG:NH1	2.51	0.44
1:B:501:ASP:N	1:B:501:ASP:OD1	2.50	0.44
1:F:114:ILE:CD1	1:F:176:VAL:HG22	2.48	0.44
1:F:52:PHE:N	1:F:55:ASP:OD2	2.47	0.44
1:A:222:LEU:HB2	1:A:223:PRO:HD3	1.98	0.43
1:E:222:LEU:HB3	1:E:223:PRO:HD3	2.00	0.43
1:E:549:THR:CG2	1:F:603:GLN:HA	2.48	0.43
1:B:423:ILE:CD1	1:C:233:ILE:HD11	2.48	0.43
1:C:46:MET:HA	1:C:51:LEU:HD12	1.99	0.43
1:D:114:ILE:CD1	1:D:176:VAL:HG22	2.48	0.43
1:E:489:LEU:HB3	1:E:531:ILE:HG21	2.00	0.43
1:E:707:ILE:HG22	1:E:708:ARG:N	2.33	0.43
1:C:427:MET:CG	1:C:430:ILE:HG21	2.48	0.43
1:B:430:ILE:HD11	1:B:437:ILE:HD12	1.99	0.43
1:C:441:VAL:O	1:C:444:SER:OG	2.26	0.43
1:E:733:ARG:NH2	1:E:737:GLU:OE2	2.52	0.43
1:D:430:ILE:HG13	1:D:431:ASP:N	2.33	0.43
1:E:65:ARG:NH1	1:E:91:ASN:O	2.51	0.43
1:A:427:MET:O	1:A:429:LEU:N	2.52	0.42
1:E:430:ILE:HD11	1:E:437:ILE:HD12	2.00	0.42
1:B:27:ILE:HG22	1:B:28:VAL:N	2.34	0.42
1:E:626:PRO:HB2	1:E:762:LEU:HD11	2.01	0.42
1:C:222:LEU:HB2	1:C:223:PRO:HD3	2.00	0.42
1:D:586:ARG:HD3	1:D:598:ASP:HA	2.01	0.42
1:A:649:ASP:O	1:A:652:SER:OG	2.37	0.42
1:F:127:THR:OG1	1:F:128:GLY:N	2.52	0.42
1:E:501:ASP:N	1:E:501:ASP:OD1	2.52	0.42
1:F:206:ILE:HG12	1:F:253:LEU:HD22	2.01	0.42
1:F:494:GLN:NE2	1:F:498:GLU:OE2	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:ARG:NH2	1:C:641:GLN:OE1	2.51	0.42
1:D:695:CYS:HB3	1:E:506:PHE:CE2	2.55	0.42
1:B:708:ARG:O	1:B:730:GLU:N	2.51	0.42
1:F:168:THR:O	1:F:171:SER:OG	2.35	0.42
1:D:222:LEU:HB2	1:D:223:PRO:HD3	2.01	0.42
1:D:429:LEU:HD12	1:D:430:ILE:N	2.35	0.41
1:B:108:VAL:HG12	1:B:173:TYR:CD1	2.54	0.41
2:F:902:AGS:H8	2:F:902:AGS:H5'1	2.01	0.41
1:D:611:MET:HE2	1:D:617:VAL:HG11	2.01	0.41
1:A:430:ILE:HG13	1:A:431:ASP:N	2.35	0.41
1:E:430:ILE:HG13	1:E:431:ASP:N	2.34	0.41
1:A:407:VAL:HG12	1:A:408:GLY:H	1.85	0.41
1:E:22:ARG:HB3	1:E:23:PRO:HD2	2.01	0.41
1:F:430:ILE:HD11	1:F:437:ILE:HD12	2.02	0.41
1:D:707:ILE:HG22	1:D:708:ARG:N	2.36	0.41
1:E:43:GLN:N	1:E:44:PRO:CD	2.84	0.41
1:F:43:GLN:N	1:F:44:PRO:CD	2.83	0.41
1:F:430:ILE:HG13	1:F:431:ASP:N	2.35	0.41
1:B:460:ASN:OD1	1:B:460:ASN:N	2.52	0.41
1:C:43:GLN:N	1:C:44:PRO:CD	2.84	0.41
1:B:225:ARG:C	1:B:227:PRO:HD3	2.41	0.41
1:B:430:ILE:HG13	1:B:431:ASP:N	2.36	0.41
1:A:43:GLN:N	1:A:44:PRO:CD	2.84	0.41
1:B:312:LYS:N	1:B:352:SER:O	2.54	0.41
1:D:553:GLY:HA2	1:D:599:ARG:NH2	2.36	0.41
1:A:403:THR:CG2	1:A:406:HIS:CG	3.05	0.41
1:D:695:CYS:HB3	1:E:506:PHE:HE2	1.86	0.40
1:F:330:THR:O	1:F:334:GLY:N	2.51	0.40
1:C:760:GLN:O	1:C:763:GLN:NE2	2.54	0.40
1:E:734:ASP:OD1	1:E:734:ASP:N	2.49	0.40
1:B:526:LEU:HD11	2:B:901:AGS:H2'	2.04	0.40
1:B:269:ILE:HG23	1:B:274:ILE:HD11	2.03	0.40
2:B:902:AGS:O2A	5:B:1002:HOH:O	2.21	0.40
1:D:43:GLN:N	1:D:44:PRO:CD	2.85	0.40
1:B:226:HIS:HB3	1:B:229:LEU:HD23	2.03	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	718/785 (92%)	682 (95%)	31 (4%)	5 (1%)	26	66
1	B	719/785 (92%)	667 (93%)	44 (6%)	8 (1%)	17	57
1	C	720/785 (92%)	673 (94%)	35 (5%)	12 (2%)	11	47
1	D	718/785 (92%)	673 (94%)	37 (5%)	8 (1%)	17	57
1	E	719/785 (92%)	668 (93%)	41 (6%)	10 (1%)	14	50
1	F	720/785 (92%)	668 (93%)	44 (6%)	8 (1%)	17	57
All	All	4314/4710 (92%)	4031 (93%)	232 (5%)	51 (1%)	16	54

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	GLU
1	B	428	ASP
1	B	615	LYS
1	C	50	GLN
1	C	352	SER
1	C	430	ILE
1	C	431	ASP
1	C	707	ILE
1	D	428	ASP
1	D	430	ILE
1	D	613	THR
1	E	428	ASP
1	F	339	ALA
1	F	428	ASP
1	A	428	ASP
1	A	430	ILE
1	B	430	ILE
1	C	340	HIS
1	C	428	ASP
1	D	340	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	424	ARG
1	D	431	ASP
1	E	430	ILE
1	F	279	ALA
1	F	430	ILE
1	B	425	LYS
1	C	614	LYS
1	E	425	LYS
1	E	431	ASP
1	F	425	LYS
1	A	431	ASP
1	B	78	SER
1	B	431	ASP
1	E	613	THR
1	E	614	LYS
1	F	312	LYS
1	F	431	ASP
1	A	432	LEU
1	C	615	LYS
1	E	73	SER
1	B	143	TYR
1	D	423	ILE
1	E	612	SER
1	F	106	PRO
1	C	708	ARG
1	D	729	PRO
1	C	350	PRO
1	C	423	ILE
1	E	186	GLY
1	E	587	GLY
1	A	186	GLY

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	616/658 (94%)	600 (97%)	16 (3%)	54 81
1	B	617/658 (94%)	591 (96%)	26 (4%)	36 73
1	C	617/658 (94%)	596 (97%)	21 (3%)	44 77
1	D	616/658 (94%)	600 (97%)	16 (3%)	54 81
1	E	616/658 (94%)	590 (96%)	26 (4%)	36 73
1	F	617/658 (94%)	602 (98%)	15 (2%)	57 83
All	All	3699/3948 (94%)	3579 (97%)	120 (3%)	46 79

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	57	VAL
1	A	230	PHE
1	A	313	ARG
1	A	338	ARG
1	A	348	ASN
1	A	349	ARG
1	A	420	LEU
1	A	428	ASP
1	A	431	ASP
1	A	433	GLU
1	A	450	ASP
1	A	556	GLU
1	A	573	VAL
1	A	624	ASN
1	A	672	LEU
1	B	40	SER
1	B	45	LYS
1	B	46	MET
1	B	47	ASP
1	B	52	PHE
1	B	55	ASP
1	B	86	ARG
1	B	90	ASN
1	B	115	HIS
1	B	173	TYR
1	B	185	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	199	ASN
1	B	222	LEU
1	B	224	LEU
1	B	225	ARG
1	B	337	GLN
1	B	429	LEU
1	B	433	GLU
1	B	442	MET
1	B	494	GLN
1	B	556	GLU
1	B	573	VAL
1	B	611	MET
1	B	616	ASN
1	B	674	PHE
1	B	744	ARG
1	C	40	SER
1	C	53	ARG
1	C	72	LEU
1	C	86	ARG
1	C	230	PHE
1	C	249	THR
1	C	261	GLU
1	C	292	GLU
1	C	336	LYS
1	C	351	ASN
1	C	420	LEU
1	C	426	LYS
1	C	442	MET
1	C	443	ASN
1	C	445	LEU
1	C	494	GLN
1	C	512	LYS
1	C	556	GLU
1	C	742	PHE
1	C	745	ARG
1	C	757	MET
1	D	40	SER
1	D	74	ASP
1	D	113	ARG
1	D	230	PHE
1	D	261	GLU
1	D	316	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	335	LEU
1	D	349	ARG
1	D	433	GLU
1	D	613	THR
1	D	651	LYS
1	D	668	LYS
1	D	693	ARG
1	D	737	GLU
1	D	744	ARG
1	D	745	ARG
1	E	40	SER
1	E	64	ARG
1	E	65	ARG
1	E	71	VAL
1	E	86	ARG
1	E	230	PHE
1	E	231	LYS
1	E	338	ARG
1	E	340	HIS
1	E	348	ASN
1	E	349	ARG
1	E	433	GLU
1	E	450	ASP
1	E	460	ASN
1	E	492	LEU
1	E	549	THR
1	E	613	THR
1	E	624	ASN
1	E	635	ARG
1	E	649	ASP
1	E	741	ARG
1	E	744	ARG
1	E	745	ARG
1	E	762	LEU
1	E	763	GLN
1	E	766	ARG
1	F	53	ARG
1	F	113	ARG
1	F	230	PHE
1	F	348	ASN
1	F	429	LEU
1	F	433	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	494	GLN
1	F	599	ARG
1	F	623	THR
1	F	635	ARG
1	F	677	LYS
1	F	741	ARG
1	F	744	ARG
1	F	745	ARG
1	F	756	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	348	ASN
1	B	616	ASN
1	D	21	ASN

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 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 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	AGS	A	901	3	26,33,33	1.52	7 (26%)	24,52,52	2.54	3 (12%)
2	AGS	A	902	3	26,33,33	1.54	7 (26%)	24,52,52	2.52	3 (12%)
2	AGS	B	901	3	26,33,33	1.53	7 (26%)	24,52,52	2.49	2 (8%)
2	AGS	B	902	3	26,33,33	1.57	7 (26%)	24,52,52	2.53	3 (12%)
2	AGS	C	901	3	26,33,33	1.50	7 (26%)	24,52,52	2.50	3 (12%)
2	AGS	C	902	3	26,33,33	1.54	7 (26%)	24,52,52	2.56	3 (12%)
2	AGS	D	901	3	26,33,33	1.49	7 (26%)	24,52,52	2.49	2 (8%)
2	AGS	D	902	3	26,33,33	1.55	7 (26%)	24,52,52	2.54	2 (8%)
2	AGS	E	901	3	26,33,33	1.49	7 (26%)	24,52,52	2.52	3 (12%)
2	AGS	E	902	3	26,33,33	1.53	7 (26%)	24,52,52	2.51	4 (16%)
2	AGS	F	901	3	26,33,33	1.51	7 (26%)	24,52,52	2.52	3 (12%)
2	AGS	F	902	3	26,33,33	1.54	7 (26%)	24,52,52	2.51	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	AGS	A	901	3	-	0/17/38/38	0/3/3/3
2	AGS	A	902	3	-	0/17/38/38	0/3/3/3
2	AGS	B	901	3	-	0/17/38/38	0/3/3/3
2	AGS	B	902	3	-	0/17/38/38	0/3/3/3
2	AGS	C	901	3	-	0/17/38/38	0/3/3/3
2	AGS	C	902	3	-	0/17/38/38	0/3/3/3
2	AGS	D	901	3	-	0/17/38/38	0/3/3/3
2	AGS	D	902	3	-	0/17/38/38	0/3/3/3
2	AGS	E	901	3	-	0/17/38/38	0/3/3/3
2	AGS	E	902	3	-	0/17/38/38	0/3/3/3
2	AGS	F	901	3	-	0/17/38/38	0/3/3/3
2	AGS	F	902	3	-	0/17/38/38	0/3/3/3

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	AGS	C2'-C1'	-3.47	1.48	1.53
2	B	902	AGS	C2'-C1'	-3.39	1.48	1.53
2	D	902	AGS	C2'-C1'	-3.38	1.48	1.53
2	F	902	AGS	C2'-C1'	-3.28	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	902	AGS	C2'-C1'	-3.28	1.48	1.53
2	B	901	AGS	C2'-C1'	-3.16	1.48	1.53
2	C	902	AGS	C2'-C1'	-3.08	1.48	1.53
2	A	901	AGS	C2'-C1'	-3.06	1.48	1.53
2	C	901	AGS	C2'-C1'	-3.03	1.48	1.53
2	F	901	AGS	C2'-C1'	-3.02	1.48	1.53
2	E	901	AGS	C2'-C1'	-2.96	1.48	1.53
2	D	901	AGS	C2'-C1'	-2.81	1.49	1.53
2	B	902	AGS	C2'-C3'	-2.62	1.46	1.53
2	C	902	AGS	C2'-C3'	-2.61	1.46	1.53
2	F	901	AGS	C2'-C3'	-2.61	1.46	1.53
2	A	901	AGS	C2'-C3'	-2.58	1.46	1.53
2	A	902	AGS	C2'-C3'	-2.53	1.46	1.53
2	F	902	AGS	C2'-C3'	-2.51	1.46	1.53
2	B	901	AGS	C2'-C3'	-2.50	1.46	1.53
2	D	902	AGS	C2'-C3'	-2.50	1.46	1.53
2	D	901	AGS	C2'-C3'	-2.46	1.46	1.53
2	E	902	AGS	C2'-C3'	-2.41	1.46	1.53
2	B	901	AGS	O4'-C4'	-2.40	1.39	1.45
2	C	901	AGS	C2'-C3'	-2.38	1.47	1.53
2	E	901	AGS	C2'-C3'	-2.34	1.47	1.53
2	C	902	AGS	O4'-C4'	-2.33	1.39	1.45
2	D	901	AGS	O4'-C4'	-2.31	1.39	1.45
2	E	902	AGS	O4'-C4'	-2.31	1.39	1.45
2	F	902	AGS	O4'-C4'	-2.30	1.39	1.45
2	F	901	AGS	O4'-C4'	-2.29	1.39	1.45
2	E	901	AGS	O4'-C4'	-2.29	1.39	1.45
2	C	901	AGS	O4'-C4'	-2.28	1.39	1.45
2	A	901	AGS	O2'-C2'	-2.28	1.37	1.43
2	D	902	AGS	O4'-C4'	-2.27	1.39	1.45
2	A	902	AGS	O4'-C4'	-2.24	1.39	1.45
2	A	901	AGS	O4'-C4'	-2.23	1.39	1.45
2	B	902	AGS	O2'-C2'	-2.21	1.37	1.43
2	D	902	AGS	O3'-C3'	-2.20	1.37	1.43
2	B	902	AGS	O4'-C4'	-2.18	1.40	1.45
2	F	901	AGS	O2'-C2'	-2.15	1.37	1.43
2	D	902	AGS	O2'-C2'	-2.15	1.37	1.43
2	C	901	AGS	O2'-C2'	-2.15	1.37	1.43
2	B	902	AGS	O3'-C3'	-2.15	1.37	1.43
2	B	901	AGS	O2'-C2'	-2.15	1.37	1.43
2	B	901	AGS	O3'-C3'	-2.13	1.37	1.43
2	F	901	AGS	O3'-C3'	-2.13	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	AGS	O2'-C2'	-2.13	1.37	1.43
2	A	902	AGS	O3'-C3'	-2.13	1.37	1.43
2	C	901	AGS	O3'-C3'	-2.12	1.38	1.43
2	A	901	AGS	O3'-C3'	-2.11	1.38	1.43
2	E	902	AGS	O2'-C2'	-2.11	1.38	1.43
2	F	902	AGS	O2'-C2'	-2.11	1.38	1.43
2	C	902	AGS	O2'-C2'	-2.10	1.38	1.43
2	E	901	AGS	O3'-C3'	-2.10	1.38	1.43
2	D	901	AGS	O2'-C2'	-2.10	1.38	1.43
2	A	902	AGS	O2'-C2'	-2.09	1.38	1.43
2	E	902	AGS	O3'-C3'	-2.09	1.38	1.43
2	C	902	AGS	O3'-C3'	-2.08	1.38	1.43
2	F	902	AGS	O3'-C3'	-2.07	1.38	1.43
2	D	901	AGS	O3'-C3'	-2.06	1.38	1.43
2	E	902	AGS	C6-N6	2.26	1.43	1.34
2	D	901	AGS	C6-N6	2.26	1.43	1.34
2	F	902	AGS	C6-N6	2.26	1.43	1.34
2	C	902	AGS	C6-N6	2.27	1.43	1.34
2	D	902	AGS	C6-N6	2.27	1.43	1.34
2	B	902	AGS	C6-N6	2.27	1.43	1.34
2	B	901	AGS	C6-N6	2.27	1.43	1.34
2	F	901	AGS	C6-N6	2.27	1.43	1.34
2	E	901	AGS	C6-N6	2.27	1.43	1.34
2	A	901	AGS	C6-N6	2.28	1.43	1.34
2	A	902	AGS	C6-N6	2.29	1.43	1.34
2	C	901	AGS	C6-N6	2.31	1.43	1.34
2	A	901	AGS	PG-S1G	2.47	1.95	1.90
2	E	901	AGS	PG-S1G	2.49	1.95	1.90
2	F	901	AGS	PG-S1G	2.53	1.95	1.90
2	C	901	AGS	PG-S1G	2.55	1.95	1.90
2	E	902	AGS	PG-S1G	2.57	1.95	1.90
2	A	902	AGS	PG-S1G	2.57	1.95	1.90
2	D	901	AGS	PG-S1G	2.58	1.95	1.90
2	C	902	AGS	PG-S1G	2.60	1.95	1.90
2	F	902	AGS	PG-S1G	2.61	1.95	1.90
2	D	902	AGS	PG-S1G	2.61	1.95	1.90
2	B	902	AGS	PG-S1G	2.63	1.95	1.90
2	B	901	AGS	PG-S1G	2.66	1.95	1.90

All (33) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	901	AGS	N3-C2-N1	-11.36	119.94	128.87
2	C	902	AGS	N3-C2-N1	-11.30	120.00	128.87
2	E	901	AGS	N3-C2-N1	-11.29	120.00	128.87
2	D	902	AGS	N3-C2-N1	-11.28	120.01	128.87
2	A	901	AGS	N3-C2-N1	-11.22	120.06	128.87
2	B	901	AGS	N3-C2-N1	-11.20	120.07	128.87
2	B	902	AGS	N3-C2-N1	-11.16	120.11	128.87
2	F	902	AGS	N3-C2-N1	-11.15	120.11	128.87
2	D	901	AGS	N3-C2-N1	-11.15	120.11	128.87
2	A	902	AGS	N3-C2-N1	-11.13	120.13	128.87
2	E	902	AGS	N3-C2-N1	-11.09	120.16	128.87
2	C	901	AGS	N3-C2-N1	-11.09	120.16	128.87
2	A	902	AGS	PB-O3B-PG	-3.64	119.49	132.71
2	D	902	AGS	PB-O3B-PG	-3.31	120.70	132.71
2	F	902	AGS	PB-O3B-PG	-3.13	121.37	132.71
2	E	902	AGS	PB-O3B-PG	-3.02	121.74	132.71
2	C	902	AGS	PB-O3B-PG	-2.93	122.08	132.71
2	A	901	AGS	PB-O3B-PG	-2.84	122.42	132.71
2	C	902	AGS	C4'-O4'-C1'	-2.73	106.75	109.64
2	C	901	AGS	PB-O3B-PG	-2.47	123.75	132.71
2	B	902	AGS	C4'-O4'-C1'	-2.46	107.03	109.64
2	B	902	AGS	PB-O3B-PG	-2.46	123.78	132.71
2	E	901	AGS	PB-O3B-PG	-2.38	124.07	132.71
2	B	901	AGS	PB-O3B-PG	-2.35	124.18	132.71
2	E	902	AGS	C4'-O4'-C1'	-2.29	107.22	109.64
2	D	901	AGS	PB-O3B-PG	-2.14	124.96	132.71
2	F	901	AGS	PB-O3B-PG	-2.13	124.97	132.71
2	A	902	AGS	C4'-O4'-C1'	-2.11	107.40	109.64
2	F	901	AGS	C4'-O4'-C1'	-2.04	107.48	109.64
2	E	902	AGS	O4'-C4'-C3'	2.06	109.34	105.16
2	E	901	AGS	O4'-C4'-C3'	2.07	109.35	105.16
2	C	901	AGS	O4'-C4'-C3'	2.22	109.66	105.16
2	A	901	AGS	O4'-C4'-C3'	2.22	109.67	105.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AGS	1	0
2	A	902	AGS	1	0
2	B	901	AGS	2	0
2	B	902	AGS	1	0
2	E	902	AGS	2	0
2	F	902	AGS	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	722/785 (91%)	0.94	112 (15%) 3 2	53, 121, 220, 294	0
1	B	723/785 (92%)	0.55	42 (5%) 26 21	53, 108, 176, 299	0
1	C	724/785 (92%)	0.60	69 (9%) 10 9	42, 113, 191, 278	0
1	D	722/785 (91%)	0.83	108 (14%) 3 2	53, 135, 220, 266	0
1	E	723/785 (92%)	0.59	51 (7%) 19 15	63, 113, 181, 272	0
1	F	724/785 (92%)	0.93	113 (15%) 3 2	47, 122, 233, 304	0
All	All	4338/4710 (92%)	0.74	495 (11%) 7 5	42, 117, 213, 304	0

All (495) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	116	VAL	12.1
1	F	24	ASN	9.8
1	F	114	ILE	8.9
1	F	102	ILE	7.5
1	D	46	MET	7.5
1	A	435	GLU	7.1
1	A	117	LEU	7.1
1	D	26	LEU	7.0
1	A	23	PRO	6.9
1	F	164	LYS	6.9
1	F	174	CYS	6.7
1	A	21	ASN	6.4
1	D	173	TYR	6.4
1	D	41	LEU	6.2
1	D	40	SER	6.1
1	F	117	LEU	6.0
1	F	76	THR	6.0
1	A	134	TYR	5.8
1	A	114	ILE	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	71	VAL	5.7
1	C	23	PRO	5.6
1	D	21	ASN	5.6
1	E	317	HIS	5.4
1	F	166	VAL	5.4
1	A	174	CYS	5.4
1	A	26	LEU	5.4
1	A	53	ARG	5.3
1	B	552	PHE	5.3
1	D	43	GLN	5.2
1	A	175	ILE	5.2
1	F	134	TYR	5.2
1	F	103	GLN	5.1
1	D	57	VAL	5.1
1	A	390	LEU	5.1
1	F	41	LEU	5.1
1	D	116	VAL	5.1
1	F	589	ASN	5.0
1	F	173	TYR	5.0
1	C	21	ASN	5.0
1	D	25	ARG	4.9
1	D	53	ARG	4.9
1	A	47	ASP	4.9
1	D	162	GLU	4.8
1	B	445	LEU	4.8
1	F	111	GLY	4.8
1	F	52	PHE	4.8
1	F	194	GLU	4.8
1	D	114	ILE	4.8
1	D	24	ASN	4.7
1	A	116	VAL	4.7
1	F	94	VAL	4.7
1	F	183	HIS	4.7
1	F	707	ILE	4.6
1	D	94	VAL	4.6
1	A	433	GLU	4.6
1	F	21	ASN	4.6
1	B	21	ASN	4.6
1	F	115	HIS	4.6
1	D	188	PRO	4.6
1	F	43	GLN	4.5
1	D	117	LEU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	26	LEU	4.4
1	A	703	ILE	4.4
1	E	72	LEU	4.4
1	D	672	LEU	4.4
1	D	165	VAL	4.4
1	F	182	ILE	4.3
1	B	102	ILE	4.3
1	B	44	PRO	4.3
1	A	186	GLY	4.3
1	F	44	PRO	4.3
1	D	47	ASP	4.3
1	D	442	MET	4.3
1	A	44	PRO	4.2
1	C	694	ALA	4.2
1	D	69	CYS	4.2
1	F	187	GLU	4.2
1	D	194	GLU	4.2
1	E	433	GLU	4.2
1	F	113	ARG	4.1
1	D	118	PRO	4.1
1	D	708	ARG	4.1
1	C	73	SER	4.1
1	C	699	ILE	4.1
1	D	23	PRO	4.1
1	A	130	LEU	4.1
1	A	729	PRO	4.0
1	D	187	GLU	4.0
1	A	182	ILE	4.0
1	C	72	LEU	4.0
1	D	52	PHE	4.0
1	A	436	THR	4.0
1	F	175	ILE	4.0
1	D	56	THR	4.0
1	C	43	GLN	4.0
1	E	50	GLN	4.0
1	C	666	VAL	4.0
1	A	316	THR	4.0
1	A	702	SER	3.9
1	F	172	PRO	3.9
1	F	128	GLY	3.9
1	A	735	HIS	3.9
1	B	551	TRP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	480	GLY	3.9
1	A	72	LEU	3.8
1	F	452	PHE	3.8
1	A	187	GLU	3.8
1	A	731	ILE	3.8
1	D	163	PHE	3.8
1	C	697	LEU	3.8
1	F	109	LYS	3.8
1	C	702	SER	3.8
1	F	179	ASP	3.7
1	A	41	LEU	3.7
1	B	47	ASP	3.7
1	C	672	LEU	3.7
1	D	164	LYS	3.7
1	F	63	LYS	3.7
1	A	57	VAL	3.7
1	F	40	SER	3.7
1	D	439	ALA	3.7
1	D	182	ILE	3.7
1	D	502	LYS	3.7
1	F	77	CYS	3.6
1	A	185	GLU	3.6
1	A	25	ARG	3.6
1	E	49	LEU	3.6
1	A	102	ILE	3.6
1	D	731	ILE	3.6
1	D	51	LEU	3.6
1	D	150	ASP	3.6
1	D	104	PRO	3.6
1	B	502	LYS	3.6
1	B	506	PHE	3.6
1	D	82	ILE	3.6
1	E	731	ILE	3.6
1	D	316	THR	3.6
1	F	57	VAL	3.5
1	F	82	ILE	3.5
1	A	434	ASP	3.5
1	A	50	GLN	3.5
1	A	188	PRO	3.5
1	E	126	ILE	3.5
1	C	703	ILE	3.5
1	C	81	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	731	ILE	3.5
1	A	127	THR	3.5
1	E	435	GLU	3.5
1	F	165	VAL	3.5
1	C	44	PRO	3.5
1	E	26	LEU	3.5
1	A	705	SER	3.5
1	F	23	PRO	3.5
1	F	73	SER	3.5
1	D	55	ASP	3.4
1	D	129	ASN	3.4
1	F	48	GLU	3.4
1	F	434	ASP	3.4
1	A	40	SER	3.4
1	E	64	ARG	3.4
1	D	191	ARG	3.4
1	A	52	PHE	3.4
1	D	73	SER	3.4
1	C	736	PHE	3.4
1	E	447	VAL	3.4
1	F	71	VAL	3.4
1	A	736	PHE	3.4
1	E	44	PRO	3.3
1	C	428	ASP	3.3
1	D	100	ILE	3.3
1	E	434	ASP	3.3
1	F	167	GLU	3.3
1	F	612	SER	3.3
1	A	176	VAL	3.3
1	F	26	LEU	3.3
1	D	102	ILE	3.3
1	F	170	PRO	3.3
1	A	446	ALA	3.3
1	D	495	TYR	3.3
1	A	389	LYS	3.3
1	A	184	CYS	3.3
1	C	682	PHE	3.3
1	E	552	PHE	3.3
1	F	316	THR	3.3
1	A	708	ARG	3.2
1	F	50	GLN	3.2
1	C	552	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	43	GLN	3.2
1	C	705	SER	3.2
1	D	189	ILE	3.2
1	C	42	SER	3.2
1	D	153	LEU	3.2
1	A	501	ASP	3.2
1	B	337	GLN	3.2
1	D	99	VAL	3.2
1	F	233	ILE	3.2
1	F	62	LYS	3.2
1	A	145	PRO	3.2
1	C	708	ARG	3.1
1	D	50	GLN	3.1
1	F	75	ASP	3.1
1	A	699	ILE	3.1
1	A	113	ARG	3.1
1	A	82	ILE	3.1
1	E	81	LYS	3.1
1	D	131	PHE	3.1
1	A	183	HIS	3.1
1	D	172	PRO	3.1
1	A	193	ASP	3.1
1	E	43	GLN	3.1
1	D	193	ASP	3.1
1	A	707	ILE	3.1
1	F	100	ILE	3.0
1	A	506	PHE	3.0
1	B	134	TYR	3.0
1	F	426	LYS	3.0
1	A	432	LEU	3.0
1	C	675	LEU	3.0
1	F	78	SER	3.0
1	A	100	ILE	3.0
1	C	698	ALA	3.0
1	C	695	CYS	3.0
1	D	119	ILE	3.0
1	D	426	LYS	3.0
1	E	747	VAL	2.9
1	C	706	GLU	2.9
1	B	230	PHE	2.9
1	E	439	ALA	2.9
1	A	162	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	2.9
1	F	231	LYS	2.9
1	F	47	ASP	2.9
1	D	499	HIS	2.9
1	F	443	ASN	2.9
1	C	143	TYR	2.9
1	D	78	SER	2.9
1	C	71	VAL	2.9
1	C	41	LEU	2.9
1	C	707	ILE	2.9
1	F	322	ARG	2.9
1	B	41	LEU	2.9
1	B	105	CYS	2.9
1	D	92	LEU	2.9
1	B	446	ALA	2.9
1	F	148	LYS	2.9
1	A	104	PRO	2.9
1	D	161	VAL	2.8
1	F	46	MET	2.8
1	C	735	HIS	2.8
1	A	439	ALA	2.8
1	F	393	ASP	2.8
1	A	64	ARG	2.8
1	F	168	THR	2.8
1	F	176	VAL	2.8
1	C	472	PRO	2.8
1	F	70	ILE	2.8
1	A	103	GLN	2.8
1	C	670	VAL	2.8
1	C	668	LYS	2.8
1	D	28	VAL	2.8
1	D	147	ARG	2.8
1	D	503	PHE	2.8
1	D	166	VAL	2.8
1	A	428	ASP	2.7
1	A	161	VAL	2.7
1	D	176	VAL	2.7
1	F	123	VAL	2.7
1	C	82	ILE	2.7
1	C	100	ILE	2.7
1	D	452	PHE	2.7
1	A	22	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	131	PHE	2.7
1	F	706	GLU	2.7
1	F	104	PRO	2.7
1	F	232	ALA	2.7
1	C	25	ARG	2.7
1	B	554	GLU	2.7
1	B	126	ILE	2.7
1	A	151	ILE	2.7
1	C	182	ILE	2.7
1	A	83	ARG	2.6
1	E	452	PHE	2.6
1	B	672	LEU	2.6
1	B	553	GLY	2.6
1	C	51	LEU	2.6
1	E	551	TRP	2.6
1	E	99	VAL	2.6
1	E	45	LYS	2.6
1	E	682	PHE	2.6
1	F	25	ARG	2.6
1	F	150	ASP	2.6
1	C	596	ALA	2.6
1	E	232	ALA	2.6
1	A	51	LEU	2.6
1	C	429	LEU	2.6
1	C	50	GLN	2.6
1	C	669	ASP	2.6
1	F	439	ALA	2.6
1	A	706	GLU	2.6
1	B	503	PHE	2.6
1	D	123	VAL	2.6
1	E	520	PRO	2.6
1	D	93	ARG	2.6
1	E	730	GLU	2.5
1	C	696	LYS	2.5
1	A	388	MET	2.5
1	D	132	GLU	2.5
1	A	237	PRO	2.5
1	F	729	PRO	2.5
1	C	667	ALA	2.5
1	A	502	LYS	2.5
1	B	58	LEU	2.5
1	E	322	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	315	LYS	2.5
1	D	44	PRO	2.5
1	E	672	LEU	2.5
1	A	694	ALA	2.5
1	B	28	VAL	2.5
1	A	504	LEU	2.5
1	E	522	CYS	2.5
1	D	498	GLU	2.5
1	C	47	ASP	2.5
1	D	79	ASP	2.5
1	E	21	ASN	2.5
1	E	130	LEU	2.5
1	E	687	LEU	2.4
1	F	112	LYS	2.4
1	D	446	ALA	2.4
1	D	113	ARG	2.4
1	A	160	ALA	2.4
1	A	267	PHE	2.4
1	F	703	ILE	2.4
1	A	500	PRO	2.4
1	A	234	GLY	2.4
1	E	51	LEU	2.4
1	F	147	ARG	2.4
1	B	340	HIS	2.4
1	E	47	ASP	2.4
1	D	29	ASP	2.4
1	A	92	LEU	2.4
1	A	46	MET	2.4
1	A	131	PHE	2.4
1	A	552	PHE	2.4
1	B	82	ILE	2.4
1	E	707	ILE	2.4
1	F	193	ASP	2.4
1	A	157	GLY	2.4
1	B	24	ASN	2.4
1	E	436	THR	2.4
1	F	428	ASP	2.4
1	F	99	VAL	2.4
1	E	158	MET	2.4
1	A	119	ILE	2.4
1	B	613	THR	2.4
1	E	316	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	701	GLU	2.4
1	E	186	GLY	2.3
1	D	48	GLU	2.3
1	F	433	GLU	2.3
1	C	597	ALA	2.3
1	C	739	ALA	2.3
1	E	588	GLY	2.3
1	D	39	VAL	2.3
1	F	79	ASP	2.3
1	B	612	SER	2.3
1	F	83	ARG	2.3
1	F	495	TYR	2.3
1	B	435	GLU	2.3
1	C	390	LEU	2.3
1	A	48	GLU	2.3
1	E	48	GLU	2.3
1	F	127	THR	2.3
1	E	42	SER	2.3
1	D	404	HIS	2.3
1	F	55	ASP	2.3
1	F	97	GLY	2.3
1	F	192	GLU	2.3
1	B	198	LEU	2.3
1	C	446	ALA	2.3
1	E	127	THR	2.3
1	A	164	LYS	2.3
1	C	101	SER	2.3
1	A	396	LEU	2.3
1	B	232	ALA	2.3
1	F	188	PRO	2.3
1	A	695	CYS	2.3
1	B	114	ILE	2.3
1	A	59	LEU	2.3
1	F	53	ARG	2.3
1	A	394	VAL	2.3
1	C	340	HIS	2.3
1	A	84	MET	2.3
1	B	390	LEU	2.3
1	E	119	ILE	2.3
1	F	110	TYR	2.3
1	F	171	SER	2.2
1	B	434	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	27	ILE	2.2
1	A	39	VAL	2.2
1	D	196	GLU	2.2
1	D	435	GLU	2.2
1	A	101	SER	2.2
1	D	130	LEU	2.2
1	F	429	LEU	2.2
1	C	46	MET	2.2
1	D	699	ILE	2.2
1	F	133	VAL	2.2
1	A	704	GLU	2.2
1	D	151	ILE	2.2
1	E	503	PHE	2.2
1	F	154	VAL	2.2
1	F	155	ARG	2.2
1	D	436	THR	2.2
1	F	199	ASN	2.2
1	D	62	LYS	2.2
1	D	186	GLY	2.2
1	C	60	LYS	2.2
1	F	81	LYS	2.2
1	A	73	SER	2.2
1	A	135	LEU	2.2
1	D	705	SER	2.2
1	A	447	VAL	2.2
1	A	730	GLU	2.2
1	B	433	GLU	2.2
1	A	696	LYS	2.2
1	D	144	ARG	2.2
1	F	126	ILE	2.2
1	A	336	LYS	2.2
1	C	767	GLY	2.2
1	D	45	LYS	2.2
1	A	503	PHE	2.1
1	A	141	GLU	2.1
1	D	126	ILE	2.1
1	F	190	LYS	2.1
1	F	266	PHE	2.1
1	D	152	PHE	2.1
1	C	435	GLU	2.1
1	F	321	GLU	2.1
1	D	84	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	768	PHE	2.1
1	E	736	PHE	2.1
1	F	143	TYR	2.1
1	D	49	LEU	2.1
1	F	163	PHE	2.1
1	D	115	HIS	2.1
1	D	443	ASN	2.1
1	D	479	ILE	2.1
1	D	666	VAL	2.1
1	A	443	ASN	2.1
1	C	663	LYS	2.1
1	D	139	PHE	2.1
1	B	439	ALA	2.1
1	D	179	ASP	2.1
1	B	479	ILE	2.1
1	B	499	HIS	2.1
1	D	72	LEU	2.1
1	C	768	PHE	2.1
1	F	80	GLU	2.1
1	D	81	LYS	2.1
1	D	428	ASP	2.1
1	C	588	GLY	2.1
1	B	36	ASN	2.1
1	E	768	PHE	2.1
1	C	613	THR	2.1
1	E	612	SER	2.1
1	A	442	MET	2.1
1	F	320	VAL	2.1
1	E	102	ILE	2.1
1	E	494	GLN	2.0
1	A	132	GLU	2.0
1	D	195	GLU	2.0
1	F	42	SER	2.0
1	F	317	HIS	2.0
1	A	510	PRO	2.0
1	B	96	LEU	2.0
1	C	199	ASN	2.0
1	D	679	THR	2.0
1	E	59	LEU	2.0
1	B	753	ARG	2.0
1	A	431	ASP	2.0
1	A	698	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	599	ARG	2.0
1	C	769	GLY	2.0
1	B	734	ASP	2.0
1	C	734	ASP	2.0
1	A	391	ALA	2.0
1	F	118	PRO	2.0
1	C	24	ASN	2.0
1	C	704	GLU	2.0
1	B	428	ASP	2.0
1	C	28	VAL	2.0
1	F	51	LEU	2.0
1	F	708	ARG	2.0
1	F	704	GLU	2.0
1	C	661	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
4	CL	F	905	1/1	0.86	0.31	0.49	98,98,98,98	0
4	CL	E	905	1/1	0.89	0.28	0.46	93,93,93,93	0
2	AGS	A	901	31/31	0.95	0.27	0.27	75,86,104,117	0
2	AGS	F	901	31/31	0.95	0.24	-0.34	47,61,80,93	0
4	CL	A	905	1/1	0.91	0.27	-0.35	87,87,87,87	0
2	AGS	A	902	31/31	0.96	0.26	-0.42	73,90,154,194	0
2	AGS	B	901	31/31	0.94	0.24	-0.45	57,88,112,122	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	AGS	E	901	31/31	0.91	0.26	-0.51	76,88,120,170	0
2	AGS	D	901	31/31	0.94	0.24	-0.52	70,99,121,158	0
4	CL	B	905	1/1	0.88	0.23	-0.62	92,92,92,92	0
4	CL	D	905	1/1	0.88	0.24	-0.66	99,99,99,99	0
2	AGS	F	902	31/31	0.95	0.24	-0.75	88,102,133,210	0
2	AGS	D	902	31/31	0.95	0.21	-0.85	68,82,106,169	0
2	AGS	C	902	31/31	0.96	0.26	-0.89	59,76,122,189	0
2	AGS	C	901	31/31	0.94	0.20	-0.97	59,100,122,152	0
2	AGS	E	902	31/31	0.96	0.20	-1.09	75,89,127,165	0
4	CL	C	905	1/1	0.86	0.19	-1.19	117,117,117,117	0
2	AGS	B	902	31/31	0.97	0.23	-1.21	55,79,132,182	0
3	MG	E	903	1/1	0.97	0.14	-1.81	81,81,81,81	0
3	MG	D	904	1/1	0.95	0.31	-	99,99,99,99	0
3	MG	C	904	1/1	0.97	0.22	-	107,107,107,107	0
3	MG	C	903	1/1	0.98	0.23	-	101,101,101,101	0
3	MG	A	903	1/1	0.94	0.12	-	186,186,186,186	0
3	MG	F	904	1/1	0.96	0.27	-	76,76,76,76	0
3	MG	A	904	1/1	0.97	0.23	-	76,76,76,76	0
3	MG	F	903	1/1	0.96	0.16	-	152,152,152,152	0
3	MG	B	903	1/1	0.98	0.17	-	119,119,119,119	0
3	MG	D	903	1/1	0.85	0.13	-	170,170,170,170	0
3	MG	B	904	1/1	0.98	0.22	-	86,86,86,86	0
3	MG	E	904	1/1	0.98	0.26	-	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.