



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2021 – 01:09 PM GMT

PDB ID : 6YAG
Title : Crystal structure of PnrA from *S. pneumoniae* in complex with thymidine
Authors : Batuecas, M.T.; Hermoso, J.A.
Deposited on : 2020-03-12
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

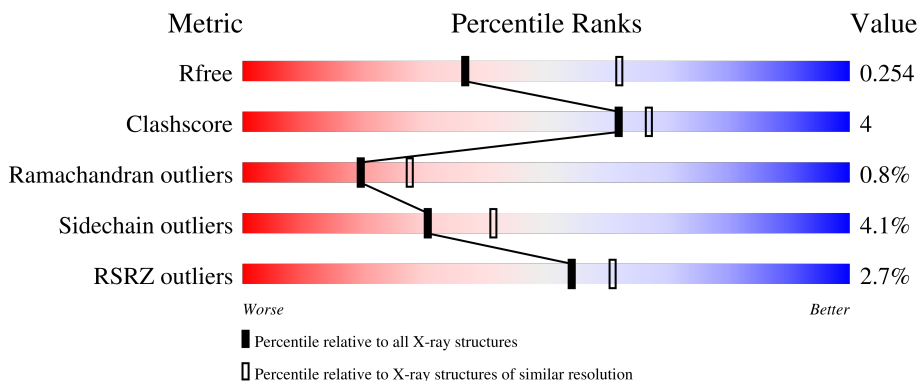
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	 85% 13% .
1	B	330	 88% 10% .
1	C	330	 88% 12% .
1	D	330	 88% 10% ..

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10201 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 Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	330	Total 2477	C 1548	N 424	O 504	S 1	0	1	0
1	A	329	Total 2463	C 1540	N 420	O 502	S 1	0	0	0
1	B	329	Total 2471	C 1545	N 423	O 502	S 1	0	1	0
1	D	328	Total 2457	C 1537	N 419	O 500	S 1	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	SER	-	expression tag	UNP A0A0H2UPF3
C	4	SER	-	expression tag	UNP A0A0H2UPF3
C	5	HIS	-	expression tag	UNP A0A0H2UPF3
C	6	HIS	-	expression tag	UNP A0A0H2UPF3
C	7	HIS	-	expression tag	UNP A0A0H2UPF3
C	8	HIS	-	expression tag	UNP A0A0H2UPF3
C	9	HIS	-	expression tag	UNP A0A0H2UPF3
C	10	HIS	-	expression tag	UNP A0A0H2UPF3
C	11	MET	-	expression tag	UNP A0A0H2UPF3
C	12	SER	-	expression tag	UNP A0A0H2UPF3
C	13	GLY	-	expression tag	UNP A0A0H2UPF3
C	14	GLU	-	expression tag	UNP A0A0H2UPF3
C	15	ASN	-	expression tag	UNP A0A0H2UPF3
C	16	LEU	-	expression tag	UNP A0A0H2UPF3
C	17	TYR	-	expression tag	UNP A0A0H2UPF3
C	18	PHE	-	expression tag	UNP A0A0H2UPF3
C	19	GLN	-	expression tag	UNP A0A0H2UPF3
C	20	GLY	-	expression tag	UNP A0A0H2UPF3
C	21	ALA	-	expression tag	UNP A0A0H2UPF3
C	22	SER	-	expression tag	UNP A0A0H2UPF3
A	3	SER	-	expression tag	UNP A0A0H2UPF3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	-	expression tag	UNP A0A0H2UPF3
A	5	HIS	-	expression tag	UNP A0A0H2UPF3
A	6	HIS	-	expression tag	UNP A0A0H2UPF3
A	7	HIS	-	expression tag	UNP A0A0H2UPF3
A	8	HIS	-	expression tag	UNP A0A0H2UPF3
A	9	HIS	-	expression tag	UNP A0A0H2UPF3
A	10	HIS	-	expression tag	UNP A0A0H2UPF3
A	11	MET	-	expression tag	UNP A0A0H2UPF3
A	12	SER	-	expression tag	UNP A0A0H2UPF3
A	13	GLY	-	expression tag	UNP A0A0H2UPF3
A	14	GLU	-	expression tag	UNP A0A0H2UPF3
A	15	ASN	-	expression tag	UNP A0A0H2UPF3
A	16	LEU	-	expression tag	UNP A0A0H2UPF3
A	17	TYR	-	expression tag	UNP A0A0H2UPF3
A	18	PHE	-	expression tag	UNP A0A0H2UPF3
A	19	GLN	-	expression tag	UNP A0A0H2UPF3
A	20	GLY	-	expression tag	UNP A0A0H2UPF3
A	21	ALA	-	expression tag	UNP A0A0H2UPF3
A	22	SER	-	expression tag	UNP A0A0H2UPF3
B	3	SER	-	expression tag	UNP A0A0H2UPF3
B	4	SER	-	expression tag	UNP A0A0H2UPF3
B	5	HIS	-	expression tag	UNP A0A0H2UPF3
B	6	HIS	-	expression tag	UNP A0A0H2UPF3
B	7	HIS	-	expression tag	UNP A0A0H2UPF3
B	8	HIS	-	expression tag	UNP A0A0H2UPF3
B	9	HIS	-	expression tag	UNP A0A0H2UPF3
B	10	HIS	-	expression tag	UNP A0A0H2UPF3
B	11	MET	-	expression tag	UNP A0A0H2UPF3
B	12	SER	-	expression tag	UNP A0A0H2UPF3
B	13	GLY	-	expression tag	UNP A0A0H2UPF3
B	14	GLU	-	expression tag	UNP A0A0H2UPF3
B	15	ASN	-	expression tag	UNP A0A0H2UPF3
B	16	LEU	-	expression tag	UNP A0A0H2UPF3
B	17	TYR	-	expression tag	UNP A0A0H2UPF3
B	18	PHE	-	expression tag	UNP A0A0H2UPF3
B	19	GLN	-	expression tag	UNP A0A0H2UPF3
B	20	GLY	-	expression tag	UNP A0A0H2UPF3
B	21	ALA	-	expression tag	UNP A0A0H2UPF3
B	22	SER	-	expression tag	UNP A0A0H2UPF3
D	3	SER	-	expression tag	UNP A0A0H2UPF3
D	4	SER	-	expression tag	UNP A0A0H2UPF3
D	5	HIS	-	expression tag	UNP A0A0H2UPF3

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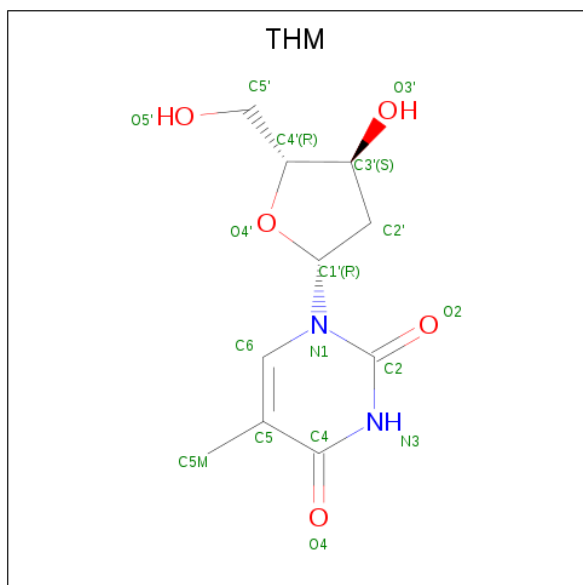
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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	HIS	-	expression tag	UNP A0A0H2UPF3
D	7	HIS	-	expression tag	UNP A0A0H2UPF3
D	8	HIS	-	expression tag	UNP A0A0H2UPF3
D	9	HIS	-	expression tag	UNP A0A0H2UPF3
D	10	HIS	-	expression tag	UNP A0A0H2UPF3
D	11	MET	-	expression tag	UNP A0A0H2UPF3
D	12	SER	-	expression tag	UNP A0A0H2UPF3
D	13	GLY	-	expression tag	UNP A0A0H2UPF3
D	14	GLU	-	expression tag	UNP A0A0H2UPF3
D	15	ASN	-	expression tag	UNP A0A0H2UPF3
D	16	LEU	-	expression tag	UNP A0A0H2UPF3
D	17	TYR	-	expression tag	UNP A0A0H2UPF3
D	18	PHE	-	expression tag	UNP A0A0H2UPF3
D	19	GLN	-	expression tag	UNP A0A0H2UPF3
D	20	GLY	-	expression tag	UNP A0A0H2UPF3
D	21	ALA	-	expression tag	UNP A0A0H2UPF3
D	22	SER	-	expression tag	UNP A0A0H2UPF3

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

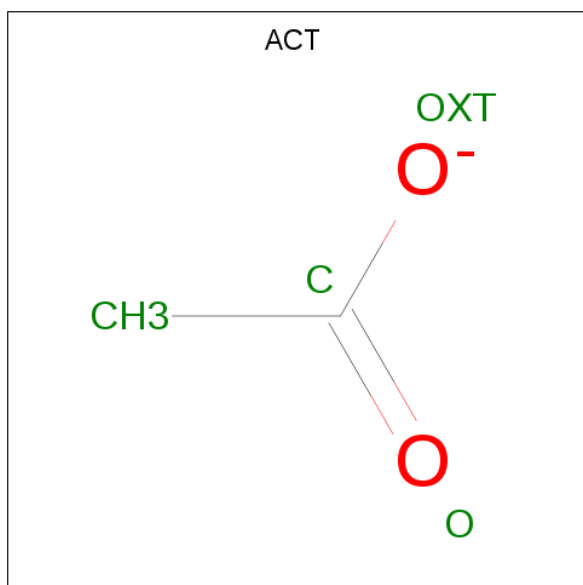
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Ni 2 2	0	0
2	A	1	Total Ni 1 1	0	0
2	D	3	Total Ni 3 3	0	0
2	C	1	Total Ni 1 1	0	0

- Molecule 3 is THYMIDINE (three-letter code: THM) (formula: C₁₀H₁₄N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	Total	C	N	O	0	0
			17	10	2	5		
3	A	1	Total	C	N	O	0	0
			17	10	2	5		
3	B	1	Total	C	N	O	0	0
			17	10	2	5		
3	D	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		


- Molecule 5 is water.

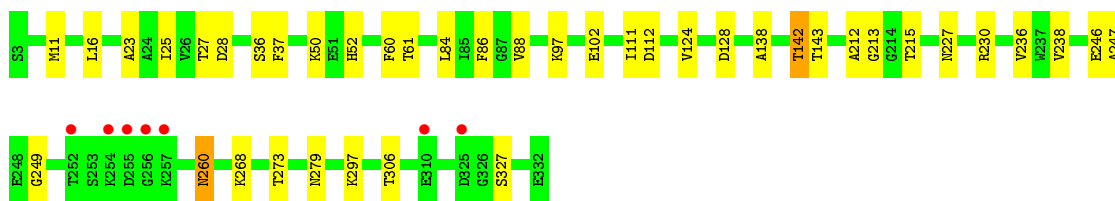
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	78	Total	O	0	0
			78	78		
5	A	80	Total	O	0	0
			80	80		
5	B	73	Total	O	0	0
			73	73		
5	D	23	Total	O	0	0
			23	23		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

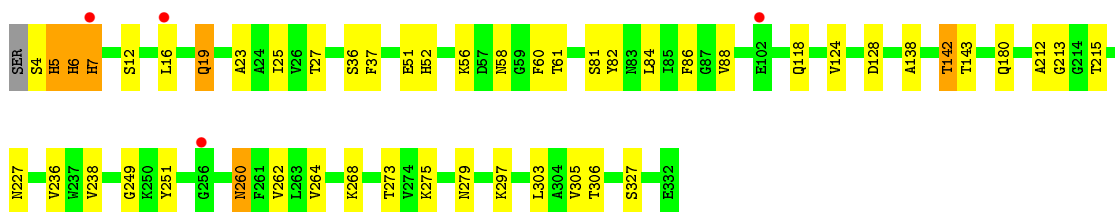
- Molecule 1: Lipoprotein

Chain C: 




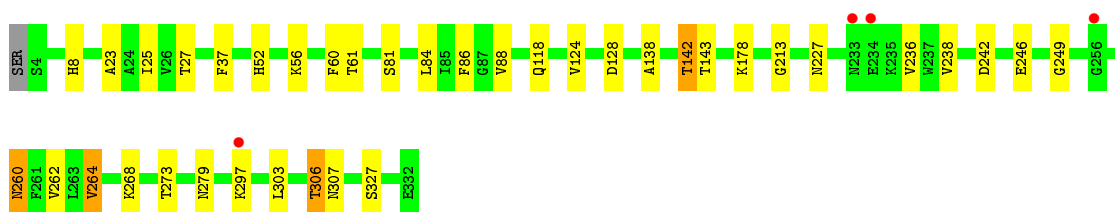
- Molecule 1: Lipoprotein

Chain A: 

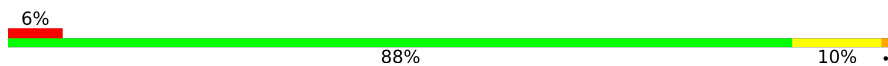


- Molecule 1: Lipoprotein

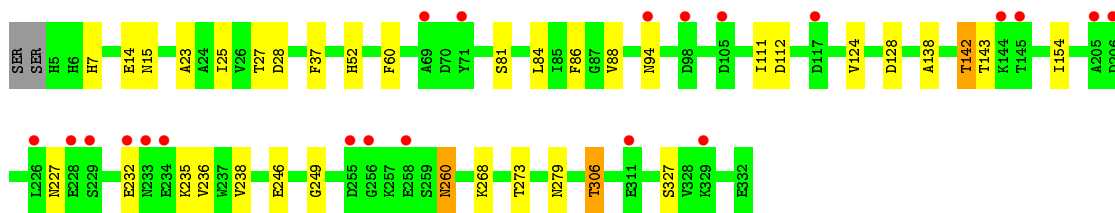
Chain B: 



- Molecule 1: Lipoprotein

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.97Å 303.82Å 128.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.55 49.16 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.21-2.55) 98.7 (49.16-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.208 , 0.255 0.211 , 0.254	Depositor DCC
R_{free} test set	2579 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10201	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, THM, ACT

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	0.68	0/2505	0.81	0/3384
1	B	0.68	0/2516	0.81	0/3398
1	C	0.70	0/2522	0.81	0/3406
1	D	0.67	0/2499	0.80	0/3376
All	All	0.68	0/10042	0.80	0/13564

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2463	0	2377	27	1
1	B	2471	0	2390	23	0
1	C	2477	0	2395	22	0
1	D	2457	0	2372	18	2
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	3	0	0	0	0
3	A	17	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	14	4	0
3	C	17	0	14	2	0
3	D	17	0	14	1	0
4	D	4	0	3	0	0
5	A	80	0	0	3	0
5	B	73	0	0	4	0
5	C	78	0	0	0	0
5	D	23	0	0	3	0
All	All	10201	0	9593	86	2

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 4.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:HG3	5:A:560:HOH:O	1.65	0.96
1:A:227:ASN:HD21	1:A:236:VAL:H	1.17	0.91
1:B:227:ASN:HD21	1:B:236:VAL:H	1.17	0.90
1:C:227:ASN:HD21	1:C:236:VAL:H	1.17	0.88
1:D:227:ASN:HD21	1:D:236:VAL:H	1.18	0.88
1:A:124:VAL:HG11	1:A:273:THR:HG21	1.72	0.71
1:B:307:ASN:OD1	5:B:501:HOH:O	2.10	0.69
1:C:124:VAL:HG11	1:C:273:THR:HG21	1.75	0.69
1:D:7:HIS:CB	5:D:511:HOH:O	2.40	0.69
1:B:118:GLN:HG3	5:B:549:HOH:O	1.92	0.68
1:B:124:VAL:HG11	1:B:273:THR:HG21	1.76	0.67
1:D:124:VAL:HG11	1:D:273:THR:HG21	1.78	0.65
1:B:213:GLY:HA3	3:B:403:THM:HM51	1.79	0.65
1:A:61:THR:HG22	1:A:82:TYR:CZ	2.34	0.63
1:D:246:GLU:HG3	1:D:306:THR:HG21	1.79	0.62
1:A:52:HIS:HE1	1:A:279:ASN:OD1	1.81	0.62
1:A:128:ASP:OD1	1:A:268:LYS:HD2	2.00	0.61
1:B:128:ASP:OD1	1:B:268:LYS:HD2	2.02	0.60
1:C:128:ASP:OD1	1:C:268:LYS:HD2	2.02	0.59
1:D:128:ASP:OD1	1:D:268:LYS:HD2	2.03	0.58
1:A:51:GLU:OE2	1:A:275:LYS:NZ	2.37	0.56
1:C:50:LYS:HE3	5:A:530:HOH:O	2.07	0.55
1:A:19:GLN:HA	1:A:19:GLN:OE1	2.07	0.54
1:D:232:GLU:O	1:D:235:LYS:HD3	2.08	0.53
1:C:11:MET:HG3	1:C:16:LEU:HD21	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ASP:HB3	3:D:403:THM:O4	2.08	0.53
1:B:52:HIS:HE1	1:B:279:ASN:OD1	1.91	0.53
1:A:227:ASN:ND2	1:A:236:VAL:H	1.99	0.53
1:D:52:HIS:HE1	1:D:279:ASN:OD1	1.92	0.53
1:C:52:HIS:HE1	1:C:279:ASN:OD1	1.92	0.52
1:D:227:ASN:ND2	1:D:236:VAL:H	1.99	0.51
1:D:7:HIS:HB3	5:D:511:HOH:O	2.07	0.51
1:D:7:HIS:CA	5:D:511:HOH:O	2.59	0.51
1:B:246:GLU:HG3	1:B:306:THR:HG21	1.92	0.51
1:B:227:ASN:ND2	1:B:236:VAL:H	1.98	0.50
1:A:4:SER:O	1:A:5:HIS:HB3	2.11	0.49
1:C:247:ALA:CB	1:A:58:ASN:HB2	2.43	0.49
1:A:6:HIS:O	1:A:7:HIS:HB2	2.12	0.48
1:B:56:LYS:HE2	1:B:61:THR:OG1	2.13	0.48
1:B:213:GLY:HA3	3:B:403:THM:C5M	2.44	0.48
1:C:227:ASN:ND2	1:C:236:VAL:H	1.98	0.48
1:C:213:GLY:HA3	3:C:502:THM:HM51	1.96	0.48
1:C:37:PHE:CE2	1:C:88:VAL:HG12	2.49	0.47
1:B:138:ALA:O	1:B:142:THR:CG2	2.63	0.47
1:C:11:MET:CG	1:C:16:LEU:HD21	2.45	0.46
1:B:37:PHE:CE2	1:B:88:VAL:HG12	2.51	0.46
1:D:138:ALA:O	1:D:142:THR:CG2	2.64	0.46
1:B:249:GLY:O	1:B:260:ASN:HA	2.16	0.45
1:D:249:GLY:O	1:D:260:ASN:HA	2.17	0.45
1:B:297:LYS:HE3	5:B:535:HOH:O	2.16	0.45
1:A:138:ALA:O	1:A:142:THR:CG2	2.64	0.45
1:A:297:LYS:HE3	5:A:536:HOH:O	2.16	0.45
1:A:37:PHE:CE2	1:A:88:VAL:HG12	2.52	0.45
1:C:138:ALA:O	1:C:142:THR:CG2	2.65	0.45
1:A:212:ALA:HB1	1:A:215:THR:HB	1.99	0.45
1:C:249:GLY:O	1:C:260:ASN:HA	2.17	0.45
1:A:249:GLY:O	1:A:260:ASN:HA	2.17	0.44
1:C:247:ALA:HA	1:A:58:ASN:HB2	1.99	0.44
1:B:23:ALA:HA	1:B:84:LEU:O	2.17	0.44
1:D:37:PHE:CE2	1:D:88:VAL:HG12	2.52	0.44
1:A:25:ILE:HG22	1:A:86:PHE:HB2	1.99	0.43
1:C:28:ASP:HB3	3:C:502:THM:O4	2.18	0.43
1:A:264:VAL:HG13	1:A:303:LEU:HD11	2.00	0.43
1:B:25:ILE:HG22	1:B:86:PHE:HB2	2.00	0.43
1:C:246:GLU:HB3	1:A:58:ASN:ND2	2.33	0.43
1:A:227:ASN:HB3	1:A:251:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ILE:HG22	1:D:86:PHE:HB2	2.00	0.42
1:C:212:ALA:HB1	1:C:215:THR:HB	2.00	0.42
1:B:213:GLY:CA	3:B:403:THM:HM51	2.46	0.42
1:C:25:ILE:HG22	1:C:86:PHE:HB2	2.02	0.42
1:A:213:GLY:HA3	3:A:401:THM:HM51	2.00	0.42
1:B:260:ASN:HD21	1:B:262:VAL:HB	1.85	0.42
1:A:23:ALA:HA	1:A:84:LEU:O	2.20	0.42
1:A:23:ALA:O	1:A:60:PHE:HA	2.21	0.41
1:C:111:ILE:O	1:C:112:ASP:HB2	2.19	0.41
1:C:23:ALA:HA	1:C:84:LEU:O	2.20	0.41
1:C:23:ALA:O	1:C:60:PHE:HA	2.20	0.41
1:D:23:ALA:HA	1:D:84:LEU:O	2.20	0.41
1:C:247:ALA:HB2	1:A:58:ASN:HB2	2.01	0.41
1:B:23:ALA:O	1:B:60:PHE:HA	2.21	0.41
1:B:264:VAL:HG13	1:B:303:LEU:HD11	2.03	0.41
1:D:23:ALA:O	1:D:60:PHE:HA	2.21	0.41
1:B:8:HIS:HD2	5:B:507:HOH:O	2.04	0.40
1:B:242:ASP:OD2	3:B:403:THM:O5'	2.26	0.40
1:A:260:ASN:ND2	1:A:262:VAL:H	2.20	0.40
1:D:111:ILE:O	1:D:112:ASP:HB2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ASN:ND2	1:D:94:ASN:ND2[4_556]	2.02	0.18
1:A:19:GLN:O	1:D:15:ASN:ND2[2_454]	2.18	0.02

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	327/330 (99%)	302 (92%)	19 (6%)	6 (2%)	8	10
1	B	328/330 (99%)	311 (95%)	16 (5%)	1 (0%)	41	51
1	C	329/330 (100%)	308 (94%)	19 (6%)	2 (1%)	25	34
1	D	326/330 (99%)	309 (95%)	16 (5%)	1 (0%)	41	51
All	All	1310/1320 (99%)	1230 (94%)	70 (5%)	10 (1%)	19	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	6	HIS
1	C	306	THR
1	A	7	HIS
1	A	306	THR
1	D	306	THR
1	C	36	SER
1	A	36	SER
1	B	306	THR
1	A	305	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/254 (100%)	241 (95%)	12 (5%)	26	35
1	B	254/254 (100%)	245 (96%)	9 (4%)	36	49
1	C	255/254 (100%)	244 (96%)	11 (4%)	29	39
1	D	252/254 (99%)	243 (96%)	9 (4%)	35	47
All	All	1014/1016 (100%)	973 (96%)	41 (4%)	30	43

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	27	THR

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Mol	Chain	Res	Type
1	C	61	THR
1	C	97	LYS
1	C	102	GLU
1	C	142	THR
1	C	143	THR
1	C	230	ARG
1	C	238	VAL
1	C	260	ASN
1	C	297	LYS
1	C	327	SER
1	A	12	SER
1	A	16	LEU
1	A	19	GLN
1	A	27	THR
1	A	56	LYS
1	A	81	SER
1	A	142	THR
1	A	143	THR
1	A	180	GLN
1	A	238	VAL
1	A	260	ASN
1	A	327	SER
1	B	27	THR
1	B	81	SER
1	B	142	THR
1	B	143	THR
1	B	178	LYS
1	B	238	VAL
1	B	260	ASN
1	B	264	VAL
1	B	327	SER
1	D	14	GLU
1	D	27	THR
1	D	81	SER
1	D	142	THR
1	D	143	THR
1	D	154	ILE
1	D	238	VAL
1	D	260	ASN
1	D	327	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	6	HIS
1	C	7	HIS
1	C	9	HIS
1	C	52	HIS
1	C	227	ASN
1	C	260	ASN
1	A	8	HIS
1	A	52	HIS
1	A	58	ASN
1	A	227	ASN
1	A	260	ASN
1	B	8	HIS
1	B	52	HIS
1	B	118	GLN
1	B	227	ASN
1	B	260	ASN
1	D	7	HIS
1	D	52	HIS
1	D	118	GLN
1	D	227	ASN
1	D	260	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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
3	THM	D	403	-	15,18,18	1.05	2 (13%)	16,26,26	3.57	2 (12%)
3	THM	A	401	-	15,18,18	1.09	2 (13%)	16,26,26	3.50	1 (6%)
4	ACT	D	405	-	1,3,3	4.25	1 (100%)	0,3,3	0.00	-
3	THM	B	403	-	15,18,18	1.09	2 (13%)	16,26,26	3.59	1 (6%)
3	THM	C	502	-	15,18,18	1.08	2 (13%)	16,26,26	3.48	2 (12%)

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
3	THM	D	403	-	-	0/3/18/18	0/2/2/2
3	THM	A	401	-	-	1/3/18/18	0/2/2/2
3	THM	B	403	-	-	2/3/18/18	0/2/2/2
3	THM	C	502	-	-	1/3/18/18	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	405	ACT	CH3-C	4.25	1.54	1.48
3	D	403	THM	C4-N3	2.63	1.37	1.33
3	A	401	THM	C4-N3	2.59	1.37	1.33
3	B	403	THM	C4-N3	2.53	1.37	1.33
3	A	401	THM	C6-C5	-2.46	1.33	1.40
3	C	502	THM	C4-N3	2.42	1.37	1.33
3	B	403	THM	C6-C5	-2.27	1.33	1.40
3	C	502	THM	C6-C5	-2.23	1.33	1.40
3	D	403	THM	C6-C5	-2.19	1.34	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	THM	C4-N3-C2	14.03	126.98	115.14
3	D	403	THM	C4-N3-C2	13.77	126.77	115.14
3	A	401	THM	C4-N3-C2	13.60	126.63	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	THM	C4-N3-C2	13.52	126.56	115.14
3	D	403	THM	C5M-C5-C6	2.20	123.32	118.68
3	C	502	THM	C5M-C5-C6	2.12	123.16	118.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	THM	C3'-C4'-C5'-O5'
3	B	403	THM	O4'-C4'-C5'-O5'
3	C	502	THM	C3'-C4'-C5'-O5'
3	A	401	THM	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	THM	1	0
3	A	401	THM	1	0
3	B	403	THM	4	0
3	C	502	THM	2	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	329/330 (99%)	0.02	4 (1%) 79 84	18, 39, 71, 136	0
1	B	329/330 (99%)	-0.06	4 (1%) 79 84	17, 41, 80, 114	0
1	C	330/330 (100%)	-0.03	7 (2%) 63 70	16, 41, 87, 109	0
1	D	328/330 (99%)	0.53	21 (6%) 19 22	30, 70, 110, 160	0
All	All	1316/1320 (99%)	0.11	36 (2%) 54 61	16, 47, 96, 160	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	HIS	8.2
1	D	256	GLY	7.3
1	D	234	GLU	5.5
1	C	310	GLU	4.4
1	A	16	LEU	4.1
1	D	233	ASN	3.7
1	D	232	GLU	3.7
1	C	252	THR	3.4
1	B	234	GLU	3.1
1	D	226	LEU	3.1
1	D	311	GLU	3.0
1	D	144	LYS	3.0
1	D	94	ASN	2.9
1	D	258	GLU	2.8
1	C	254	LYS	2.8
1	D	71	TYR	2.8
1	B	233	ASN	2.8
1	C	325	ASP	2.7
1	D	255	ASP	2.7
1	C	256	GLY	2.6
1	D	205	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	329	LYS	2.4
1	D	98	ASP	2.4
1	D	228	GLU	2.4
1	A	256	GLY	2.4
1	B	256	GLY	2.3
1	A	102	GLU	2.3
1	D	145	THR	2.3
1	D	229	SER	2.3
1	D	206	ASP	2.2
1	D	105	ASP	2.2
1	C	255	ASP	2.1
1	B	297	LYS	2.1
1	C	257	LYS	2.1
1	D	69	ALA	2.0
1	D	117	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	D	405	4/4	0.91	0.24	68,73,73,75	0
2	NI	D	401	1/1	0.95	0.10	48,48,48,48	0
3	THM	A	401	17/17	0.95	0.13	23,29,34,39	0
3	THM	D	403	17/17	0.96	0.14	42,46,47,51	0
3	THM	C	502	17/17	0.96	0.13	24,29,34,36	0
3	THM	B	403	17/17	0.97	0.12	28,30,31,32	0
2	NI	D	402	1/1	0.98	0.17	46,46,46,46	0
2	NI	B	402	1/1	0.98	0.28	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	B	401	1/1	0.99	0.12	17,17,17,17	0
2	NI	A	402	1/1	0.99	0.07	46,46,46,46	0
2	NI	D	404	1/1	0.99	0.06	100,100,100,100	0
2	NI	C	501	1/1	1.00	0.14	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.