



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:49 AM GMT

PDB ID : 2C9D
Title : LUMAZINE SYNTHASE FROM MYCOBACTERIUM TUBERCULOSIS
BOUND TO 3-(1,3,7-TRIHYDRO-9-D-RIBITYL-2,6,8-PURINETRION
E-7-YL)HEXANE 1-PHOSPHATE
Authors : Morgunova, E.; Illarionov, B.; Jin, G.; Haase, I.; Fischer, M.; Cushman, M.;
Bacher, A.; Ladenstein, R.
Deposited on : 2005-12-09
Resolution : 2.80 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>

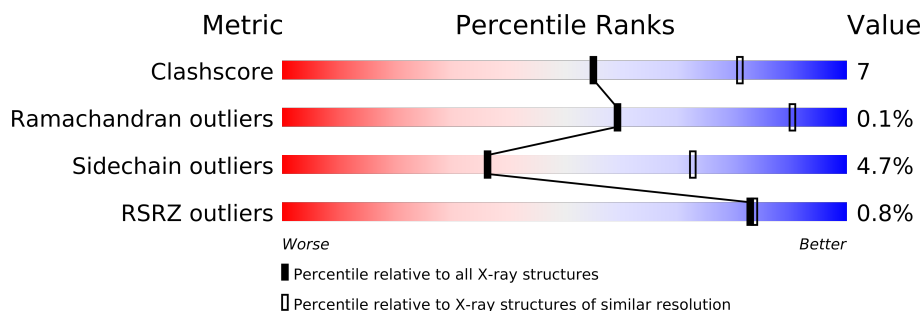
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	160	
1	B	160	
1	C	160	
1	D	160	
1	E	160	
1	F	160	
1	G	160	
1	H	160	
1	I	160	
1	J	160	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MPD	J	1164	-	X

2 Entry composition

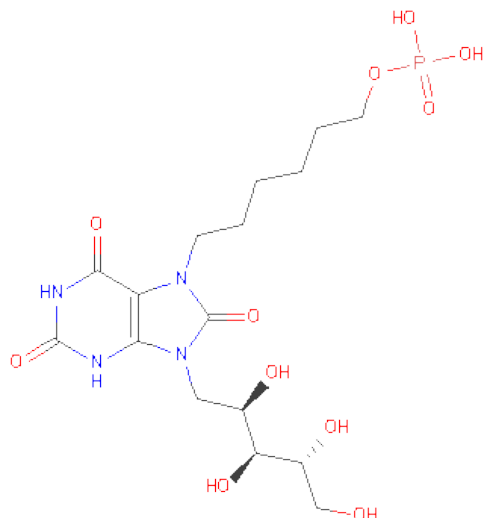
There are 5 unique types of molecules in this entry. The entry contains 11482 atoms, of which 0 are hydrogen and 0 are deuterium.

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 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	B	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	C	146	Total	C	N	O	S	0	0	0
			1055	651	193	208	3			
1	D	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	E	146	Total	C	N	O	S	0	0	0
			1055	651	193	208	3			
1	F	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	G	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	H	146	Total	C	N	O	S	0	0	0
			1055	651	193	208	3			
1	I	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	J	146	Total	C	N	O	S	0	0	0
			1055	651	193	208	3			

- Molecule 2 is 3-(1,3,7-TRIHYDRO-9-D-RIBITYL-2,6,8-PURINETRIONE-7-YL) HEXANE 1-PHOSPHATE (three-letter code: PHR) (formula: C₁₆H₂₇N₄O₁₁P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	B	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	C	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	D	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	E	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	F	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	G	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	H	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	I	1	Total	C	N	O	P	0	0
			32	16	4	11	1		
2	J	1	Total	C	N	O	P	0	0
			32	16	4	11	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

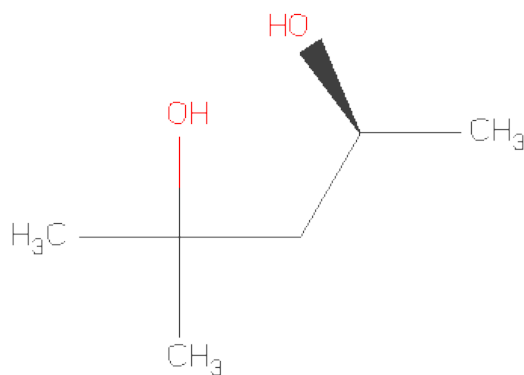
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	K	0	0
			1	1		
3	J	3	Total	K	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total K 1 1	0	0
3	E	2	Total K 2 2	0	0
3	H	1	Total K 1 1	0	0
3	B	3	Total K 3 3	0	0
3	I	1	Total K 1 1	0	0
3	C	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	F	1	Total K 1 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	J	1	Total C O 8 6 2	0	0

- Molecule 5 is water.

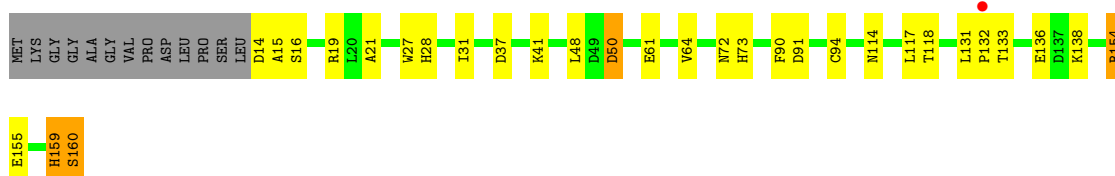
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total 58	O 58	0	0
5	B	59	Total 59	O 59	0	0
5	C	51	Total 51	O 51	0	0
5	D	33	Total 33	O 33	0	0
5	E	49	Total 49	O 49	0	0
5	F	56	Total 56	O 56	0	0
5	G	55	Total 55	O 55	0	0
5	H	61	Total 61	O 61	0	0
5	I	60	Total 60	O 60	0	0
5	J	49	Total 49	O 49	0	0

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: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain A: 



- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain B: 



- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain C: 



- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain D: 



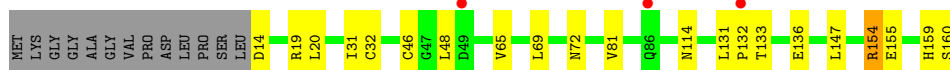
- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain E: 



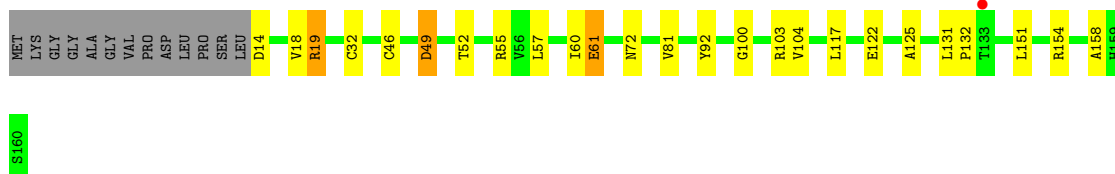
- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain F: 



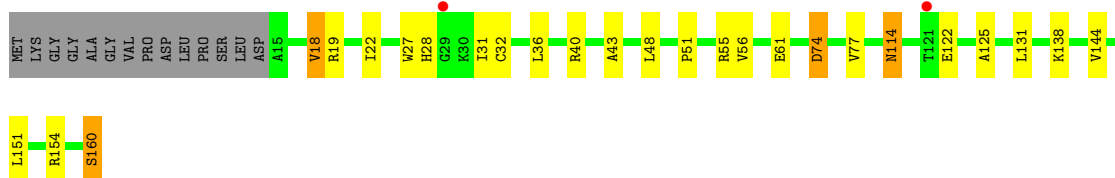
- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain G:



- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain H:



- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain I:



- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINESYNTHASE

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.95Å 79.96Å 88.35Å 64.27° 64.39° 62.81°	Depositor
Resolution (Å)	12.00 – 2.80 44.58 – 2.30	Depositor EDS
% Data completeness (in resolution range)	82.0 (12.00-2.80) 60.7 (44.58-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.259 , 0.326 0.265 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.7	EDS
Estimated twinning fraction	0.000 for -h+k,-h,-h+l 0.000 for -k,h-k,-k+l 0.014 for h,h-k,h-l 0.016 for -h+k,k,k-l 0.397 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57102 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11482	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.80% 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: PHR, K, MPD

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	0.46	1/1075 (0.1%)	0.54	0/1467
1	B	0.43	0/1075	0.53	0/1467
1	C	0.41	0/1067	0.54	0/1456
1	D	0.47	1/1075 (0.1%)	0.55	0/1467
1	E	0.42	0/1067	0.55	0/1456
1	F	0.61	2/1075 (0.2%)	0.54	1/1467 (0.1%)
1	G	0.42	0/1075	0.55	0/1467
1	H	0.65	1/1067 (0.1%)	0.55	0/1456
1	I	0.43	0/1075	0.51	0/1467
1	J	0.42	0/1067	0.60	2/1456 (0.1%)
All	All	0.48	5/10718 (0.0%)	0.55	3/14626 (0.0%)

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	A	0	1
1	C	0	1
1	E	0	1
1	J	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	160	SER	CB-OG	16.79	1.64	1.42
1	F	160	SER	CB-OG	14.25	1.60	1.42
1	D	160	SER	C-O	6.50	1.35	1.23
1	A	160	SER	C-O	5.17	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	160	SER	CA-CB	-5.14	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	159	HIS	C-N-CA	7.55	140.58	121.70
1	J	160	SER	N-CA-C	-7.46	90.85	111.00
1	F	160	SER	N-CA-CB	5.27	118.40	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	HIS	Peptide
1	C	159	HIS	Peptide
1	E	159	HIS	Peptide
1	J	159	HIS	Peptide

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	1063	0	1074	18	0
1	B	1063	0	1074	20	0
1	C	1055	0	1070	16	0
1	D	1063	0	1074	15	0
1	E	1055	0	1070	15	0
1	F	1063	0	1074	14	0
1	G	1063	0	1074	17	0
1	H	1055	0	1070	23	0
1	I	1063	0	1074	16	0
1	J	1055	0	1070	11	0
2	A	32	0	25	0	0
2	B	32	0	25	1	0
2	C	32	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	32	0	25	0	0
2	E	32	0	25	1	0
2	F	32	0	25	0	0
2	G	32	0	25	1	0
2	H	32	0	25	0	0
2	I	32	0	25	0	0
2	J	32	0	25	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	3	0	0	0	0
4	A	8	0	14	0	0
4	J	8	0	14	0	0
5	A	58	0	0	6	0
5	B	59	0	0	7	0
5	C	51	0	0	7	0
5	D	33	0	0	1	0
5	E	49	0	0	7	0
5	F	56	0	0	6	0
5	G	55	0	0	7	0
5	H	61	0	0	10	0
5	I	60	0	0	5	0
5	J	49	0	0	4	0
All	All	11482	0	11002	148	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 7.

All (148) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:160:SER:CB	1:H:160:SER:OG	1.64	1.45
1:B:57:LEU:HA	5:B:2024:HOH:O	1.61	1.00
1:G:60:ILE:HG12	5:G:2030:HOH:O	1.64	0.96
1:H:43:ALA:HB1	5:H:2022:HOH:O	1.67	0.92
1:A:117:LEU:HD12	5:A:2051:HOH:O	1.77	0.84
1:G:49:ASP:HA	5:G:2018:HOH:O	1.79	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:52:THR:HG23	1:I:160:SER:HB2	1.61	0.81
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.45	0.81
1:B:26:SER:HB2	5:B:2024:HOH:O	1.80	0.80
1:F:155:GLU:O	1:F:159:HIS:HE1	1.64	0.79
1:F:14:ASP:O	1:F:46:CYS:O	2.01	0.77
1:G:32:CYS:SG	1:G:55:ARG:NH2	2.57	0.77
1:C:160:SER:HB2	5:J:2021:HOH:O	1.86	0.75
1:A:117:LEU:HD21	1:A:138:LYS:HG3	1.67	0.74
1:C:43:ALA:HB1	5:C:2013:HOH:O	1.87	0.74
1:A:64:VAL:HG13	5:A:2018:HOH:O	1.86	0.73
1:I:112:ILE:HB	5:I:2041:HOH:O	1.89	0.71
1:A:31:ILE:HG21	5:A:2051:HOH:O	1.89	0.71
1:B:128:ARG:HG2	1:B:128:ARG:HH11	1.57	0.69
1:F:31:ILE:CG2	5:F:2045:HOH:O	2.41	0.69
1:G:92:TYR:O	5:G:2029:HOH:O	2.11	0.68
1:F:31:ILE:HG21	5:F:2045:HOH:O	1.93	0.68
1:C:112:ILE:HD12	5:C:2025:HOH:O	1.94	0.67
1:E:50:ASP:HB2	5:E:2017:HOH:O	1.94	0.66
1:I:130:GLY:HA3	1:I:137:ASP:OD2	1.96	0.65
1:C:25:SER:HB2	5:C:2051:HOH:O	1.96	0.65
1:D:19:ARG:CZ	1:I:154:ARG:HH22	2.12	0.63
1:B:128:ARG:CG	1:B:128:ARG:HH11	2.11	0.63
1:H:160:SER:CB	1:H:160:SER:HG	2.07	0.62
1:I:155:GLU:O	1:I:159:HIS:HE1	1.83	0.62
1:B:131:LEU:HB3	1:B:132:PRO:HD2	1.83	0.60
5:D:2020:HOH:O	1:E:98:THR:HG21	2.00	0.60
1:H:48:LEU:O	5:H:2022:HOH:O	2.16	0.60
1:I:83:ILE:HB	5:I:2012:HOH:O	2.02	0.60
1:F:155:GLU:O	1:F:159:HIS:CE1	2.51	0.59
1:J:127:ASP:HB3	5:J:2040:HOH:O	2.02	0.59
1:E:27:TRP:HD1	1:E:28:HIS:CD2	2.20	0.59
1:B:155:GLU:O	1:B:159:HIS:CE1	2.55	0.59
1:A:155:GLU:O	1:A:159:HIS:HE1	1.86	0.59
1:H:138:LYS:HG3	5:H:2054:HOH:O	2.03	0.58
1:J:130:GLY:HA3	1:J:137:ASP:OD2	2.03	0.58
1:H:160:SER:OG	1:H:160:SER:CA	2.48	0.58
1:H:22:ILE:HG22	1:H:77:VAL:HB	1.85	0.58
1:A:94:CYS:HB2	5:E:2031:HOH:O	2.03	0.58
1:B:155:GLU:O	1:B:159:HIS:HE1	1.87	0.58
1:A:14:ASP:O	1:A:16:SER:N	2.36	0.57
1:D:128:ARG:HG3	1:D:128:ARG:NH1	2.19	0.57
1:A:131:LEU:HB3	1:A:132:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:61:GLU:OE1	2:G:791:PHR:O21	2.21	0.57
1:E:72:ASN:HB2	5:E:2026:HOH:O	2.03	0.57
1:H:144:VAL:HB	5:H:2053:HOH:O	2.06	0.56
1:J:128:ARG:HD2	5:J:2041:HOH:O	2.06	0.56
1:D:131:LEU:HB3	1:D:132:PRO:HD2	1.88	0.55
1:C:58:GLY:HA2	5:C:2051:HOH:O	2.07	0.55
1:C:131:LEU:HB3	1:C:132:PRO:HD2	1.89	0.54
1:D:81:VAL:HG12	1:D:117:LEU:HB2	1.88	0.54
1:I:131:LEU:HB3	1:I:132:PRO:HD2	1.90	0.54
1:E:32:CYS:SG	5:E:2021:HOH:O	2.59	0.53
1:H:18:VAL:HG22	1:H:48:LEU:HD11	1.91	0.53
1:J:135:ALA:HB3	5:J:2037:HOH:O	2.08	0.53
1:B:149:THR:HG21	5:B:2054:HOH:O	2.08	0.53
1:I:21:ALA:HB2	1:I:73:HIS:CD2	2.43	0.53
1:A:91:ASP:HA	5:E:2031:HOH:O	2.09	0.52
1:F:65:VAL:O	1:F:69:LEU:HG	2.10	0.52
1:B:72:ASN:HD21	1:F:154:ARG:NH1	2.09	0.51
1:B:57:LEU:HD12	5:B:2024:HOH:O	2.10	0.51
1:H:51:PRO:HD2	5:H:2019:HOH:O	2.10	0.51
1:J:36:LEU:O	1:J:40:ARG:HG3	2.10	0.50
1:F:131:LEU:HB3	1:F:132:PRO:HD2	1.94	0.50
1:E:155:GLU:O	1:E:159:HIS:HE1	1.94	0.50
1:C:160:SER:HB3	1:J:52:THR:HG23	1.93	0.50
1:B:31:ILE:HG13	5:B:2008:HOH:O	2.12	0.50
1:A:50:ASP:HB2	5:A:2013:HOH:O	2.12	0.50
1:E:58:GLY:HA3	2:E:791:PHR:H11	1.94	0.49
1:B:128:ARG:CG	1:B:128:ARG:NH1	2.75	0.49
1:A:21:ALA:HB2	1:A:73:HIS:CD2	2.47	0.49
1:A:27:TRP:HD1	1:A:28:HIS:CD2	2.31	0.49
1:B:154:ARG:HG3	5:F:2001:HOH:O	2.13	0.48
1:G:151:LEU:HG	5:G:2047:HOH:O	2.13	0.48
1:D:160:SER:HB2	1:I:52:THR:HG23	1.94	0.48
1:F:31:ILE:HG23	5:F:2045:HOH:O	2.11	0.48
1:G:18:VAL:HG11	5:G:2047:HOH:O	2.13	0.48
1:F:20:LEU:HD22	1:F:147:LEU:HD21	1.96	0.48
1:D:94:CYS:O	1:D:98:THR:HG23	2.14	0.48
1:F:19:ARG:NH1	5:F:2001:HOH:O	2.46	0.48
1:C:86:GLN:HG3	5:C:2033:HOH:O	2.14	0.47
1:E:131:LEU:HB3	1:E:132:PRO:HD2	1.95	0.47
1:C:66:ALA:HB1	5:C:2025:HOH:O	2.15	0.47
1:A:61:GLU:HG3	5:B:2054:HOH:O	2.12	0.47
1:D:40:ARG:HH22	1:D:53:VAL:HG21	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:27:TRP:HD1	1:H:28:HIS:CD2	2.32	0.47
1:G:125:ALA:HB3	5:G:2040:HOH:O	2.15	0.47
1:B:156:LEU:HD22	1:G:158:ALA:HB1	1.96	0.47
1:C:19:ARG:CZ	1:J:154:ARG:HH12	2.28	0.47
1:C:108:SER:HA	5:C:2038:HOH:O	2.15	0.46
1:J:18:VAL:HG22	1:J:48:LEU:HD11	1.98	0.46
1:J:27:TRP:HD1	1:J:28:HIS:CD2	2.34	0.46
1:C:160:SER:HB3	1:J:52:THR:HA	1.98	0.46
1:E:154:ARG:HH22	1:H:19:ARG:NH1	2.14	0.46
1:F:32:CYS:HB2	5:F:2003:HOH:O	2.16	0.46
1:B:140:ALA:O	1:B:144:VAL:HG23	2.16	0.45
1:G:81:VAL:HG22	1:G:117:LEU:HD12	1.98	0.45
1:A:31:ILE:CG2	5:A:2051:HOH:O	2.58	0.45
1:G:32:CYS:SG	1:G:55:ARG:CZ	3.04	0.45
1:H:36:LEU:HD22	1:H:55:ARG:NH2	2.32	0.45
1:H:114:ASN:HD22	1:H:114:ASN:C	2.21	0.45
1:D:154:ARG:HD2	5:I:2032:HOH:O	2.16	0.45
1:H:28:HIS:HB3	1:H:31:ILE:HD12	1.99	0.45
1:C:27:TRP:HD1	1:C:28:HIS:CD2	2.34	0.44
1:I:138:LYS:HG3	5:I:2047:HOH:O	2.16	0.44
1:H:19:ARG:N	1:H:74:ASP:OD2	2.41	0.44
1:C:61:GLU:HG2	1:D:149:THR:OG1	2.18	0.44
1:B:87:THR:HB	1:B:88:PRO:HD2	2.00	0.44
1:D:160:SER:HB2	1:I:52:THR:HA	1.99	0.44
1:E:117:LEU:HD21	1:E:138:LYS:HG3	2.00	0.44
1:G:100:GLY:O	1:G:104:VAL:HG23	2.17	0.44
1:A:160:SER:HB2	1:G:52:THR:HA	1.99	0.43
1:D:117:LEU:HD21	1:D:138:LYS:HG3	2.00	0.43
1:H:122:GLU:HG3	5:H:2050:HOH:O	2.18	0.43
1:B:32:CYS:SG	1:B:55:ARG:NH1	2.87	0.43
5:A:2033:HOH:O	1:B:118:THR:HB	2.18	0.43
1:D:31:ILE:HG21	1:D:81:VAL:HG11	2.01	0.43
1:J:131:LEU:HB3	1:J:132:PRO:HD2	2.00	0.43
1:B:19:ARG:CZ	1:F:19:ARG:HH21	2.32	0.42
1:G:122:GLU:HG2	5:G:2040:HOH:O	2.19	0.42
1:H:125:ALA:HB3	5:H:2050:HOH:O	2.19	0.42
1:E:97:VAL:HG11	5:E:2036:HOH:O	2.19	0.42
1:H:32:CYS:HB2	5:H:2008:HOH:O	2.19	0.42
1:A:154:ARG:NH1	1:G:19:ARG:HH12	2.18	0.42
1:C:15:ALA:O	1:C:18:VAL:HG13	2.20	0.42
1:I:27:TRP:HD1	1:I:28:HIS:CD2	2.37	0.42
1:C:137:ASP:O	1:C:141:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:19:ARG:NH1	5:I:2006:HOH:O	2.53	0.42
1:E:116:VAL:HB	5:E:2036:HOH:O	2.20	0.41
1:H:51:PRO:HD3	5:H:2022:HOH:O	2.21	0.41
1:G:131:LEU:HB3	1:G:132:PRO:HD2	2.03	0.41
1:A:37:ASP:O	1:A:41:LYS:HG2	2.20	0.41
1:D:72:ASN:HD22	1:I:157:ARG:HB2	1.86	0.41
1:H:40:ARG:HG2	5:H:2018:HOH:O	2.19	0.41
1:B:15:ALA:HB1	5:B:2001:HOH:O	2.19	0.41
1:H:61:GLU:HG2	1:I:149:THR:OG1	2.21	0.41
1:E:154:ARG:HH22	1:H:19:ARG:HH11	1.69	0.41
2:B:791:PHR:H152	2:B:791:PHR:H181	1.31	0.41
1:G:14:ASP:O	1:G:46:CYS:O	2.39	0.40
1:F:31:ILE:HG21	1:F:81:VAL:HG21	2.02	0.40
1:E:158:ALA:HB1	1:I:156:LEU:HD22	2.03	0.40
1:E:21:ALA:HB2	1:E:73:HIS:CD2	2.56	0.40
1:A:90:PHE:CZ	1:A:118:THR:HG23	2.57	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	145/160 (91%)	138 (95%)	6 (4%)	1 (1%)	30	69
1	B	145/160 (91%)	139 (96%)	6 (4%)	0	100	100
1	C	144/160 (90%)	138 (96%)	6 (4%)	0	100	100
1	D	145/160 (91%)	138 (95%)	7 (5%)	0	100	100
1	E	144/160 (90%)	138 (96%)	6 (4%)	0	100	100
1	F	145/160 (91%)	139 (96%)	6 (4%)	0	100	100
1	G	145/160 (91%)	139 (96%)	6 (4%)	0	100	100
1	H	144/160 (90%)	138 (96%)	6 (4%)	0	100	100
1	I	145/160 (91%)	138 (95%)	6 (4%)	1 (1%)	30	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	144/160 (90%)	138 (96%)	6 (4%)	0	100	100
All	All	1446/1600 (90%)	1383 (96%)	61 (4%)	2 (0%)	59	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ALA
1	I	15	ALA

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	111/120 (92%)	103 (93%)	8 (7%)	21	50
1	B	111/120 (92%)	108 (97%)	3 (3%)	57	89
1	C	110/120 (92%)	103 (94%)	7 (6%)	25	58
1	D	111/120 (92%)	109 (98%)	2 (2%)	71	94
1	E	110/120 (92%)	107 (97%)	3 (3%)	57	89
1	F	111/120 (92%)	105 (95%)	6 (5%)	31	66
1	G	111/120 (92%)	104 (94%)	7 (6%)	25	59
1	H	110/120 (92%)	103 (94%)	7 (6%)	25	58
1	I	111/120 (92%)	104 (94%)	7 (6%)	25	59
1	J	110/120 (92%)	108 (98%)	2 (2%)	71	94
All	All	1106/1200 (92%)	1054 (95%)	52 (5%)	36	73

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	48	LEU
1	A	50	ASP
1	A	72	ASN
1	A	114	ASN

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Mol	Chain	Res	Type
1	A	133	THR
1	A	136	GLU
1	A	154	ARG
1	B	72	ASN
1	B	133	THR
1	B	136	GLU
1	C	18	VAL
1	C	50	ASP
1	C	114	ASN
1	C	123	GLU
1	C	149	THR
1	C	154	ARG
1	C	155	GLU
1	D	114	ASN
1	D	123	GLU
1	E	32	CYS
1	E	57	LEU
1	E	114	ASN
1	F	48	LEU
1	F	72	ASN
1	F	114	ASN
1	F	133	THR
1	F	136	GLU
1	F	154	ARG
1	G	19	ARG
1	G	49	ASP
1	G	57	LEU
1	G	61	GLU
1	G	72	ASN
1	G	103	ARG
1	G	154	ARG
1	H	18	VAL
1	H	56	VAL
1	H	74	ASP
1	H	114	ASN
1	H	131	LEU
1	H	151	LEU
1	H	154	ARG
1	I	18	VAL
1	I	50	ASP
1	I	72	ASN
1	I	86	GLN

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Mol	Chain	Res	Type
1	I	114	ASN
1	I	117	LEU
1	I	154	ARG
1	J	19	ARG
1	J	114	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	159	HIS
1	B	72	ASN
1	B	159	HIS
1	C	99	GLN
1	C	114	ASN
1	D	72	ASN
1	D	114	ASN
1	E	89	HIS
1	E	159	HIS
1	F	72	ASN
1	F	159	HIS
1	G	72	ASN
1	G	86	GLN
1	G	99	GLN
1	G	159	HIS
1	H	114	ASN
1	H	159	HIS
1	I	72	ASN
1	I	86	GLN
1	I	114	ASN
1	I	159	HIS
1	J	28	HIS
1	J	99	GLN
1	J	159	HIS

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 29 ligands modelled in this entry, 17 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	$\# Z > 2$
4	MPD	A	1163	-	7,7,7	0.27	0	10,10,10	0.24	0
2	PHR	A	791	-	31,33,33	1.58	5 (16%)	40,47,47	4.07	13 (32%)
2	PHR	B	791	-	31,33,33	1.69	5 (16%)	40,47,47	3.82	14 (35%)
2	PHR	C	791	-	31,33,33	1.64	5 (16%)	40,47,47	3.76	13 (32%)
2	PHR	D	791	-	31,33,33	1.66	5 (16%)	40,47,47	4.00	13 (32%)
2	PHR	E	791	-	31,33,33	1.71	5 (16%)	40,47,47	3.78	13 (32%)
2	PHR	F	791	-	31,33,33	1.52	5 (16%)	40,47,47	4.07	14 (35%)
2	PHR	G	791	-	31,33,33	1.58	5 (16%)	40,47,47	3.78	14 (35%)
2	PHR	H	791	-	31,33,33	1.59	5 (16%)	40,47,47	3.89	14 (35%)
2	PHR	I	791	-	31,33,33	1.68	5 (16%)	40,47,47	3.86	12 (30%)
4	MPD	J	1164	-	7,7,7	0.26	0	10,10,10	0.32	0
2	PHR	J	791	-	31,33,33	1.66	5 (16%)	40,47,47	3.88	15 (37%)

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
4	MPD	A	1163	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PHR	A	791	-	-	0/25/57/57	0/0/2/2
2	PHR	B	791	-	-	0/25/57/57	0/0/2/2
2	PHR	C	791	-	-	0/25/57/57	0/0/2/2
2	PHR	D	791	-	-	2/25/57/57	0/0/2/2
2	PHR	E	791	-	-	0/25/57/57	0/0/2/2
2	PHR	F	791	-	-	0/25/57/57	0/0/2/2
2	PHR	G	791	-	-	0/25/57/57	0/0/2/2
2	PHR	H	791	-	-	0/25/57/57	0/0/2/2
2	PHR	I	791	-	-	2/25/57/57	0/0/2/2
4	MPD	J	1164	-	-	0/5/5/5	0/0/0/0
2	PHR	J	791	-	-	0/25/57/57	0/0/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	791	PHR	C9-C4	6.11	1.49	1.43
2	J	791	PHR	C9-C4	6.03	1.49	1.43
2	I	791	PHR	C9-C4	6.00	1.49	1.43
2	B	791	PHR	C9-C4	5.85	1.49	1.43
2	C	791	PHR	C9-C4	5.66	1.49	1.43
2	D	791	PHR	C9-C4	5.62	1.49	1.43
2	H	791	PHR	C9-C4	5.37	1.48	1.43
2	A	791	PHR	C9-C4	5.37	1.48	1.43
2	G	791	PHR	C9-C4	4.92	1.48	1.43
2	F	791	PHR	C9-C4	4.81	1.48	1.43
2	D	791	PHR	C4-N3	-4.24	1.35	1.39
2	E	791	PHR	C4-N3	-4.21	1.35	1.39
2	C	791	PHR	C4-N3	-4.16	1.35	1.39
2	B	791	PHR	C4-N3	-4.07	1.35	1.39
2	I	791	PHR	C4-N3	-4.01	1.35	1.39
2	G	791	PHR	C4-N3	-3.82	1.35	1.39
2	A	791	PHR	C4-N3	-3.69	1.35	1.39
2	H	791	PHR	C4-N3	-3.66	1.35	1.39
2	J	791	PHR	C4-N3	-3.66	1.35	1.39
2	D	791	PHR	O4-C6	3.60	1.29	1.22
2	F	791	PHR	C4-N3	-3.57	1.36	1.39
2	B	791	PHR	O4-C6	3.54	1.29	1.22
2	H	791	PHR	O4-C6	3.54	1.29	1.22
2	I	791	PHR	O4-C6	3.52	1.29	1.22
2	J	791	PHR	O4-C6	3.52	1.29	1.22
2	E	791	PHR	O4-C6	3.51	1.29	1.22
2	C	791	PHR	O4-C6	3.50	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	791	PHR	O4-C6	3.40	1.29	1.22
2	G	791	PHR	O4-C6	3.36	1.29	1.22
2	G	791	PHR	C6-N5	-3.33	1.34	1.38
2	A	791	PHR	C6-N5	-3.30	1.34	1.38
2	F	791	PHR	O4-C6	3.29	1.28	1.22
2	F	791	PHR	C6-N5	-3.27	1.34	1.38
2	G	791	PHR	C6-N7	-3.19	1.34	1.38
2	H	791	PHR	C6-N5	-3.10	1.34	1.38
2	B	791	PHR	C6-N5	-3.07	1.34	1.38
2	J	791	PHR	C6-N5	-3.07	1.34	1.38
2	E	791	PHR	C6-N5	-3.05	1.34	1.38
2	D	791	PHR	C6-N5	-3.03	1.34	1.38
2	C	791	PHR	C6-N5	-3.02	1.34	1.38
2	I	791	PHR	C6-N5	-3.01	1.34	1.38
2	F	791	PHR	C6-N7	-2.90	1.35	1.38
2	B	791	PHR	C6-N7	-2.88	1.35	1.38
2	J	791	PHR	C6-N7	-2.86	1.35	1.38
2	E	791	PHR	C6-N7	-2.82	1.35	1.38
2	D	791	PHR	C6-N7	-2.80	1.35	1.38
2	H	791	PHR	C6-N7	-2.77	1.35	1.38
2	I	791	PHR	C6-N7	-2.73	1.35	1.38
2	C	791	PHR	C6-N7	-2.69	1.35	1.38
2	A	791	PHR	C6-N7	-2.53	1.35	1.38

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	791	PHR	O2-C4-C9	-14.81	121.60	127.62
2	B	791	PHR	C8-N7-C6	-13.68	104.12	117.13
2	A	791	PHR	O2-C4-C9	-13.54	122.11	127.62
2	I	791	PHR	C8-N7-C6	-13.39	104.39	117.13
2	D	791	PHR	C8-N7-C6	-13.34	104.44	117.13
2	E	791	PHR	C8-N7-C6	-13.33	104.45	117.13
2	J	791	PHR	C8-N7-C6	-13.21	104.56	117.13
2	A	791	PHR	C8-N7-C6	-13.14	104.64	117.13
2	C	791	PHR	C8-N7-C6	-13.12	104.65	117.13
2	H	791	PHR	C8-N7-C6	-12.86	104.90	117.13
2	F	791	PHR	C8-N7-C6	-12.74	105.02	117.13
2	G	791	PHR	C8-N7-C6	-12.63	105.12	117.13
2	H	791	PHR	O2-C4-C9	-12.52	122.53	127.62
2	G	791	PHR	O2-C4-C9	-12.49	122.54	127.62
2	J	791	PHR	O2-C4-C9	-11.63	122.89	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	791	PHR	O2-C4-C9	-11.50	122.94	127.62
2	I	791	PHR	O2-C4-C9	-10.84	123.21	127.62
2	C	791	PHR	O2-C4-C9	-10.34	123.41	127.62
2	B	791	PHR	O2-C4-C9	-10.25	123.45	127.62
2	E	791	PHR	O2-C4-C9	-10.06	123.53	127.62
2	A	791	PHR	C9-N5-C6	-9.70	102.58	111.14
2	H	791	PHR	C9-N5-C6	-9.55	102.72	111.14
2	F	791	PHR	C9-N5-C6	-9.41	102.84	111.14
2	D	791	PHR	C9-N5-C6	-9.40	102.85	111.14
2	C	791	PHR	C9-N5-C6	-9.39	102.86	111.14
2	I	791	PHR	C9-N5-C6	-9.36	102.89	111.14
2	E	791	PHR	C9-N5-C6	-9.32	102.92	111.14
2	J	791	PHR	C9-N5-C6	-9.11	103.10	111.14
2	B	791	PHR	C9-N5-C6	-9.01	103.20	111.14
2	G	791	PHR	C9-N5-C6	-8.87	103.31	111.14
2	A	791	PHR	N7-C6-N5	7.79	117.37	106.26
2	D	791	PHR	N7-C6-N5	7.73	117.28	106.26
2	I	791	PHR	N7-C6-N5	7.69	117.23	106.26
2	E	791	PHR	N7-C6-N5	7.67	117.20	106.26
2	B	791	PHR	N7-C6-N5	7.65	117.16	106.26
2	C	791	PHR	N7-C6-N5	7.62	117.13	106.26
2	H	791	PHR	N7-C6-N5	7.53	117.00	106.26
2	J	791	PHR	N7-C6-N5	7.49	116.94	106.26
2	F	791	PHR	N7-C6-N5	7.34	116.73	106.26
2	G	791	PHR	N7-C6-N5	7.12	116.41	106.26
2	D	791	PHR	C10-N7-C8	5.79	131.39	125.50
2	B	791	PHR	C10-N7-C8	5.08	130.67	125.50
2	D	791	PHR	C4-N3-C2	-4.91	121.94	126.17
2	J	791	PHR	C4-N3-C2	-4.90	121.94	126.17
2	J	791	PHR	N3-C2-N1	4.69	123.77	115.85
2	B	791	PHR	C15-N5-C6	4.62	128.86	122.37
2	D	791	PHR	C9-C4-N3	4.54	116.95	114.61
2	I	791	PHR	C10-N7-C8	4.45	130.02	125.50
2	D	791	PHR	N3-C2-N1	4.43	123.34	115.85
2	B	791	PHR	N3-C2-N1	4.39	123.27	115.85
2	E	791	PHR	N3-C2-N1	4.34	123.18	115.85
2	C	791	PHR	N3-C2-N1	4.27	123.06	115.85
2	E	791	PHR	C4-N3-C2	-4.26	122.50	126.17
2	I	791	PHR	C4-N3-C2	-4.24	122.51	126.17
2	B	791	PHR	C4-N3-C2	-4.18	122.56	126.17
2	G	791	PHR	C15-N5-C6	4.17	128.24	122.37
2	I	791	PHR	N3-C2-N1	4.14	122.84	115.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	791	PHR	C15-N5-C6	4.14	128.19	122.37
2	G	791	PHR	N3-C2-N1	4.11	122.78	115.85
2	A	791	PHR	C4-N3-C2	-4.10	122.63	126.17
2	H	791	PHR	N3-C2-N1	4.08	122.74	115.85
2	A	791	PHR	C9-C4-N3	4.08	116.71	114.61
2	A	791	PHR	O4-C6-N5	-4.07	120.77	126.74
2	C	791	PHR	C10-N7-C8	4.06	129.63	125.50
2	F	791	PHR	N3-C2-N1	3.98	122.58	115.85
2	A	791	PHR	N3-C2-N1	3.98	122.57	115.85
2	F	791	PHR	C4-N3-C2	-3.96	122.75	126.17
2	I	791	PHR	C9-C4-N3	3.96	116.65	114.61
2	A	791	PHR	C10-N7-C8	3.95	129.52	125.50
2	C	791	PHR	C4-N3-C2	-3.93	122.78	126.17
2	A	791	PHR	C15-N5-C9	3.93	130.01	125.78
2	D	791	PHR	O4-C6-N7	-3.89	121.02	126.74
2	H	791	PHR	C15-N5-C6	3.89	127.84	122.37
2	J	791	PHR	C15-N5-C6	3.89	127.84	122.37
2	B	791	PHR	O4-C6-N7	-3.89	121.03	126.74
2	E	791	PHR	C15-N5-C6	3.87	127.82	122.37
2	C	791	PHR	C15-N5-C6	3.85	127.79	122.37
2	H	791	PHR	C4-N3-C2	-3.79	122.90	126.17
2	E	791	PHR	O4-C6-N5	-3.78	121.19	126.74
2	I	791	PHR	C15-N5-C6	3.72	127.61	122.37
2	I	791	PHR	O4-C6-N5	-3.71	121.30	126.74
2	J	791	PHR	O4-C6-N7	-3.69	121.32	126.74
2	C	791	PHR	O4-C6-N7	-3.69	121.33	126.74
2	H	791	PHR	O4-C6-N7	-3.66	121.37	126.74
2	E	791	PHR	C10-N7-C8	3.65	129.22	125.50
2	D	791	PHR	C15-N5-C9	3.65	129.71	125.78
2	D	791	PHR	C15-N5-C6	3.61	127.45	122.37
2	F	791	PHR	O4-C6-N5	-3.59	121.46	126.74
2	I	791	PHR	O4-C6-N7	-3.59	121.47	126.74
2	A	791	PHR	C15-N5-C6	3.58	127.41	122.37
2	C	791	PHR	O4-C6-N5	-3.54	121.55	126.74
2	G	791	PHR	C4-N3-C2	-3.50	123.15	126.17
2	E	791	PHR	O4-C6-N7	-3.49	121.61	126.74
2	H	791	PHR	C10-N7-C8	3.48	129.04	125.50
2	H	791	PHR	O4-C6-N5	-3.48	121.63	126.74
2	E	791	PHR	C9-C4-N3	3.47	116.40	114.61
2	I	791	PHR	C15-N5-C9	3.46	129.51	125.78
2	D	791	PHR	O4-C6-N5	-3.43	121.70	126.74
2	J	791	PHR	O4-C6-N5	-3.41	121.73	126.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	791	PHR	C9-C4-N3	3.41	116.36	114.61
2	H	791	PHR	C15-N5-C9	3.40	129.44	125.78
2	G	791	PHR	O4-C6-N5	-3.37	121.79	126.74
2	G	791	PHR	O4-C6-N7	-3.36	121.80	126.74
2	B	791	PHR	O4-C6-N5	-3.36	121.81	126.74
2	F	791	PHR	O4-C6-N7	-3.36	121.81	126.74
2	F	791	PHR	C9-C4-N3	3.35	116.33	114.61
2	C	791	PHR	C15-N5-C9	3.32	129.36	125.78
2	A	791	PHR	O4-C6-N7	-3.32	121.86	126.74
2	C	791	PHR	C9-C4-N3	3.27	116.29	114.61
2	F	791	PHR	O2-C4-N3	3.26	122.07	117.93
2	E	791	PHR	C15-N5-C9	3.24	129.27	125.78
2	J	791	PHR	C10-N7-C8	3.06	128.62	125.50
2	J	791	PHR	C15-N5-C9	3.04	129.05	125.78
2	H	791	PHR	C9-C4-N3	3.01	116.16	114.61
2	G	791	PHR	O2-C4-N3	2.99	121.72	117.93
2	F	791	PHR	C15-N5-C9	2.97	128.97	125.78
2	G	791	PHR	C10-N7-C6	2.94	128.23	122.83
2	J	791	PHR	O1-C2-N1	-2.91	117.52	121.80
2	H	791	PHR	O2-C4-N3	2.66	121.31	117.93
2	F	791	PHR	C10-N7-C6	2.65	127.70	122.83
2	A	791	PHR	O2-C4-N3	2.56	121.17	117.93
2	G	791	PHR	O1-C2-N1	-2.55	118.06	121.80
2	G	791	PHR	C15-N5-C9	2.48	128.45	125.78
2	B	791	PHR	C9-C4-N3	2.39	115.84	114.61
2	J	791	PHR	O2-C4-N3	2.22	120.74	117.93
2	G	791	PHR	C9-C4-N3	2.20	115.74	114.61
2	B	791	PHR	O2-C4-N3	2.19	120.70	117.93
2	J	791	PHR	C10-N7-C6	2.17	126.81	122.83
2	F	791	PHR	O1-C2-N1	-2.16	118.63	121.80
2	B	791	PHR	O1-C2-N1	-2.15	118.64	121.80
2	E	791	PHR	O1-C2-N1	-2.13	118.67	121.80
2	C	791	PHR	O1-C2-N3	-2.09	117.48	121.76
2	D	791	PHR	O1-C2-N3	-2.05	117.56	121.76
2	H	791	PHR	O1-C2-N1	-2.03	118.82	121.80
2	B	791	PHR	C15-N5-C9	2.01	127.94	125.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	791	PHR	C11-C10-N7-C8

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Mol	Chain	Res	Type	Atoms
2	I	791	PHR	C11-C10-N7-C8
2	D	791	PHR	C11-C10-N7-C6
2	I	791	PHR	C11-C10-N7-C6

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	147/160 (91%)	-0.14	1 (0%) 84 85	31, 32, 33, 34	0
1	B	147/160 (91%)	-0.20	1 (0%) 84 85	31, 32, 32, 34	0
1	C	146/160 (91%)	-0.28	1 (0%) 84 85	31, 32, 32, 33	0
1	D	147/160 (91%)	-0.19	1 (0%) 84 85	31, 32, 32, 34	0
1	E	146/160 (91%)	-0.13	2 (1%) 72 72	31, 32, 32, 33	0
1	F	147/160 (91%)	-0.16	3 (2%) 62 63	31, 32, 32, 33	0
1	G	147/160 (91%)	-0.22	1 (0%) 84 85	30, 32, 32, 33	0
1	H	146/160 (91%)	-0.27	2 (1%) 72 72	31, 32, 32, 33	0
1	I	147/160 (91%)	-0.22	0 100 100	30, 32, 32, 33	0
1	J	146/160 (91%)	-0.10	0 100 100	31, 32, 32, 33	0
All	All	1466/1600 (91%)	-0.19	12 (0%) 83 83	30, 32, 32, 34	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	29	GLY	4.1
1	H	121	THR	3.1
1	G	133	THR	2.6
1	B	160	SER	2.5
1	F	132	PRO	2.3
1	F	49	ASP	2.2
1	E	132	PRO	2.2
1	A	132	PRO	2.2
1	D	44	ALA	2.1
1	F	86	GLN	2.1
1	H	29	GLY	2.0
1	C	160	SER	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
4	MPD	J	1164	8/8	0.23	10.69	38,38,39,40	0
4	MPD	A	1163	8/8	0.22	1.74	39,40,40,40	0
2	PHR	D	791	32/32	0.19	0.70	36,37,38,39	0
2	PHR	G	791	32/32	0.17	0.38	31,35,41,41	0
2	PHR	A	791	32/32	0.18	0.15	35,38,40,40	0
2	PHR	E	791	32/32	0.18	0.05	31,32,35,36	0
2	PHR	C	791	32/32	0.16	-0.04	33,36,39,40	0
2	PHR	J	791	32/32	0.18	-0.06	33,33,34,34	0
2	PHR	I	791	32/32	0.15	-0.18	29,32,37,37	0
2	PHR	F	791	32/32	0.16	-0.36	34,35,37,38	0
2	PHR	H	791	32/32	0.15	-0.37	32,34,35,36	0
3	K	I	1161	1/1	0.11	-0.74	29,29,29,29	0
3	K	G	1161	1/1	0.15	-0.86	29,29,29,29	0
2	PHR	B	791	32/32	0.13	-1.03	30,34,37,37	0
3	K	J	1163	1/1	0.10	-1.37	51,51,51,51	0
3	K	B	1161	1/1	0.13	-1.42	32,32,32,32	0
3	K	C	1161	1/1	0.09	-2.21	29,29,29,29	0
3	K	B	1162	1/1	0.09	-2.24	31,31,31,31	0
3	K	H	1161	1/1	0.11	-2.39	31,31,31,31	0
3	K	A	1161	1/1	0.07	-2.40	30,30,30,30	0
3	K	C	1162	1/1	0.06	-2.57	36,36,36,36	0
3	K	E	1162	1/1	0.06	-2.82	38,38,38,38	0
3	K	B	1163	1/1	0.05	-2.86	32,32,32,32	0
3	K	F	1161	1/1	0.08	-2.91	32,32,32,32	0
3	K	A	1162	1/1	0.06	-3.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	K	E	1161	1/1	0.11	-3.11	30,30,30,30	0
3	K	J	1161	1/1	0.10	-3.33	50,50,50,50	0
3	K	J	1162	1/1	0.08	-3.40	31,31,31,31	0
3	K	D	1161	1/1	0.07	-3.43	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.