



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:08 PM GMT

PDB ID : 3Q9T
Title : Crystal structure analysis of formate oxidase
Authors : Doubayashi, D.; Ootake, T.; Maeda, Y.; Oki, M.; Tokunaga, Y.; Sakurai, A.;
Nagaosa, Y.; Mikami, B.; Uchida, H.
Deposited on : 2011-01-09
Resolution : 2.24 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>

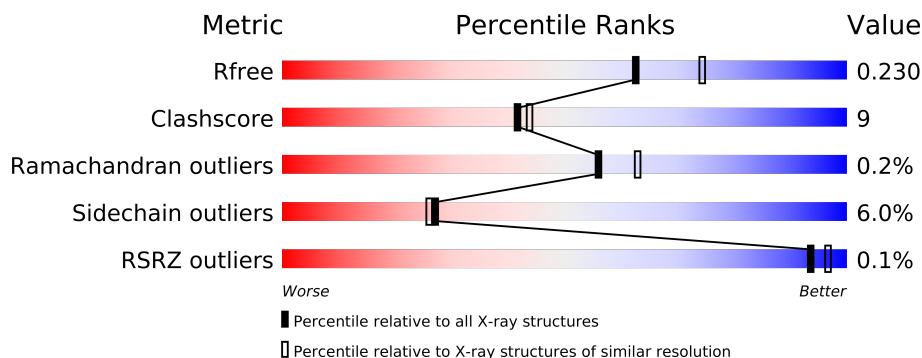
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.24 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	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

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	577	<div><div></div><div></div></div>
1	B	577	<div><div></div><div></div></div>
1	C	577	<div><div></div><div></div></div>

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

Mol	Type	Chain	Res	Geometry	Electron density
3	MRD	A	581	-	X
3	MRD	A	582	-	X
4	ACT	A	1	-	X

2 Entry composition i

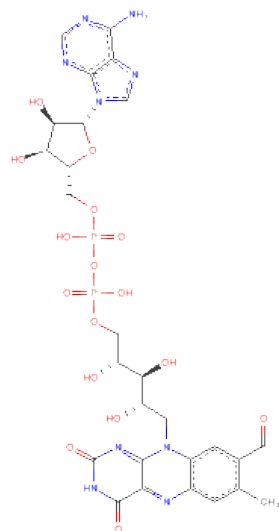
There are 7 unique types of molecules in this entry. The entry contains 14820 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Choline dehydrogenase and related flavoproteins.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	8	9	0
			4590	2910	800	860	20			
1	B	577	Total	C	N	O	S	8	7	0
			4571	2899	793	858	21			
1	C	577	Total	C	N	O	S	0	5	0
			4562	2893	791	858	20			

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL(2R,3S,4S)-5-(8-FORMYL-7-METHYL-2,4-DIOXO-3,4-DIHYDROBENZO[G]PTERIDIN-10(2H)-YL)-2,3,4-TRIHIDROXYPENTYLDIHYDROGEN DIPHOSPHATE (three-letter code: FAY) (formula: C₂₇H₃₁N₉O₁₆P₂).



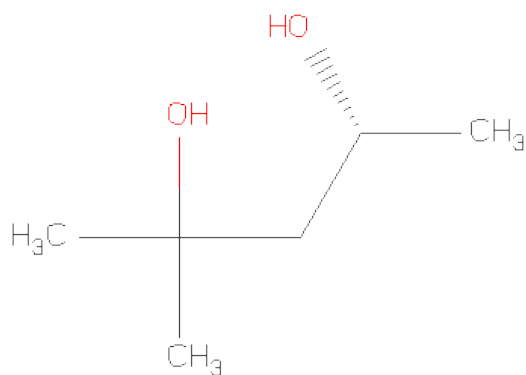
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			54	27	9	16	2		
2	B	1	Total	C	N	O	P	0	0
			54	27	9	16	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			54	27	9	16	2		

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



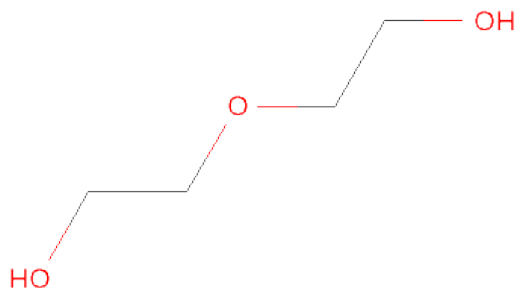
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		

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



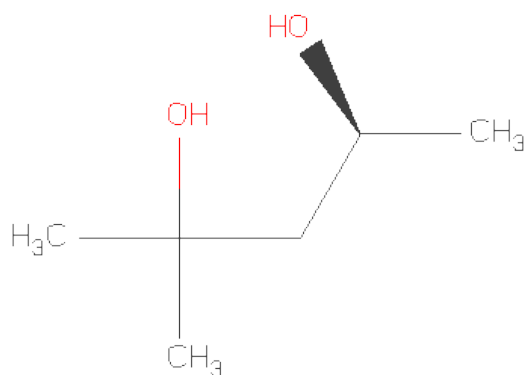
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 7 is water.

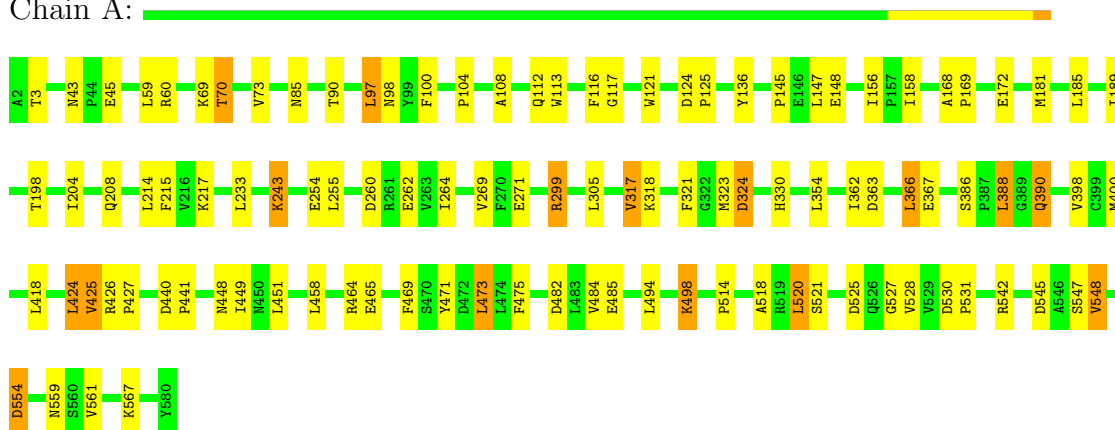
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	406	Total	O	0	0
			406	406		
7	B	265	Total	O	0	0
			265	265		
7	C	229	Total	O	0	0
			229	229		

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.

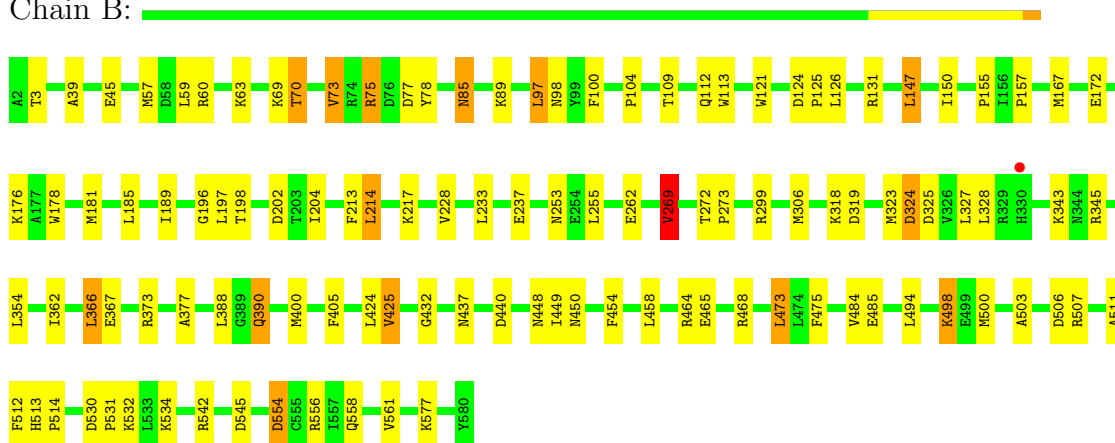
- Molecule 1: Choline dehydrogenase and related flavoproteins

Chain A:



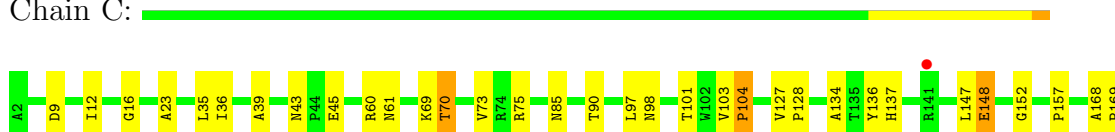
- Molecule 1: Choline dehydrogenase and related flavoproteins

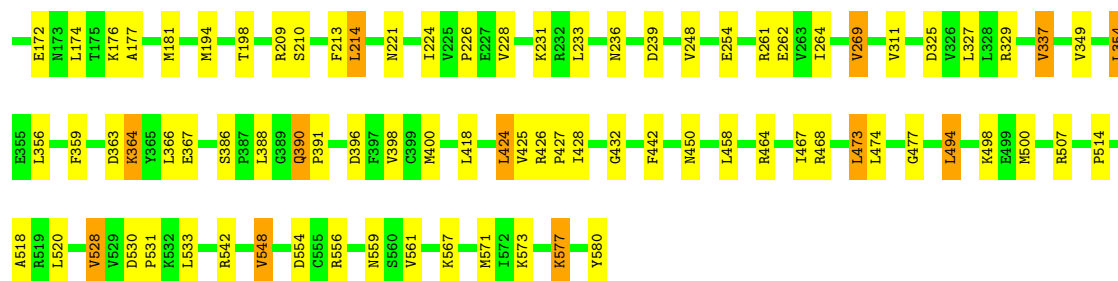
Chain B:



- Molecule 1: Choline dehydrogenase and related flavoproteins

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	156.68Å 156.02Å 184.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.24 49.53 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.52-2.24) 98.4 (49.53-2.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.184 , 0.236 0.179 , 0.230	Depositor DCC
R_{free} test set	5337 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.5	EDS
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 106556 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14820	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: MRD, MPD, FAY, PEG, 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	0.41	0/4724	0.61	1/6405 (0.0%)
1	B	0.37	0/4702	0.56	1/6375 (0.0%)
1	C	0.34	0/4687	0.54	0/6355
All	All	0.38	0/14113	0.57	2/19135 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	VAL	CB-CA-C	-6.31	99.41	111.40
1	A	473	LEU	CA-CB-CG	5.67	128.33	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	4590	0	4525	84	0
1	B	4571	0	4503	77	0
1	C	4562	0	4488	80	0
2	A	54	0	29	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	54	0	29	7	0
2	C	54	0	29	5	0
3	A	16	0	28	12	0
4	A	4	0	3	1	0
5	B	7	0	10	1	0
6	C	8	0	14	3	0
7	A	406	0	0	11	0
7	B	265	0	0	12	0
7	C	229	0	0	5	0
All	All	14820	0	13658	251	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 9.

All (251) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:325:ASP:HB3	1:C:329:ARG:HH21	1.20	1.00
3:A:581:MRD:H1C2	3:A:581:MRD:H5C3	1.43	0.99
1:A:299[A]:ARG:HH11	1:A:299[A]:ARG:HB2	1.29	0.96
1:B:390[B]:GLN:H	1:B:390[B]:GLN:HE21	1.14	0.95
1:B:327:LEU:HB2	1:B:400:MET:HE3	1.53	0.88
1:B:327:LEU:HB2	1:B:400:MET:CE	2.10	0.81
1:B:485:GLU:HG2	7:B:715:HOH:O	1.81	0.79
3:A:581:MRD:H1C1	7:A:909:HOH:O	1.83	0.78
1:C:12:ILE:HG13	1:C:23:ALA:HB2	1.65	0.78
1:A:390[B]:GLN:HE21	1:A:390[B]:GLN:H	1.30	0.77
1:A:318:LYS:HE2	1:A:482:ASP:O	1.83	0.77
1:C:325:ASP:HB3	1:C:329:ARG:NH2	2.00	0.77
1:A:299[A]:ARG:HH11	1:A:299[A]:ARG:CB	1.98	0.76
1:C:364[A]:LYS:O	1:C:364[A]:LYS:HD3	1.87	0.75
1:C:236:ASN:HB3	1:C:239:ASP:HB3	1.68	0.74
1:C:327:LEU:HB2	1:C:400:MET:HE1	1.70	0.73
1:B:262:GLU:OE1	1:B:542:ARG:HD2	1.88	0.73
1:C:327:LEU:HB2	1:C:400:MET:CE	2.19	0.72
3:A:581:MRD:H1C2	3:A:581:MRD:C5	2.20	0.71
1:B:75[A]:ARG:HD3	1:B:77:ASP:OD1	1.91	0.71
1:B:63:LYS:HE2	7:B:725:HOH:O	1.90	0.71
1:C:498:LYS:HE3	7:C:735:HOH:O	1.91	0.71
1:C:567:LYS:HE3	1:C:571:MET:HE3	1.72	0.69
1:C:337:VAL:CG1	1:C:349:VAL:HG23	2.23	0.69
1:B:390[B]:GLN:NE2	1:B:390[B]:GLN:H	1.91	0.69
1:B:437[A]:ASN:ND2	1:B:448[A]:ASN:OD1	2.26	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:181:MET:HE2	7:C:759:HOH:O	1.93	0.68
1:B:299:ARG:HG2	7:B:638:HOH:O	1.92	0.68
3:A:581:MRD:C1	3:A:581:MRD:H5C3	2.22	0.68
1:B:388:LEU:H	1:B:390[B]:GLN:HE22	1.43	0.67
1:B:328:LEU:HG	1:B:400:MET:CE	2.24	0.67
1:C:337:VAL:HG13	1:C:349:VAL:HG23	1.76	0.67
1:A:262:GLU:OE1	1:A:542:ARG:HD2	1.95	0.65
1:A:386:SER:HB3	1:A:390[A]:GLN:HG2	1.79	0.64
1:B:561:VAL:HG21	2:B:600:FAY:H5'A	1.79	0.63
6:C:1:MPD:O2	6:C:1:MPD:H52	1.98	0.62
1:C:157:PRO:HD2	1:C:210:SER:HB3	1.81	0.62
1:B:318[B]:LYS:HD3	1:B:319:ASP:O	2.00	0.62
1:B:464:ARG:HD2	1:B:465:GLU:OE2	1.99	0.61
3:A:581:MRD:H1C3	7:A:730:HOH:O	2.00	0.61
1:C:236:ASN:HB3	1:C:239:ASP:CB	2.31	0.61
1:C:386:SER:CB	1:C:390[A]:GLN:HG2	2.31	0.61
1:B:328:LEU:HG	1:B:400:MET:HE2	1.81	0.60
1:A:363:ASP:O	1:A:367:GLU:HG2	1.99	0.60
1:C:533:LEU:HD22	1:C:548:VAL:HG21	1.82	0.60
1:B:425:VAL:HG13	1:B:554:ASP:HA	1.84	0.60
1:A:471:TYR:HD1	3:A:581:MRD:H5C2	1.67	0.60
1:A:324:ASP:HA	1:A:400:MET:CE	2.32	0.59
1:C:494:LEU:HD23	6:C:1:MPD:H52	1.84	0.59
1:C:494:LEU:HD23	6:C:1:MPD:C5	2.32	0.59
1:A:386:SER:CB	1:A:390[A]:GLN:HG2	2.33	0.58
1:B:437[A]:ASN:OD1	1:B:448[A]:ASN:ND2	2.36	0.58
1:C:530:ASP:HB2	1:C:531:PRO:HD2	1.84	0.58
1:A:70:THR:HB	1:A:449:ILE:HB	1.85	0.58
1:A:424:LEU:HD13	1:A:427:PRO:HB3	1.86	0.58
1:A:324:ASP:HA	1:A:400:MET:HE2	1.85	0.57
1:B:306:MET:HE3	7:B:790:HOH:O	2.05	0.57
1:A:299[A]:ARG:CG	1:A:299[A]:ARG:HH11	2.18	0.57
1:C:530:ASP:HB2	1:C:531:PRO:CD	2.36	0.56
1:B:196:GLY:HA2	7:B:876:HOH:O	2.05	0.56
1:A:269:VAL:HG11	1:A:514:PRO:HB2	1.87	0.56
1:A:425:VAL:HG13	1:A:554:ASP:HA	1.87	0.56
1:A:124:ASP:HB2	1:A:125:PRO:HD3	1.88	0.56
1:A:485:GLU:HG2	7:A:750:HOH:O	2.05	0.56
1:C:518:ALA:HA	1:C:528:VAL:CG1	2.36	0.56
1:B:131:ARG:HD3	1:B:150:ILE:HA	1.89	0.55
1:A:156:ILE:HD11	1:A:215:PHE:CE2	2.42	0.55
1:A:181:MET:HE3	7:A:888:HOH:O	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:9:ASP:O	1:C:261:ARG:HB2	2.07	0.55
1:C:386:SER:HB3	1:C:390[A]:GLN:HG2	1.88	0.55
1:C:567:LYS:CE	1:C:571:MET:HE3	2.37	0.55
1:C:269:VAL:HG21	1:C:514:PRO:HG2	1.89	0.55
1:B:70:THR:HB	1:B:449:ILE:HB	1.90	0.54
1:C:464:ARG:HD3	1:C:468:ARG:NH2	2.22	0.54
1:B:155:PRO:O	1:B:157:PRO:HD3	2.08	0.54
1:C:101:THR:HB	1:C:556:ARG:HD2	1.90	0.54
1:A:475:PHE:CZ	1:A:484:VAL:HG11	2.44	0.53
1:B:507:ARG:HD2	7:B:618:HOH:O	2.09	0.52
1:A:136:TYR:CD2	1:A:148:GLU:HA	2.44	0.52
1:A:330:HIS:HD2	7:A:588:HOH:O	1.92	0.52
1:A:271:GLU:OE2	4:A:1:ACT:O	2.28	0.52
1:A:471:TYR:HB3	3:A:581:MRD:C5	2.40	0.52
1:A:45[A]:GLU:OE2	1:A:217:LYS:HD2	2.09	0.52
1:A:388:LEU:H	1:A:390[B]:GLN:HE22	1.58	0.52
1:B:113:TRP:HB2	1:B:121:TRP:O	2.10	0.52
1:C:264:ILE:HD12	1:C:264:ILE:N	2.25	0.51
1:C:221:ASN:N	1:C:221:ASN:OD1	2.43	0.51
1:C:269:VAL:HG22	7:C:589:HOH:O	2.11	0.51
1:C:60:ARG:O	1:C:61:ASN:HB2	2.10	0.51
2:C:600:FAY:O4'	2:C:600:FAY:C1'	2.58	0.51
1:A:299[A]:ARG:NH1	1:A:299[A]:ARG:HB2	2.13	0.51
1:B:60:ARG:HD2	7:B:738:HOH:O	2.10	0.51
1:B:213:PHE:CD2	1:B:214:LEU:HD13	2.46	0.51
1:A:390[A]:GLN:HG3	1:A:426:ARG:HD2	1.93	0.51
1:A:156:ILE:HD11	1:A:215:PHE:HE2	1.75	0.51
1:A:530:ASP:HB2	1:A:531:PRO:CD	2.41	0.51
1:C:518:ALA:HA	1:C:528:VAL:HG13	1.93	0.50
1:B:124:ASP:HB2	1:B:125:PRO:HD3	1.92	0.50
1:B:45[A]:GLU:CD	1:B:45[A]:GLU:H	2.15	0.50
1:A:464:ARG:HD2	1:A:465:GLU:OE2	2.11	0.50
1:A:299[A]:ARG:NH2	1:A:525:ASP:OD1	2.44	0.50
1:A:45[B]:GLU:CD	1:A:45[B]:GLU:H	2.15	0.50
1:C:231:LYS:HE3	1:C:254:GLU:OE1	2.12	0.50
3:A:582:MRD:H4	1:C:428:ILE:HD12	1.93	0.50
1:A:113:TRP:HB2	1:A:121:TRP:O	2.12	0.50
1:A:330:HIS:CD2	7:A:588:HOH:O	2.65	0.49
1:C:573:LYS:HE2	1:C:580:TYR:CE2	2.46	0.49
1:C:168:ALA:HB3	1:C:169:PRO:HD3	1.94	0.49
1:C:390[A]:GLN:HG3	1:C:426:ARG:HD2	1.93	0.49
1:A:318:LYS:NZ	7:A:750:HOH:O	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:520[A]:LEU:HD12	1:A:521:SER:N	2.28	0.49
1:A:471:TYR:HB3	3:A:581:MRD:H5C1	1.94	0.49
1:C:327:LEU:HB2	1:C:400:MET:HE3	1.93	0.49
1:A:60:ARG:HD2	7:A:664:HOH:O	2.12	0.49
1:B:432:GLY:HA3	1:B:450:ASN:O	2.12	0.49
3:A:581:MRD:C1	3:A:581:MRD:C5	2.88	0.48
1:C:386:SER:OG	1:C:390[A]:GLN:HG2	2.12	0.48
1:B:189:ILE:HD13	1:B:198:THR:HG21	1.94	0.48
1:B:57:MET:HE1	1:B:405:PHE:CD2	2.49	0.48
1:C:424:LEU:HD13	1:C:427:PRO:HB3	1.95	0.48
1:A:471:TYR:CD1	3:A:581:MRD:H5C2	2.48	0.48
1:C:224:ILE:HG22	1:C:226:PRO:HD3	1.95	0.48
1:C:390[A]:GLN:H	1:C:390[A]:GLN:CD	2.16	0.48
1:A:121:TRP:CH2	1:A:567:LYS:HD3	2.49	0.48
1:A:98:ASN:HB2	2:A:600:FAY:C5X	2.44	0.48
1:A:323:MET:C	1:A:400:MET:HE3	2.34	0.48
1:B:464:ARG:HG3	1:B:500:MET:HB3	1.96	0.48
1:B:45[B]:GLU:CD	1:B:217:LYS:HZ2	2.17	0.48
1:C:69:LYS:O	1:C:70:THR:HG22	2.14	0.48
1:A:362:ILE:HG13	1:A:366:LEU:HD22	1.96	0.47
1:A:330:HIS:CE1	7:A:705:HOH:O	2.67	0.47
1:A:108:ALA:O	1:A:112[B]:GLN:HG2	2.14	0.47
1:B:109:THR:O	1:B:112:GLN:HB2	2.14	0.47
1:C:134:ALA:O	1:C:152:GLY:N	2.47	0.47
1:A:117:GLY:N	1:A:520[A]:LEU:HD11	2.30	0.47
1:C:16:GLY:HA3	2:C:600:FAY:O5B	2.15	0.47
1:B:178:TRP:CE2	1:B:197:LEU:HB2	2.49	0.46
1:C:464:ARG:HG3	1:C:500:MET:HB3	1.96	0.46
5:B:1:PEG:H32	5:B:1:PEG:H11	1.58	0.46
1:A:305:LEU:HD21	1:A:451:LEU:HD23	1.97	0.46
1:B:327:LEU:HB2	1:B:400:MET:HE1	1.95	0.46
1:A:561:VAL:HG21	2:A:600:FAY:H5'A	1.98	0.46
1:C:103:VAL:HG23	1:C:104:PRO:HD2	1.98	0.46
1:B:545:ASP:HB2	2:B:600:FAY:O2P	2.16	0.46
1:C:507:ARG:HD2	7:C:597:HOH:O	2.16	0.46
1:A:530:ASP:HB2	1:A:531:PRO:HD2	1.98	0.46
1:B:498:LYS:HA	1:B:498:LYS:HD2	1.52	0.46
1:B:475:PHE:CZ	1:B:484:VAL:HG11	2.50	0.46
1:B:530:ASP:HB2	1:B:531:PRO:CD	2.46	0.46
1:C:432:GLY:HA3	1:C:450:ASN:O	2.16	0.46
2:B:600:FAY:C1'	2:B:600:FAY:O4'	2.64	0.45
1:B:69:LYS:O	1:B:70:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:ALA:HB3	1:A:169:PRO:HD3	1.96	0.45
1:C:127:VAL:HB	1:C:128:PRO:HD3	1.98	0.45
1:A:390[A]:GLN:H	1:A:390[A]:GLN:CD	2.20	0.45
1:B:202:ASP:C	1:B:204:ILE:H	2.20	0.45
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.85	0.45
1:C:473:LEU:HD13	1:C:474:LEU:CD2	2.47	0.45
1:B:513:HIS:CE1	1:B:556:ARG:HG2	2.51	0.45
1:A:521:SER:HB3	1:A:527:GLY:HA3	1.98	0.45
1:B:181:MET:HG3	1:B:473:LEU:HD23	1.98	0.45
1:A:145:PRO:O	1:A:148:GLU:HG2	2.17	0.45
1:A:260:ASP:OD2	3:A:582:MRD:H5C2	2.16	0.45
1:B:362:ILE:HG13	1:B:366:LEU:HD22	1.99	0.45
1:B:75[B]:ARG:HD2	1:B:454:PHE:O	2.16	0.45
1:A:156:ILE:CD1	1:A:215:PHE:HE2	2.30	0.45
1:A:70:THR:HG23	1:A:85:ASN:CB	2.47	0.44
1:A:398:VAL:O	1:A:418:LEU:HD12	2.17	0.44
1:C:577:LYS:HD2	1:C:577:LYS:HA	1.76	0.44
1:C:354:LEU:HD11	1:C:396:ASP:HB3	2.00	0.44
1:B:511:ALA:O	1:B:512:PHE:HB2	2.17	0.44
1:B:39:ALA:HA	1:B:228:VAL:O	2.18	0.44
1:B:98:ASN:HB2	2:B:600:FAY:N5	2.33	0.44
1:A:59:LEU:HD13	1:A:97:LEU:HB3	2.00	0.44
1:B:503:ALA:O	1:B:507:ARG:HB2	2.18	0.44
2:A:600:FAY:C1'	2:A:600:FAY:O4'	2.65	0.44
1:C:35:LEU:HD12	1:C:36:ILE:N	2.33	0.44
1:B:425:VAL:HG13	1:B:554:ASP:CA	2.48	0.44
1:B:59:LEU:HD13	1:B:97:LEU:HB3	1.99	0.44
1:C:262:GLU:OE2	1:C:542:ARG:NH1	2.51	0.44
1:A:264:ILE:HD12	1:A:264:ILE:N	2.33	0.44
1:B:70:THR:HG23	1:B:85:ASN:CB	2.47	0.43
1:C:363:ASP:O	1:C:367:GLU:HG2	2.19	0.43
1:A:498:LYS:HD2	1:A:498:LYS:HA	1.84	0.43
1:C:567:LYS:NZ	1:C:571:MET:CE	2.81	0.43
1:C:98:ASN:HB2	2:C:600:FAY:C5X	2.48	0.43
1:A:269:VAL:HA	1:A:547:SER:HB3	2.00	0.43
1:B:272:THR:N	1:B:273:PRO:HD2	2.33	0.43
1:C:561:VAL:HG21	2:C:600:FAY:H5'A	2.01	0.43
1:B:388:LEU:H	1:B:390[B]:GLN:NE2	2.11	0.43
1:C:248:VAL:HB	1:C:442:PHE:HZ	1.82	0.43
1:B:534:LYS:HE2	7:B:712:HOH:O	2.19	0.43
1:A:254:GLU:OE1	1:B:440:ASP:OD2	2.36	0.43
1:A:390[A]:GLN:HG3	1:A:426:ARG:CD	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:469:PHE:CD2	1:A:469:PHE:C	2.92	0.43
1:C:311:VAL:HG11	1:C:467:ILE:HD11	2.00	0.43
1:C:136:TYR:CD2	1:C:148:GLU:HA	2.54	0.43
1:B:167:MET:CE	1:B:323:MET:SD	3.07	0.43
1:C:157:PRO:HD2	1:C:210:SER:CB	2.48	0.42
1:C:174:LEU:HD23	1:C:356:LEU:HD12	2.00	0.42
1:C:398:VAL:O	1:C:418:LEU:HD12	2.19	0.42
1:C:45[A]:GLU:H	1:C:45[A]:GLU:CD	2.22	0.42
1:B:532:LYS:HB3	1:B:542:ARG:HH21	1.84	0.42
1:A:299[A]:ARG:CG	1:A:299[A]:ARG:NH1	2.80	0.42
1:B:367:GLU:O	1:B:373:ARG:HD3	2.20	0.42
1:B:73:VAL:HG23	1:B:75[A]:ARG:HG2	2.01	0.42
1:A:70:THR:HG23	1:A:85:ASN:HB2	2.01	0.42
1:C:396:ASP:CG	1:C:556:ARG:HH21	2.23	0.42
1:A:156:ILE:CD1	1:A:215:PHE:CE2	3.02	0.42
1:A:116:PHE:C	1:A:520[A]:LEU:HD11	2.40	0.42
1:A:100:PHE:CG	1:A:204:ILE:HD11	2.54	0.42
1:A:243:LYS:HE2	7:A:920:HOH:O	2.18	0.42
1:A:189:ILE:HD13	1:A:198:THR:HG21	2.01	0.42
1:C:43:ASN:HA	1:C:45[A]:GLU:OE2	2.19	0.42
1:C:518:ALA:HA	1:C:528:VAL:HG11	2.01	0.42
1:B:324:ASP:OD1	1:B:324:ASP:N	2.51	0.42
1:C:137:HIS:HE1	7:C:688:HOH:O	2.03	0.42
1:B:78:TYR:OH	1:B:506:ASP:HA	2.19	0.42
1:B:89:LYS:NZ	7:B:872:HOH:O	2.48	0.42
1:A:545:ASP:O	1:A:548:VAL:HB	2.20	0.42
1:A:518:ALA:HB1	1:A:528:VAL:CG2	2.50	0.41
1:A:425:VAL:HG13	1:A:554:ASP:CA	2.50	0.41
1:A:475:PHE:CE1	1:A:484:VAL:HG11	2.55	0.41
1:C:39:ALA:HB2	2:C:600:FAY:C2A	2.50	0.41
1:B:98:ASN:HB2	2:B:600:FAY:C5X	2.50	0.41
1:C:364[A]:LYS:C	1:C:364[A]:LYS:HD3	2.36	0.41
1:A:43:ASN:HA	1:A:45[B]:GLU:OE2	2.21	0.41
1:B:377:ALA:HB2	7:B:771:HOH:O	2.20	0.41
1:B:269:VAL:HG21	1:B:514:PRO:HG2	2.01	0.41
1:B:39:ALA:HB2	2:B:600:FAY:C2A	2.51	0.41
1:C:262:GLU:OE1	1:C:542:ARG:HD2	2.21	0.41
1:B:237:GLU:HG3	7:B:586:HOH:O	2.19	0.41
1:C:12:ILE:HD13	1:C:264:ILE:HB	2.02	0.41
1:A:448[B]:ASN:OD1	7:A:751:HOH:O	2.22	0.41
1:B:558:GLN:HB3	2:B:600:FAY:C2	2.51	0.41
1:B:253:ASN:ND2	7:B:687:HOH:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:317:VAL:HG13	1:A:321:PHE:HB2	2.02	0.41
1:B:100:PHE:CG	1:B:204:ILE:HD11	2.56	0.41
1:A:158:ILE:HG13	1:A:158:ILE:O	2.17	0.41
1:C:177:ALA:HB1	1:C:477:GLY:HA3	2.02	0.41
1:C:213:PHE:CD2	1:C:214:LEU:HD13	2.55	0.41
1:A:69:LYS:O	1:A:70:THR:HG22	2.20	0.40
1:C:39:ALA:HA	1:C:228:VAL:O	2.21	0.40
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.86	0.40
1:B:464:ARG:HD3	1:B:468:ARG:NH2	2.36	0.40
1:C:194:MET:O	1:C:359:PHE:HB2	2.21	0.40
1:C:390[A]:GLN:HB2	1:C:391:PRO:CD	2.52	0.40
1:C:176:LYS:HE3	1:C:176:LYS:HB2	1.68	0.40
1:A:440:ASP:HA	1:A:441:PRO:HD2	1.82	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	584/577 (101%)	560 (96%)	22 (4%)	2 (0%)	50	54
1	B	582/577 (101%)	551 (95%)	30 (5%)	1 (0%)	56	63
1	C	580/577 (100%)	543 (94%)	36 (6%)	1 (0%)	56	63
All	All	1746/1731 (101%)	1654 (95%)	88 (5%)	4 (0%)	56	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	C	104	PRO
1	B	104	PRO
1	A	104	PRO

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	501/492 (102%)	469 (94%)	32 (6%)	25	23
1	B	499/492 (101%)	468 (94%)	31 (6%)	26	24
1	C	497/492 (101%)	463 (93%)	34 (7%)	22	20
All	All	1497/1476 (101%)	1400 (94%)	97 (6%)	27	22

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	70	THR
1	A	73	VAL
1	A	97	LEU
1	A	147	LEU
1	A	172	GLU
1	A	185	LEU
1	A	208	GLN
1	A	214	LEU
1	A	233	LEU
1	A	243	LYS
1	A	255	LEU
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	317	VAL
1	A	324	ASP
1	A	354	LEU
1	A	366	LEU
1	A	388	LEU
1	A	390[A]	GLN
1	A	390[B]	GLN
1	A	424	LEU
1	A	425	VAL
1	A	458	LEU
1	A	473	LEU
1	A	494	LEU
1	A	498	LYS

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Mol	Chain	Res	Type
1	A	520[A]	LEU
1	A	520[B]	LEU
1	A	548	VAL
1	A	554	ASP
1	A	559	ASN
1	B	3	THR
1	B	70	THR
1	B	73	VAL
1	B	75[A]	ARG
1	B	75[B]	ARG
1	B	85	ASN
1	B	97	LEU
1	B	147	LEU
1	B	172	GLU
1	B	176	LYS
1	B	185	LEU
1	B	214	LEU
1	B	233	LEU
1	B	255	LEU
1	B	269	VAL
1	B	324	ASP
1	B	325	ASP
1	B	343	LYS
1	B	345	ARG
1	B	354	LEU
1	B	366	LEU
1	B	390[A]	GLN
1	B	390[B]	GLN
1	B	424	LEU
1	B	425	VAL
1	B	458	LEU
1	B	473	LEU
1	B	494	LEU
1	B	498	LYS
1	B	554	ASP
1	B	577	LYS
1	C	70	THR
1	C	73	VAL
1	C	75[A]	ARG
1	C	75[B]	ARG
1	C	85	ASN
1	C	90	THR

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Mol	Chain	Res	Type
1	C	97	LEU
1	C	147	LEU
1	C	148	GLU
1	C	172	GLU
1	C	198	THR
1	C	209	ARG
1	C	214	LEU
1	C	233	LEU
1	C	269	VAL
1	C	337	VAL
1	C	354	LEU
1	C	364[A]	LYS
1	C	364[B]	LYS
1	C	366	LEU
1	C	388	LEU
1	C	390[A]	GLN
1	C	390[B]	GLN
1	C	424	LEU
1	C	425	VAL
1	C	458	LEU
1	C	473	LEU
1	C	494	LEU
1	C	520	LEU
1	C	528	VAL
1	C	548	VAL
1	C	554	ASP
1	C	559	ASN
1	C	577	LYS

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

Mol	Chain	Res	Type
1	B	183	GLN
1	B	253	ASN
1	B	559	ASN

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 ⓘ

8 ligands are modelled in this entry.

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	ACT	A	1	-	1,3,3	1.98	0	0,3,3	0.00	-
3	MRD	A	581	-	7,7,7	0.27	0	10,10,10	0.66	0
3	MRD	A	582	-	7,7,7	0.41	0	10,10,10	0.39	0
2	FAY	A	600	-	59,59,59	1.27	6 (10%)	86,90,90	2.05	16 (18%)
5	PEG	B	1	-	6,6,6	0.59	0	5,5,5	1.01	1 (20%)
2	FAY	B	600	-	59,59,59	1.24	5 (8%)	86,90,90	2.02	20 (23%)
6	MPD	C	1	-	7,7,7	0.25	0	10,10,10	0.43	0
2	FAY	C	600	-	59,59,59	1.16	6 (10%)	86,90,90	1.98	18 (20%)

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	ACT	A	1	-	-	0/0/0/0	0/0/0/0
3	MRD	A	581	-	-	0/5/5/5	0/0/0/0
3	MRD	A	582	-	-	0/5/5/5	0/0/0/0
2	FAY	A	600	-	-	0/36/52/52	0/1/6/6
5	PEG	B	1	-	-	0/4/4/4	0/0/0/0
2	FAY	B	600	-	-	0/36/52/52	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	C	1	-	-	0/5/5/5	0/0/0/0
2	FAY	C	600	-	-	0/36/52/52	0/1/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAY	C1'-N10	4.72	1.53	1.48
2	B	600	FAY	C1'-N10	4.67	1.53	1.48
2	C	600	FAY	C1'-N10	3.78	1.52	1.48
2	A	600	FAY	C1'-C2'	3.66	1.55	1.51
2	C	600	FAY	C2A-N3A	3.48	1.39	1.32
2	A	600	FAY	C2A-N3A	3.45	1.39	1.32
2	B	600	FAY	C2A-N3A	3.24	1.38	1.32
2	B	600	FAY	C5'-C4'	2.90	1.56	1.51
2	B	600	FAY	C1'-C2'	2.80	1.54	1.51
2	C	600	FAY	C2A-N1A	2.54	1.38	1.33
2	A	600	FAY	C2A-N1A	2.43	1.38	1.33
2	A	600	FAY	C5'-C4'	2.26	1.55	1.51
2	B	600	FAY	C2A-N1A	2.20	1.38	1.33
2	C	600	FAY	C5'-C4'	2.20	1.55	1.51
2	C	600	FAY	C6-C5X	-2.19	1.39	1.41
2	C	600	FAY	C5X-N5	2.07	1.38	1.35
2	A	600	FAY	O2'-C2'	-2.04	1.38	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAY	N3A-C2A-N1A	-9.85	120.47	128.71
2	C	600	FAY	N3A-C2A-N1A	-9.52	120.75	128.71
2	B	600	FAY	N3A-C2A-N1A	-9.18	121.04	128.71
2	B	600	FAY	C4X-C10-N1	-5.84	116.90	122.73
2	A	600	FAY	C4X-C10-N1	-5.71	117.02	122.73
2	A	600	FAY	C2-N1-C10	5.08	120.10	114.98
2	A	600	FAY	C9A-N10-C10	-4.99	116.87	121.77
2	C	600	FAY	C1'-N10-C9A	4.95	123.69	118.87
2	B	600	FAY	C9A-N10-C10	-4.77	117.08	121.77
2	B	600	FAY	C1'-C2'-C3'	4.72	123.31	109.82
2	A	600	FAY	C1'-C2'-C3'	4.41	122.42	109.82
2	B	600	FAY	C2-N1-C10	4.24	119.25	114.98
2	C	600	FAY	C2-N1-C10	4.19	119.20	114.98
2	A	600	FAY	N3A-C4A-N9A	4.10	132.83	125.43
2	C	600	FAY	N3A-C4A-N9A	4.08	132.81	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	FAY	C4X-C10-N1	-4.02	118.71	122.73
2	B	600	FAY	N3A-C4A-N9A	3.60	131.94	125.43
2	C	600	FAY	C9A-N10-C10	-3.60	118.23	121.77
2	C	600	FAY	C1'-C2'-C3'	3.60	120.12	109.82
2	B	600	FAY	PA-O3P-P	-3.53	121.33	131.68
2	A	600	FAY	C7-C8-C8M	-3.41	117.63	123.36
2	A	600	FAY	C4-N3-C2	-3.28	118.65	125.39
2	B	600	FAY	C5X-C9A-N10	3.24	120.00	116.80
2	C	600	FAY	C5X-C9A-N10	3.20	119.95	116.80
2	B	600	FAY	C4A-C5A-N7A	-3.11	106.86	109.52
2	C	600	FAY	O4B-C1B-N9A	3.05	111.28	108.44
2	B	600	FAY	C4-N3-C2	-3.03	119.17	125.39
2	C	600	FAY	C4-N3-C2	-2.96	119.31	125.39
2	A	600	FAY	C4-C4X-C10	2.94	121.70	116.95
2	A	600	FAY	C5X-C9A-N10	2.93	119.69	116.80
2	C	600	FAY	PA-O3P-P	-2.93	123.10	131.68
2	B	600	FAY	C7-C8-C8M	-2.73	118.77	123.36
2	A	600	FAY	O3'-C3'-C2'	2.70	115.55	108.74
2	C	600	FAY	C7-C8-C8M	-2.64	118.92	123.36
2	A	600	FAY	PA-O3P-P	-2.63	123.96	131.68
2	C	600	FAY	C2'-C1'-N10	-2.63	108.96	112.45
2	B	600	FAY	C5A-C4A-N3A	-2.56	120.13	125.70
2	A	600	FAY	C1'-N10-C9A	2.55	121.36	118.87
2	C	600	FAY	C5A-C4A-N3A	-2.55	120.14	125.70
2	A	600	FAY	C6-C5X-N5	-2.51	116.05	118.97
2	C	600	FAY	C9-C8-C7	2.46	120.56	118.38
2	B	600	FAY	C1'-N10-C9A	2.43	121.24	118.87
2	B	600	FAY	O4B-C1B-N9A	2.34	110.61	108.44
2	A	600	FAY	C5A-C4A-N3A	-2.30	120.69	125.70
2	B	600	FAY	C4X-N5-C5X	2.26	119.23	116.69
2	B	600	FAY	O4'-C4'-C3'	-2.23	103.50	109.05
2	B	600	FAY	C8-C9-C9A	2.20	121.17	117.90
2	A	600	FAY	N7A-C8A-N9A	-2.20	108.15	114.36
2	C	600	FAY	C4A-C5A-N7A	-2.19	107.64	109.52
2	C	600	FAY	N7A-C8A-N9A	-2.19	108.15	114.36
2	B	600	FAY	N1-C10-N10	2.10	121.50	115.97
2	B	600	FAY	C4-C4X-C10	2.09	120.32	116.95
2	C	600	FAY	C2A-N3A-C4A	2.08	119.93	114.01
2	B	600	FAY	N7A-C8A-N9A	-2.07	108.52	114.36
5	B	1	PEG	C3-O2-C2	-2.00	104.58	113.38

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	577/577 (100%)	-0.70	0 100 100	15, 22, 36, 57	0
1	B	577/577 (100%)	-0.48	1 (0%) 93 96	16, 29, 49, 79	0
1	C	577/577 (100%)	-0.30	1 (0%) 93 96	19, 36, 54, 81	0
All	All	1731/1731 (100%)	-0.49	2 (0%) 93 96	15, 28, 50, 81	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	HIS	3.0
1	C	141	ARG	2.6

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(\AA^2)	Q<0.9
4	ACT	A	1	4/4	0.27	24.72	28,29,30,36	0
3	MRD	A	582	8/8	0.34	11.04	24,49,56,57	0
3	MRD	A	581	8/8	0.14	2.12	27,37,46,46	0
6	MPD	C	1	8/8	0.19	1.74	29,35,40,42	0
2	FAY	A	600	54/54	0.10	1.14	14,19,26,28	0
2	FAY	C	600	54/54	0.11	0.80	21,31,40,42	0
2	FAY	B	600	54/54	0.12	0.71	15,22,31,35	0
5	PEG	B	1	7/7	0.15	-0.65	41,45,55,57	0

6.5 Other polymers

There are no such residues in this entry.