



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:36 PM GMT

PDB ID : 4KLN
Title : Structure of p97 N-D1 A232E mutant in complex with ATPgS
Authors : Xia, D.; Tang, W.K.
Deposited on : 2013-05-07
Resolution : 2.62 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

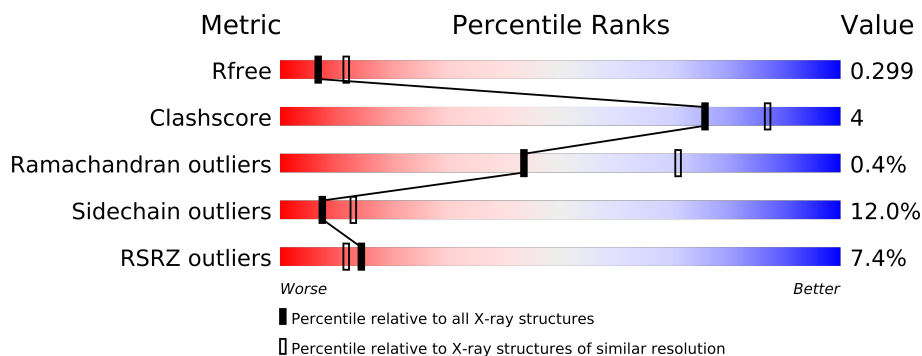
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.62 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}	66092	1940 (2.64-2.60)
Clashscore	79885	2404 (2.64-2.60)
Ramachandran outliers	78287	2360 (2.64-2.60)
Sidechain outliers	78261	2360 (2.64-2.60)
RSRZ outliers	66119	1939 (2.64-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	489	
1	B	489	
1	C	489	
1	D	489	
1	E	489	
1	F	489	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21556 atoms, of which 0 are hydrogen and 0 are deuterium.

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	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	B	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	C	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	D	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	E	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	F	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			

There are 54 discrepancies between the modelled and reference sequences:

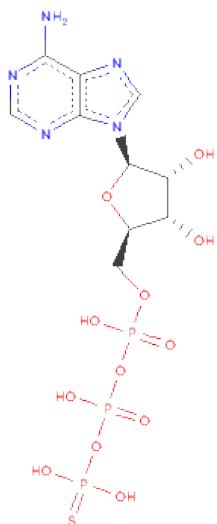
Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLU	ALA	ENGINEERED MUTATION	UNP P55072
A	482	ARG	-	EXPRESSION TAG	UNP P55072
A	483	SER	-	EXPRESSION TAG	UNP P55072
A	484	HIS	-	EXPRESSION TAG	UNP P55072
A	485	HIS	-	EXPRESSION TAG	UNP P55072
A	486	HIS	-	EXPRESSION TAG	UNP P55072
A	487	HIS	-	EXPRESSION TAG	UNP P55072
A	488	HIS	-	EXPRESSION TAG	UNP P55072
A	489	HIS	-	EXPRESSION TAG	UNP P55072
B	232	GLU	ALA	ENGINEERED MUTATION	UNP P55072
B	482	ARG	-	EXPRESSION TAG	UNP P55072
B	483	SER	-	EXPRESSION TAG	UNP P55072
B	484	HIS	-	EXPRESSION TAG	UNP P55072
B	485	HIS	-	EXPRESSION TAG	UNP P55072
B	486	HIS	-	EXPRESSION TAG	UNP P55072
B	487	HIS	-	EXPRESSION TAG	UNP P55072
B	488	HIS	-	EXPRESSION TAG	UNP P55072

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	489	HIS	-	EXPRESSION TAG	UNP P55072
C	232	GLU	ALA	ENGINEERED MUTATION	UNP P55072
C	482	ARG	-	EXPRESSION TAG	UNP P55072
C	483	SER	-	EXPRESSION TAG	UNP P55072
C	484	HIS	-	EXPRESSION TAG	UNP P55072
C	485	HIS	-	EXPRESSION TAG	UNP P55072
C	486	HIS	-	EXPRESSION TAG	UNP P55072
C	487	HIS	-	EXPRESSION TAG	UNP P55072
C	488	HIS	-	EXPRESSION TAG	UNP P55072
C	489	HIS	-	EXPRESSION TAG	UNP P55072
D	232	GLU	ALA	ENGINEERED MUTATION	UNP P55072
D	482	ARG	-	EXPRESSION TAG	UNP P55072
D	483	SER	-	EXPRESSION TAG	UNP P55072
D	484	HIS	-	EXPRESSION TAG	UNP P55072
D	485	HIS	-	EXPRESSION TAG	UNP P55072
D	486	HIS	-	EXPRESSION TAG	UNP P55072
D	487	HIS	-	EXPRESSION TAG	UNP P55072
D	488	HIS	-	EXPRESSION TAG	UNP P55072
D	489	HIS	-	EXPRESSION TAG	UNP P55072
E	232	GLU	ALA	ENGINEERED MUTATION	UNP P55072
E	482	ARG	-	EXPRESSION TAG	UNP P55072
E	483	SER	-	EXPRESSION TAG	UNP P55072
E	484	HIS	-	EXPRESSION TAG	UNP P55072
E	485	HIS	-	EXPRESSION TAG	UNP P55072
E	486	HIS	-	EXPRESSION TAG	UNP P55072
E	487	HIS	-	EXPRESSION TAG	UNP P55072
E	488	HIS	-	EXPRESSION TAG	UNP P55072
E	489	HIS	-	EXPRESSION TAG	UNP P55072
F	232	GLU	ALA	ENGINEERED MUTATION	UNP P55072
F	482	ARG	-	EXPRESSION TAG	UNP P55072
F	483	SER	-	EXPRESSION TAG	UNP P55072
F	484	HIS	-	EXPRESSION TAG	UNP P55072
F	485	HIS	-	EXPRESSION TAG	UNP P55072
F	486	HIS	-	EXPRESSION TAG	UNP P55072
F	487	HIS	-	EXPRESSION TAG	UNP P55072
F	488	HIS	-	EXPRESSION TAG	UNP P55072
F	489	HIS	-	EXPRESSION TAG	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORICACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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

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

- Molecule 4 is water.

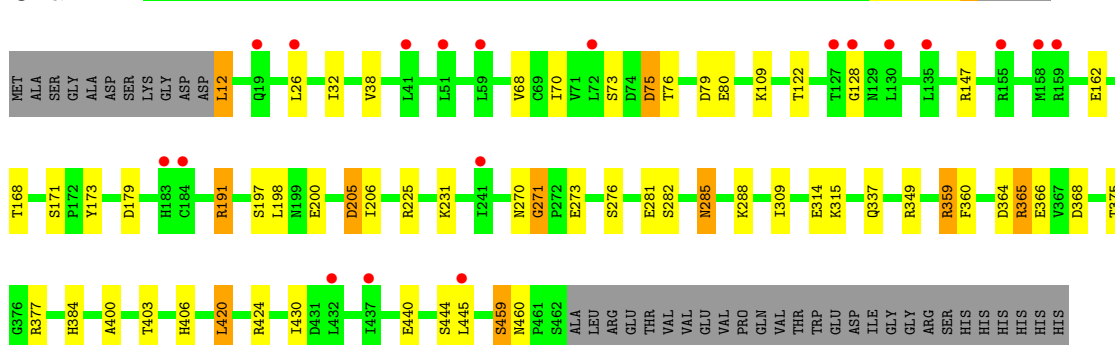
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	B	28	Total 28	O 28	0	0
4	C	30	Total 30	O 30	0	0
4	D	26	Total 26	O 26	0	0
4	E	25	Total 25	O 25	0	0
4	F	24	Total 24	O 24	0	0

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.

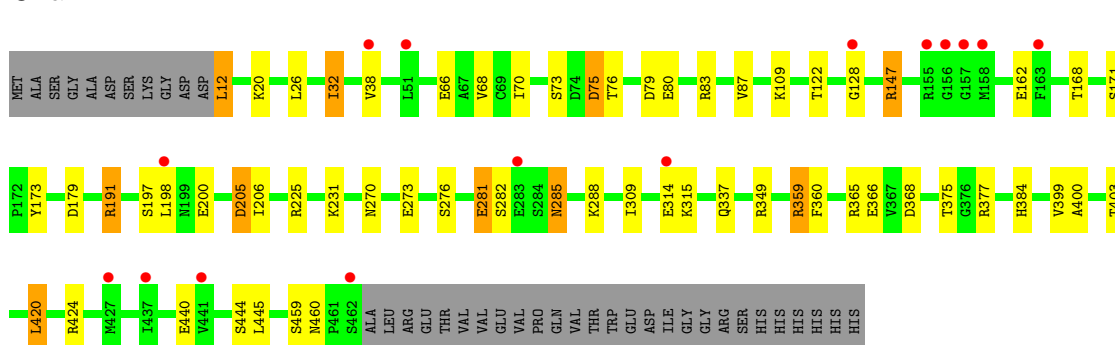
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain A:



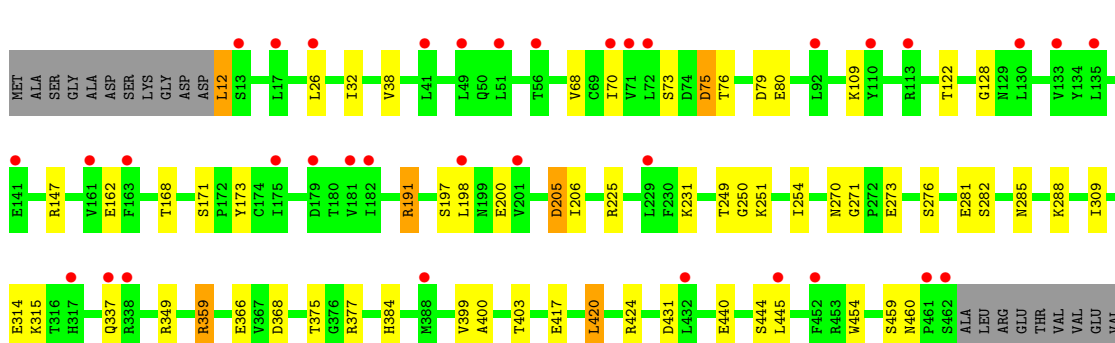
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B:



- Molecule 1: Transitional endoplasmic reticulum ATPase

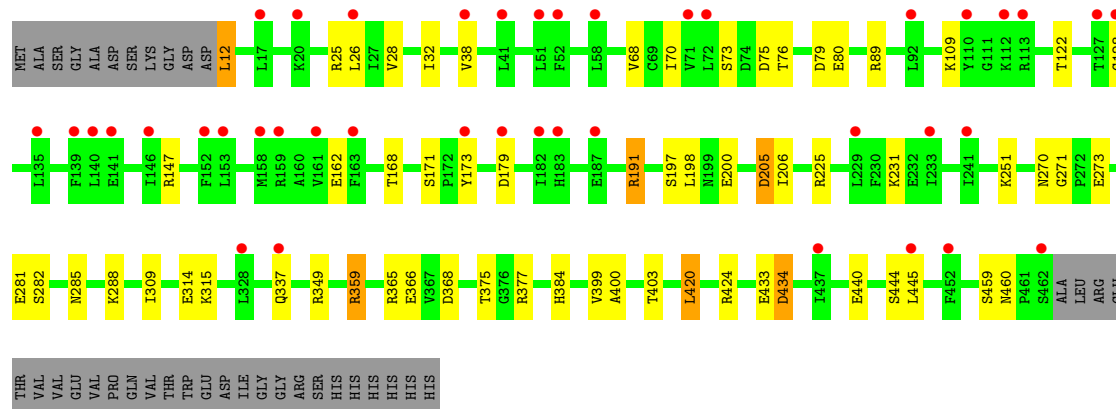
Chain C:



PRO
GLN
VAL
THR
TRP
GLU
ASP
ILE
GLY
GLY
ARG
SER
HIS
HIS
HIS
HIS
HIS

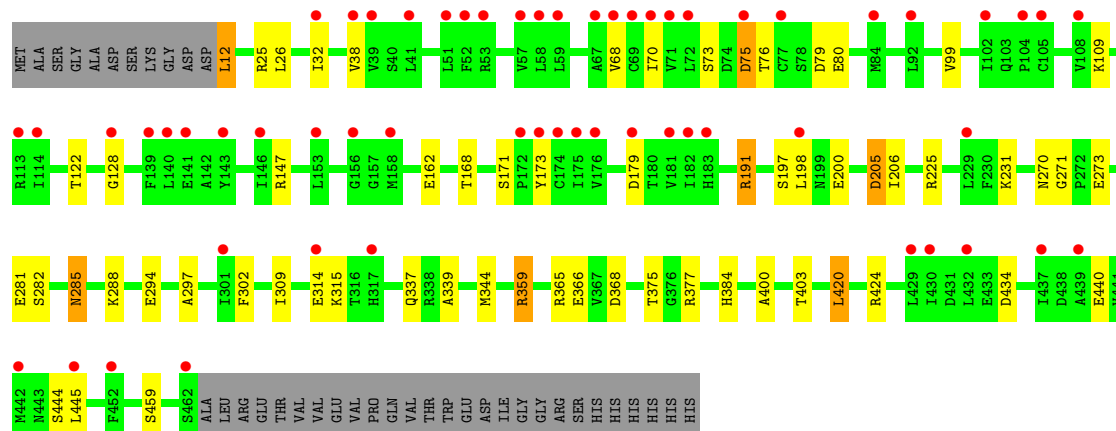
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



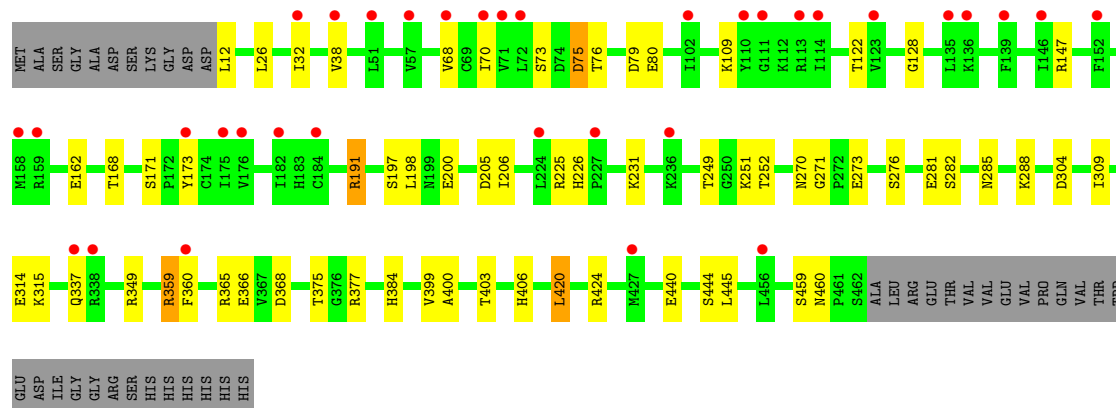
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.15Å 104.51Å 109.53Å 98.11° 90.55° 92.72°	Depositor
Resolution (Å)	46.29 – 2.62 46.24 – 2.62	Depositor EDS
% Data completeness (in resolution range)	83.1 (46.29-2.62) 83.2 (46.24-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.274 , 0.289 0.285 , 0.299	Depositor DCC
R_{free} test set	4959 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.8	EDS
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 99906 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21556	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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	0.29	0/3587	0.55	1/4846 (0.0%)
1	B	0.31	1/3587 (0.0%)	0.56	1/4846 (0.0%)
1	C	0.30	0/3587	0.55	1/4846 (0.0%)
1	D	0.29	0/3587	0.55	1/4846 (0.0%)
1	E	0.29	0/3587	0.55	1/4846 (0.0%)
1	F	0.31	0/3587	0.55	0/4846
All	All	0.30	1/21522 (0.0%)	0.55	5/29076 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	ASN	CG-OD1	-5.75	1.11	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	12	LEU	CA-CB-CG	5.21	127.28	115.30
1	E	12	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	12	LEU	CA-CB-CG	5.17	127.19	115.30
1	C	12	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3533	0	0	16	0
1	B	3533	0	0	15	0
1	C	3533	0	0	15	0
1	D	3533	0	0	16	0
1	E	3533	0	0	13	0
1	F	3533	0	0	13	0
2	A	31	0	12	2	0
2	B	31	0	12	1	0
2	C	31	0	12	2	0
2	D	31	0	12	3	0
2	E	31	0	12	1	0
2	F	31	0	12	2	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
4	A	33	0	0	0	0
4	B	28	0	0	0	0
4	C	30	0	0	0	0
4	D	26	0	0	3	0
4	E	25	0	0	0	0
4	F	24	0	0	0	0
All	All	21556	0	72	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (84) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:800:AGS:S1G	1:C:359:ARG:CG	2.55	0.95
2:E:800:AGS:S1G	1:F:359:ARG:CG	2.59	0.90
1:A:359:ARG:CG	2:F:800:AGS:S1G	2.63	0.87
1:C:399:VAL:O	1:C:403:THR:CG2	2.30	0.79
2:C:800:AGS:S1G	1:D:359:ARG:CG	2.73	0.77
2:A:800:AGS:S1G	1:B:359:ARG:CG	2.72	0.76
1:D:399:VAL:O	1:D:403:THR:CG2	2.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:377:ARG:CD	1:C:403:THR:OG1	2.38	0.70
2:D:800:AGS:S1G	1:E:359:ARG:CG	2.79	0.70
1:F:377:ARG:NH1	1:F:400:ALA:O	2.28	0.66
1:D:377:ARG:CD	1:D:403:THR:OG1	2.47	0.62
1:F:403:THR:O	1:F:406:HIS:ND1	2.34	0.60
1:B:281:GLU:O	1:B:285:ASN:ND2	2.36	0.59
1:A:377:ARG:NH1	1:A:400:ALA:O	2.38	0.56
1:F:252:THR:OG1	1:F:304:ASP:OD2	2.25	0.55
1:E:297:ALA:CB	1:E:339:ALA:O	2.57	0.53
1:B:377:ARG:NH1	1:B:400:ALA:O	2.43	0.52
1:D:377:ARG:NH1	1:D:400:ALA:O	2.43	0.52
1:F:270:ASN:O	1:F:273:GLU:N	2.43	0.51
1:C:377:ARG:NH1	1:C:400:ALA:O	2.44	0.51
1:F:399:VAL:O	1:F:403:THR:CG2	2.59	0.51
1:A:270:ASN:O	1:A:273:GLU:N	2.43	0.51
1:B:162:GLU:OE2	1:B:191:ARG:NH2	2.46	0.48
1:D:162:GLU:OE2	1:D:191:ARG:NH2	2.47	0.48
1:E:162:GLU:OE2	1:E:191:ARG:NH2	2.46	0.48
1:D:89:ARG:CD	4:D:917:HOH:O	2.62	0.48
1:C:162:GLU:OE2	1:C:191:ARG:NH2	2.47	0.48
1:C:270:ASN:O	1:C:273:GLU:N	2.47	0.48
1:D:270:ASN:O	1:D:273:GLU:N	2.47	0.48
1:C:249:THR:OG1	1:C:251:LYS:CE	2.62	0.47
1:B:377:ARG:CD	1:B:403:THR:OG1	2.63	0.47
1:B:32:ILE:CG2	1:B:83:ARG:NH1	2.76	0.47
1:A:360:PHE:CE1	2:F:800:AGS:H4'	2.50	0.47
1:A:162:GLU:OE2	1:A:191:ARG:NH2	2.46	0.47
1:F:162:GLU:OE2	1:F:191:ARG:NH2	2.48	0.47
1:D:28:VAL:CG2	4:D:917:HOH:O	2.63	0.47
1:D:251:LYS:NZ	2:D:800:AGS:O3G	2.48	0.47
1:E:377:ARG:CD	1:E:403:THR:OG1	2.63	0.47
1:B:270:ASN:O	1:B:273:GLU:N	2.47	0.46
1:A:420:LEU:O	1:A:424:ARG:N	2.48	0.46
1:A:430:ILE:O	1:B:20:LYS:NZ	2.49	0.46
1:E:270:ASN:O	1:E:273:GLU:N	2.49	0.46
1:F:420:LEU:O	1:F:424:ARG:N	2.49	0.46
1:E:377:ARG:NH1	1:E:400:ALA:O	2.50	0.45
1:E:420:LEU:O	1:E:424:ARG:N	2.50	0.45
1:F:249:THR:OG1	1:F:251:LYS:CE	2.64	0.45
1:D:434:ASP:N	1:D:434:ASP:OD1	2.50	0.45
1:A:360:PHE:CD1	1:A:360:PHE:C	2.90	0.45
1:A:273:GLU:O	1:A:276:SER:OG	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:431:ASP:OD2	1:D:25:ARG:NH2	2.49	0.44
1:C:251:LYS:CE	2:C:800:AGS:O2B	2.66	0.44
1:D:433:GLU:CG	1:E:25:ARG:NH2	2.81	0.43
1:E:302:PHE:CE2	1:E:344:MET:CE	3.01	0.43
2:A:800:AGS:H4'	1:B:360:PHE:CE1	2.54	0.43
1:F:273:GLU:O	1:F:276:SER:OG	2.36	0.43
1:A:364:ASP:O	1:A:365:ARG:CD	2.65	0.43
1:D:420:LEU:O	1:D:424:ARG:N	2.52	0.43
1:C:273:GLU:O	1:C:276:SER:OG	2.37	0.43
1:B:399:VAL:O	1:B:403:THR:CG2	2.67	0.42
1:B:273:GLU:O	1:B:276:SER:OG	2.37	0.42
1:A:205:ASP:OD1	1:A:205:ASP:N	2.52	0.42
1:C:205:ASP:N	1:C:205:ASP:OD1	2.52	0.42
1:E:285:ASN:ND2	1:E:285:ASN:N	2.68	0.42
1:E:205:ASP:OD1	1:E:205:ASP:N	2.53	0.42
1:B:66:GLU:OE1	1:B:147:ARG:NH1	2.52	0.42
1:D:251:LYS:CE	2:D:800:AGS:O2B	2.68	0.42
1:A:406:HIS:NE2	1:A:459:SER:OG	2.52	0.42
1:E:434:ASP:O	1:F:226:HIS:CE1	2.73	0.42
1:A:377:ARG:NE	1:A:403:THR:O	2.53	0.41
1:C:420:LEU:O	1:C:424:ARG:N	2.53	0.41
1:B:75:ASP:N	1:B:75:ASP:OD1	2.53	0.41
1:A:270:ASN:O	1:A:271:GLY:C	2.59	0.41
1:C:75:ASP:OD1	1:C:75:ASP:N	2.53	0.41
1:D:205:ASP:N	1:D:205:ASP:OD1	2.53	0.41
1:A:75:ASP:OD1	1:A:75:ASP:N	2.54	0.41
1:F:75:ASP:N	1:F:75:ASP:OD1	2.53	0.41
1:D:89:ARG:CG	4:D:917:HOH:O	2.69	0.41
1:F:360:PHE:CD1	1:F:360:PHE:C	2.94	0.41
1:E:75:ASP:OD1	1:E:75:ASP:N	2.54	0.41
1:A:285:ASN:N	1:A:285:ASN:ND2	2.69	0.40
1:C:250:GLY:O	1:C:254:ILE:CG1	2.70	0.40
1:C:417:GLU:OE2	1:C:454:TRP:CZ3	2.75	0.40
1:B:205:ASP:N	1:B:205:ASP:OD1	2.55	0.40
1:B:420:LEU:O	1:B:424:ARG:N	2.54	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	449/489 (92%)	426 (95%)	21 (5%)	2 (0%)	43	71
1	B	449/489 (92%)	427 (95%)	21 (5%)	1 (0%)	56	81
1	C	449/489 (92%)	425 (95%)	22 (5%)	2 (0%)	43	71
1	D	449/489 (92%)	428 (95%)	19 (4%)	2 (0%)	43	71
1	E	449/489 (92%)	427 (95%)	20 (4%)	2 (0%)	43	71
1	F	449/489 (92%)	429 (96%)	18 (4%)	2 (0%)	43	71
All	All	2694/2934 (92%)	2562 (95%)	121 (4%)	11 (0%)	43	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	B	128	GLY
1	E	128	GLY
1	C	128	GLY
1	D	128	GLY
1	F	128	GLY
1	A	271	GLY
1	F	271	GLY
1	C	271	GLY
1	D	271	GLY
1	E	271	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	388/419 (93%)	341 (88%)	47 (12%)	7	13
1	B	388/419 (93%)	341 (88%)	47 (12%)	7	13
1	C	388/419 (93%)	343 (88%)	45 (12%)	8	14
1	D	388/419 (93%)	340 (88%)	48 (12%)	7	12
1	E	388/419 (93%)	341 (88%)	47 (12%)	7	13
1	F	388/419 (93%)	342 (88%)	46 (12%)	8	13
All	All	2328/2514 (93%)	2048 (88%)	280 (12%)	7	13

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	26	LEU
1	A	32	ILE
1	A	38	VAL
1	A	68	VAL
1	A	70	ILE
1	A	73	SER
1	A	75	ASP
1	A	76	THR
1	A	79	ASP
1	A	80	GLU
1	A	109	LYS
1	A	122	THR
1	A	147	ARG
1	A	168	THR
1	A	171	SER
1	A	173	TYR
1	A	179	ASP
1	A	191	ARG
1	A	197	SER
1	A	198	LEU
1	A	200	GLU
1	A	205	ASP
1	A	206	ILE
1	A	225	ARG
1	A	231	LYS
1	A	281	GLU
1	A	282	SER
1	A	285	ASN
1	A	288	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	309	ILE
1	A	314	GLU
1	A	315	LYS
1	A	337	GLN
1	A	349	ARG
1	A	359	ARG
1	A	365	ARG
1	A	366	GLU
1	A	368	ASP
1	A	375	THR
1	A	384	HIS
1	A	420	LEU
1	A	440	GLU
1	A	444	SER
1	A	445	LEU
1	A	459	SER
1	A	460	ASN
1	B	12	LEU
1	B	26	LEU
1	B	32	ILE
1	B	38	VAL
1	B	68	VAL
1	B	70	ILE
1	B	73	SER
1	B	75	ASP
1	B	76	THR
1	B	79	ASP
1	B	80	GLU
1	B	87	VAL
1	B	109	LYS
1	B	122	THR
1	B	147	ARG
1	B	168	THR
1	B	171	SER
1	B	173	TYR
1	B	179	ASP
1	B	191	ARG
1	B	197	SER
1	B	198	LEU
1	B	200	GLU
1	B	205	ASP
1	B	206	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	225	ARG
1	B	231	LYS
1	B	281	GLU
1	B	282	SER
1	B	288	LYS
1	B	309	ILE
1	B	314	GLU
1	B	315	LYS
1	B	337	GLN
1	B	349	ARG
1	B	359	ARG
1	B	365	ARG
1	B	366	GLU
1	B	368	ASP
1	B	375	THR
1	B	384	HIS
1	B	420	LEU
1	B	440	GLU
1	B	444	SER
1	B	445	LEU
1	B	459	SER
1	B	460	ASN
1	C	12	LEU
1	C	26	LEU
1	C	32	ILE
1	C	38	VAL
1	C	68	VAL
1	C	70	ILE
1	C	73	SER
1	C	75	ASP
1	C	76	THR
1	C	79	ASP
1	C	80	GLU
1	C	109	LYS
1	C	122	THR
1	C	147	ARG
1	C	168	THR
1	C	171	SER
1	C	173	TYR
1	C	191	ARG
1	C	197	SER
1	C	198	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	200	GLU
1	C	205	ASP
1	C	206	ILE
1	C	225	ARG
1	C	231	LYS
1	C	281	GLU
1	C	282	SER
1	C	285	ASN
1	C	288	LYS
1	C	309	ILE
1	C	314	GLU
1	C	315	LYS
1	C	337	GLN
1	C	349	ARG
1	C	359	ARG
1	C	366	GLU
1	C	368	ASP
1	C	375	THR
1	C	384	HIS
1	C	420	LEU
1	C	440	GLU
1	C	444	SER
1	C	445	LEU
1	C	459	SER
1	C	460	ASN
1	D	12	LEU
1	D	26	LEU
1	D	32	ILE
1	D	38	VAL
1	D	68	VAL
1	D	70	ILE
1	D	73	SER
1	D	75	ASP
1	D	76	THR
1	D	79	ASP
1	D	80	GLU
1	D	109	LYS
1	D	122	THR
1	D	147	ARG
1	D	168	THR
1	D	171	SER
1	D	173	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	179	ASP
1	D	191	ARG
1	D	197	SER
1	D	198	LEU
1	D	200	GLU
1	D	205	ASP
1	D	206	ILE
1	D	225	ARG
1	D	231	LYS
1	D	281	GLU
1	D	282	SER
1	D	285	ASN
1	D	288	LYS
1	D	309	ILE
1	D	314	GLU
1	D	315	LYS
1	D	337	GLN
1	D	349	ARG
1	D	359	ARG
1	D	365	ARG
1	D	366	GLU
1	D	368	ASP
1	D	375	THR
1	D	384	HIS
1	D	420	LEU
1	D	434	ASP
1	D	440	GLU
1	D	444	SER
1	D	445	LEU
1	D	459	SER
1	D	460	ASN
1	E	12	LEU
1	E	26	LEU
1	E	32	ILE
1	E	38	VAL
1	E	68	VAL
1	E	70	ILE
1	E	73	SER
1	E	75	ASP
1	E	76	THR
1	E	79	ASP
1	E	80	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	99	VAL
1	E	109	LYS
1	E	122	THR
1	E	147	ARG
1	E	168	THR
1	E	171	SER
1	E	173	TYR
1	E	179	ASP
1	E	191	ARG
1	E	197	SER
1	E	198	LEU
1	E	200	GLU
1	E	205	ASP
1	E	206	ILE
1	E	225	ARG
1	E	231	LYS
1	E	281	GLU
1	E	282	SER
1	E	285	ASN
1	E	288	LYS
1	E	294	GLU
1	E	309	ILE
1	E	314	GLU
1	E	315	LYS
1	E	337	GLN
1	E	359	ARG
1	E	365	ARG
1	E	366	GLU
1	E	368	ASP
1	E	375	THR
1	E	384	HIS
1	E	420	LEU
1	E	440	GLU
1	E	444	SER
1	E	445	LEU
1	E	459	SER
1	F	12	LEU
1	F	26	LEU
1	F	32	ILE
1	F	38	VAL
1	F	68	VAL
1	F	70	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	73	SER
1	F	75	ASP
1	F	76	THR
1	F	79	ASP
1	F	80	GLU
1	F	109	LYS
1	F	122	THR
1	F	147	ARG
1	F	168	THR
1	F	171	SER
1	F	173	TYR
1	F	191	ARG
1	F	197	SER
1	F	198	LEU
1	F	200	GLU
1	F	205	ASP
1	F	206	ILE
1	F	225	ARG
1	F	231	LYS
1	F	281	GLU
1	F	282	SER
1	F	285	ASN
1	F	288	LYS
1	F	309	ILE
1	F	314	GLU
1	F	315	LYS
1	F	337	GLN
1	F	349	ARG
1	F	359	ARG
1	F	365	ARG
1	F	366	GLU
1	F	368	ASP
1	F	375	THR
1	F	384	HIS
1	F	420	LEU
1	F	440	GLU
1	F	444	SER
1	F	445	LEU
1	F	459	SER
1	F	460	ASN

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 chains 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, 6 are monoatomic - leaving 6 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	800	3	33,33,33	1.92	5 (15%)	52,52,52	3.74	10 (19%)
2	AGS	B	800	3	33,33,33	1.90	5 (15%)	52,52,52	3.76	11 (21%)
2	AGS	C	800	3	33,33,33	1.91	5 (15%)	52,52,52	4.21	12 (23%)
2	AGS	D	800	3	33,33,33	1.92	4 (12%)	52,52,52	3.71	11 (21%)
2	AGS	E	800	3	33,33,33	1.86	4 (12%)	52,52,52	3.74	12 (23%)
2	AGS	F	800	3	33,33,33	2.08	4 (12%)	52,52,52	4.09	10 (19%)

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	800	3	-	0/21/38/38	0/1/3/3
2	AGS	B	800	3	-	0/21/38/38	0/1/3/3
2	AGS	C	800	3	-	0/21/38/38	0/1/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	D	800	3	-	0/21/38/38	0/1/3/3
2	AGS	E	800	3	-	0/21/38/38	0/1/3/3
2	AGS	F	800	3	-	0/21/38/38	0/1/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	800	AGS	PG-S1G	9.75	2.08	1.90
2	D	800	AGS	PG-S1G	8.33	2.06	1.90
2	A	800	AGS	PG-S1G	8.32	2.06	1.90
2	C	800	AGS	PG-S1G	8.02	2.05	1.90
2	B	800	AGS	PG-S1G	8.01	2.05	1.90
2	E	800	AGS	PG-S1G	7.95	2.05	1.90
2	B	800	AGS	PG-O3G	-4.32	1.47	1.56
2	C	800	AGS	PG-O3G	-4.31	1.47	1.56
2	E	800	AGS	PG-O3G	-4.23	1.47	1.56
2	A	800	AGS	PG-O3G	-4.22	1.47	1.56
2	D	800	AGS	PG-O3G	-4.20	1.47	1.56
2	F	800	AGS	PG-O3G	-4.09	1.47	1.56
2	C	800	AGS	C5-C4	3.55	1.48	1.40
2	E	800	AGS	C5-C4	3.20	1.47	1.40
2	B	800	AGS	C5-C4	3.20	1.47	1.40
2	A	800	AGS	C5-C4	3.14	1.47	1.40
2	D	800	AGS	C5-C4	3.14	1.47	1.40
2	F	800	AGS	C5-C4	3.02	1.47	1.40
2	C	800	AGS	C4-N9	-2.55	1.34	1.37
2	B	800	AGS	C4-N9	-2.50	1.34	1.37
2	E	800	AGS	C4-N9	-2.43	1.34	1.37
2	D	800	AGS	C4-N9	-2.38	1.34	1.37
2	A	800	AGS	C4-N9	-2.32	1.34	1.37
2	F	800	AGS	C4-N9	-2.28	1.34	1.37
2	B	800	AGS	PG-O2G	2.10	1.61	1.56
2	C	800	AGS	PG-O2G	2.08	1.61	1.56
2	A	800	AGS	PG-O2G	2.01	1.61	1.56

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	AGS	O3B-PG-S1G	-27.40	102.38	114.53
2	F	800	AGS	O3B-PG-S1G	-25.94	103.02	114.53
2	B	800	AGS	O3B-PG-S1G	-23.39	104.15	114.53
2	E	800	AGS	O3B-PG-S1G	-23.06	104.30	114.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	AGS	O3B-PG-S1G	-23.01	104.32	114.53
2	D	800	AGS	O3B-PG-S1G	-22.84	104.40	114.53
2	F	800	AGS	N3-C2-N1	-6.89	122.94	128.71
2	D	800	AGS	N3-C2-N1	-6.81	123.01	128.71
2	A	800	AGS	N3-C2-N1	-6.79	123.03	128.71
2	C	800	AGS	N3-C2-N1	-6.67	123.13	128.71
2	E	800	AGS	N3-C2-N1	-6.56	123.22	128.71
2	B	800	AGS	N3-C2-N1	-6.56	123.23	128.71
2	F	800	AGS	N3-C4-N9	5.45	135.28	125.43
2	D	800	AGS	N3-C4-N9	5.39	135.16	125.43
2	A	800	AGS	N3-C4-N9	5.38	135.15	125.43
2	E	800	AGS	N3-C4-N9	5.37	135.12	125.43
2	B	800	AGS	N3-C4-N9	5.34	135.08	125.43
2	C	800	AGS	N3-C4-N9	5.12	134.68	125.43
2	A	800	AGS	O2G-PG-S1G	-4.92	107.54	112.73
2	E	800	AGS	O2G-PG-S1G	-4.91	107.56	112.73
2	D	800	AGS	O2G-PG-S1G	-4.86	107.61	112.73
2	F	800	AGS	O3G-PG-S1G	-4.59	107.89	112.73
2	B	800	AGS	O2G-PG-S1G	-4.52	107.97	112.73
2	C	800	AGS	O2G-PG-S1G	-4.15	108.35	112.73
2	A	800	AGS	O3G-PG-S1G	-4.07	108.44	112.73
2	E	800	AGS	O3G-PG-S1G	-4.06	108.44	112.73
2	F	800	AGS	O2G-PG-S1G	-3.64	108.89	112.73
2	B	800	AGS	O3G-PG-S1G	-3.60	108.94	112.73
2	D	800	AGS	O3G-PG-S1G	-3.54	109.00	112.73
2	F	800	AGS	C5-C4-N3	-3.50	118.07	125.70
2	A	800	AGS	C5-C4-N3	-3.44	118.20	125.70
2	F	800	AGS	PA-O3A-PB	-3.41	121.68	131.68
2	E	800	AGS	C5-C4-N3	-3.37	118.37	125.70
2	B	800	AGS	C5-C4-N3	-3.35	118.40	125.70
2	D	800	AGS	C5-C4-N3	-3.33	118.45	125.70
2	A	800	AGS	C4-C5-N7	-3.29	106.71	109.52
2	E	800	AGS	C4-C5-N7	-3.25	106.74	109.52
2	F	800	AGS	C4-C5-N7	-3.25	106.74	109.52
2	E	800	AGS	PA-O3A-PB	-3.22	122.25	131.68
2	B	800	AGS	C4-C5-N7	-3.15	106.82	109.52
2	A	800	AGS	PA-O3A-PB	-3.14	122.48	131.68
2	D	800	AGS	C4-C5-N7	-3.11	106.86	109.52
2	C	800	AGS	O3G-PG-S1G	-3.10	109.47	112.73
2	D	800	AGS	PA-O3A-PB	-3.07	122.69	131.68
2	C	800	AGS	C5-C4-N3	-3.05	119.07	125.70
2	C	800	AGS	PA-O3A-PB	-3.00	122.87	131.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	AGS	PA-O3A-PB	-2.96	123.00	131.68
2	F	800	AGS	C2-N3-C4	2.70	121.69	114.01
2	A	800	AGS	C2-N3-C4	2.64	121.53	114.01
2	D	800	AGS	C2-N3-C4	2.59	121.39	114.01
2	E	800	AGS	C2-N3-C4	2.56	121.30	114.01
2	B	800	AGS	O4'-C1'-N9	2.54	110.80	108.44
2	B	800	AGS	C2-N3-C4	2.53	121.21	114.01
2	A	800	AGS	C3'-C2'-C1'	2.49	104.80	100.91
2	C	800	AGS	C4-C5-N7	-2.47	107.41	109.52
2	D	800	AGS	O4'-C1'-N9	2.44	110.71	108.44
2	E	800	AGS	O4'-C1'-N9	2.43	110.70	108.44
2	C	800	AGS	C2-N3-C4	2.42	120.91	114.01
2	B	800	AGS	C3'-C2'-C1'	2.37	104.61	100.91
2	E	800	AGS	C3'-C2'-C1'	2.36	104.61	100.91
2	F	800	AGS	C3'-C2'-C1'	2.36	104.60	100.91
2	C	800	AGS	O4'-C1'-N9	2.31	110.58	108.44
2	D	800	AGS	C3'-C2'-C1'	2.25	104.42	100.91
2	C	800	AGS	C3'-C2'-C1'	2.23	104.40	100.91
2	C	800	AGS	PB-O3B-PG	-2.18	124.36	131.81
2	E	800	AGS	PB-O3B-PG	-2.13	124.53	131.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	451/489 (92%)	0.37	19 (4%)	35	30	47, 81, 123, 137	0
1	B	451/489 (92%)	0.38	15 (3%)	44	41	47, 77, 110, 129	0
1	C	451/489 (92%)	0.49	35 (7%)	13	10	43, 89, 130, 150	0
1	D	451/489 (92%)	0.58	41 (9%)	9	7	45, 95, 144, 163	0
1	E	451/489 (92%)	0.89	58 (12%)	4	3	52, 93, 156, 173	0
1	F	451/489 (92%)	0.54	34 (7%)	14	11	37, 89, 132, 152	0
All	All	2706/2934 (92%)	0.54	202 (7%)	14	11	37, 86, 136, 173	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	41	LEU	8.0
1	E	173	TYR	7.2
1	E	437	ILE	6.8
1	E	72	LEU	6.5
1	E	51	LEU	6.4
1	E	69	CYS	5.8
1	D	41	LEU	5.7
1	B	314	GLU	5.5
1	E	143	TYR	5.2
1	F	72	LEU	5.0
1	E	71	VAL	5.0
1	F	158	MET	4.9
1	E	114	ILE	4.9
1	A	72	LEU	4.8
1	E	32	ILE	4.8
1	E	429	LEU	4.8
1	D	20	LYS	4.6
1	A	158	MET	4.6
1	E	52	PHE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	462	SER	4.5
1	E	128	GLY	4.5
1	A	437	ILE	4.5
1	D	135	LEU	4.5
1	E	442	MET	4.4
1	E	182	ILE	4.3
1	B	158	MET	4.3
1	C	72	LEU	4.3
1	D	128	GLY	4.3
1	E	75	ASP	4.1
1	E	439	ALA	4.0
1	F	139	PHE	4.0
1	F	114	ILE	4.0
1	E	141	GLU	3.9
1	C	161	VAL	3.9
1	F	182	ILE	3.9
1	E	77	CYS	3.9
1	D	72	LEU	3.8
1	E	146	ILE	3.8
1	D	58	LEU	3.7
1	E	104	PRO	3.7
1	E	183	HIS	3.7
1	A	128	GLY	3.7
1	E	198	LEU	3.6
1	C	182	ILE	3.6
1	D	26	LEU	3.6
1	D	153	LEU	3.6
1	C	130	LEU	3.6
1	F	32	ILE	3.6
1	D	113	ARG	3.5
1	F	111	GLY	3.5
1	A	51	LEU	3.5
1	F	68	VAL	3.5
1	A	155	ARG	3.5
1	E	38	VAL	3.5
1	E	113	ARG	3.4
1	E	158	MET	3.4
1	E	432	LEU	3.4
1	E	39	VAL	3.4
1	E	57	VAL	3.4
1	B	462	SER	3.4
1	F	175	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	338	ARG	3.3
1	E	105	CYS	3.3
1	B	157	GLY	3.3
1	C	338	ARG	3.3
1	C	133	VAL	3.3
1	D	112	LYS	3.3
1	C	317	HIS	3.2
1	F	38	VAL	3.2
1	F	113	ARG	3.2
1	C	51	LEU	3.2
1	B	283	GLU	3.2
1	E	70	ILE	3.2
1	C	26	LEU	3.2
1	F	152	PHE	3.1
1	C	141	GLU	3.1
1	E	139	PHE	3.1
1	D	163	PHE	3.0
1	B	51	LEU	3.0
1	D	182	ILE	3.0
1	C	452	PHE	3.0
1	F	173	TYR	3.0
1	D	437	ILE	3.0
1	E	84	MET	3.0
1	C	71	VAL	3.0
1	C	135	LEU	3.0
1	E	314	GLU	3.0
1	D	173	TYR	3.0
1	E	229	LEU	3.0
1	F	227	PRO	3.0
1	F	337	GLN	2.9
1	D	92	LEU	2.9
1	B	441	VAL	2.9
1	F	71	VAL	2.9
1	F	184	CYS	2.9
1	A	445	LEU	2.9
1	E	156	GLY	2.9
1	C	163	PHE	2.8
1	D	17	LEU	2.8
1	F	51	LEU	2.8
1	F	70	ILE	2.8
1	C	17	LEU	2.8
1	E	59	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	127	THR	2.8
1	E	58	LEU	2.7
1	D	127	THR	2.7
1	E	153	LEU	2.7
1	E	67	ALA	2.7
1	D	445	LEU	2.7
1	D	152	PHE	2.7
1	E	68	VAL	2.7
1	F	57	VAL	2.7
1	E	317	HIS	2.7
1	C	461	PRO	2.6
1	E	462	SER	2.6
1	B	155	ARG	2.6
1	E	181	VAL	2.6
1	D	51	LEU	2.6
1	F	136	LYS	2.6
1	A	41	LEU	2.6
1	F	427	MET	2.6
1	E	102	ILE	2.6
1	D	146	ILE	2.6
1	B	437	ILE	2.5
1	C	56	THR	2.5
1	C	70	ILE	2.5
1	F	360	PHE	2.5
1	B	156	GLY	2.5
1	C	445	LEU	2.5
1	C	113	ARG	2.5
1	D	52	PHE	2.5
1	C	110	TYR	2.5
1	C	179	ASP	2.5
1	C	49	LEU	2.5
1	C	92	LEU	2.5
1	A	135	LEU	2.4
1	D	452	PHE	2.4
1	D	110	TYR	2.4
1	E	176	VAL	2.4
1	D	38	VAL	2.4
1	D	71	VAL	2.4
1	D	158	MET	2.4
1	C	41	LEU	2.4
1	C	198	LEU	2.4
1	C	229	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	241	ILE	2.3
1	B	128	GLY	2.3
1	D	139	PHE	2.3
1	C	337	GLN	2.3
1	F	135	LEU	2.3
1	C	181	VAL	2.3
1	F	224	LEU	2.3
1	C	175	ILE	2.3
1	C	201	VAL	2.3
1	E	174	CYS	2.3
1	D	179	ASP	2.3
1	E	92	LEU	2.3
1	A	19	GLN	2.3
1	A	184	CYS	2.3
1	E	108	VAL	2.2
1	E	140	LEU	2.2
1	F	102	ILE	2.2
1	B	427	MET	2.2
1	D	141	GLU	2.2
1	D	337	GLN	2.2
1	D	328	LEU	2.2
1	E	179	ASP	2.2
1	E	53	ARG	2.2
1	A	130	LEU	2.2
1	F	110	TYR	2.2
1	A	183	HIS	2.2
1	D	187	GLU	2.2
1	E	172	PRO	2.2
1	E	175	ILE	2.2
1	D	183	HIS	2.1
1	F	456	LEU	2.1
1	C	388	MET	2.1
1	D	161	VAL	2.1
1	E	430	ILE	2.1
1	F	146	ILE	2.1
1	E	452	PHE	2.1
1	A	26	LEU	2.1
1	F	236	LYS	2.1
1	C	13	SER	2.1
1	D	233	ILE	2.1
1	A	432	LEU	2.1
1	F	159	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	445	LEU	2.1
1	E	301	ILE	2.1
1	C	432	LEU	2.1
1	D	140	LEU	2.1
1	D	229	LEU	2.1
1	D	241	ILE	2.1
1	A	59	LEU	2.1
1	B	38	VAL	2.0
1	D	159	ARG	2.0
1	B	198	LEU	2.0
1	A	159	ARG	2.0
1	C	462	SER	2.0
1	F	176	VAL	2.0
1	B	163	PHE	2.0
1	F	123	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	D	801	1/1	0.20	1.39	24,24,24,24	0
3	MG	B	801	1/1	0.19	1.35	14,14,14,14	0
3	MG	E	801	1/1	0.19	0.09	19,19,19,19	0
3	MG	F	801	1/1	0.20	-0.29	4,4,4,4	0
2	AGS	A	800	31/31	0.18	-0.29	24,27,29,29	0
2	AGS	E	800	31/31	0.19	-0.31	39,40,42,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	AGS	D	800	31/31	0.17	-0.45	34,43,45,46	0
2	AGS	B	800	31/31	0.17	-0.57	28,29,30,30	0
3	MG	A	801	1/1	0.16	-0.71	12,12,12,12	0
3	MG	C	801	1/1	0.18	-0.78	13,13,13,13	0
2	AGS	C	800	31/31	0.17	-0.81	25,31,36,37	0
2	AGS	F	800	31/31	0.18	-0.86	12,12,13,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.