



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:55 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

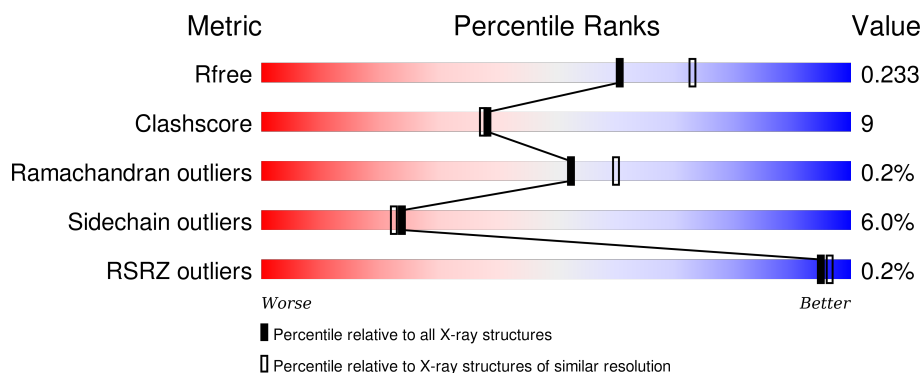
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (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. 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	577	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 16%, yellow 16%, green 82%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 82% 16% </div> </div>
1	B	577	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 17%, orange 17%, yellow 17%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 80% 17% </div> </div>
1	C	577	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 18%, orange 18%, yellow 18%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 80% 18% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition [i](#)

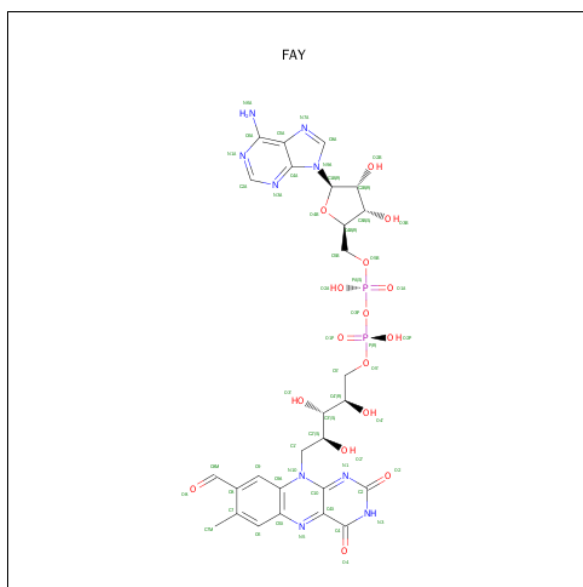
There are 7 unique types of molecules in this entry. The entry contains 14820 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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-TRIHYDROXYPENTYL DIHYDROGEN DIPHOSPHATE (three-letter code: FAY) (formula: C₂₇H₃₁N₉O₁₆P₂).



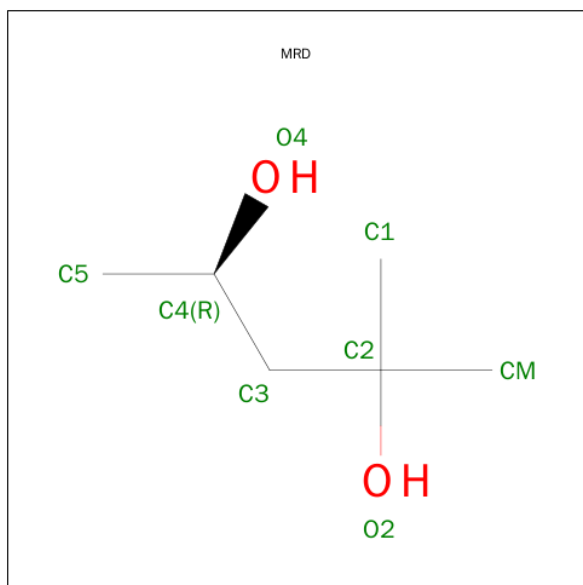
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			54	27	9	16	2		
2	B	1	Total	C	N	O	P	0	0
			54	27	9	16	2		

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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: $C_6H_{14}O_2$).



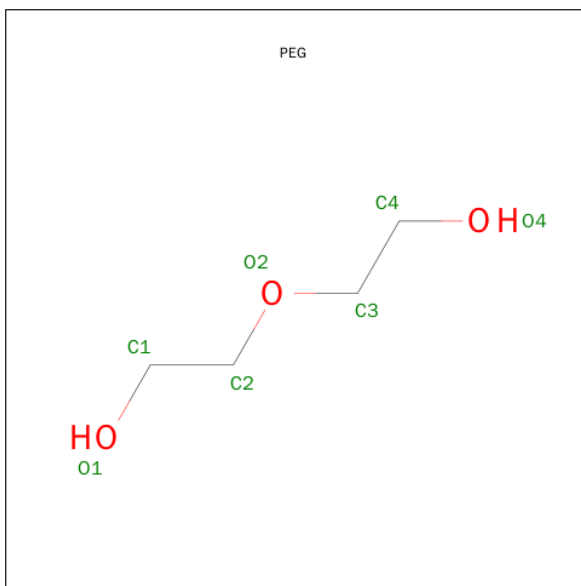
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		

- 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: C₄H₁₀O₃).



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: C₆H₁₄O₂).



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

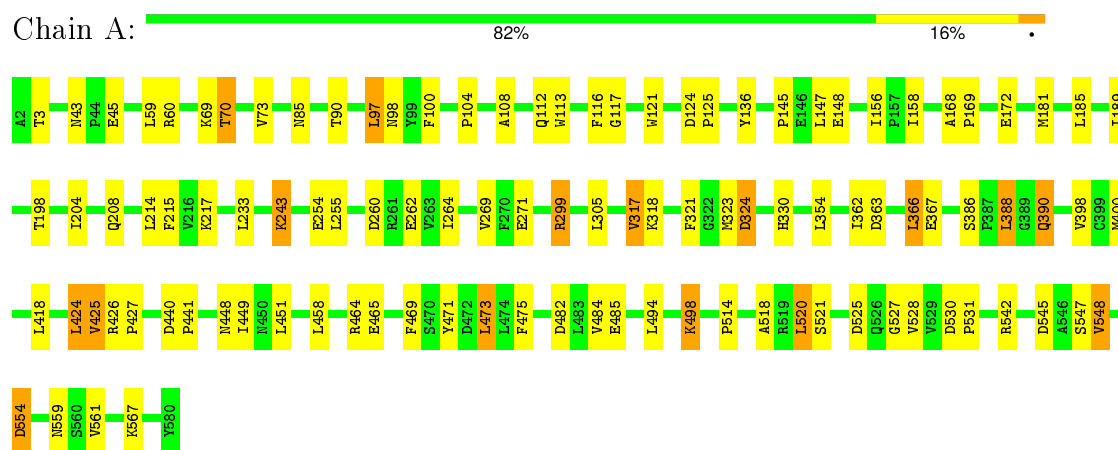
- Molecule 7 is water.

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		

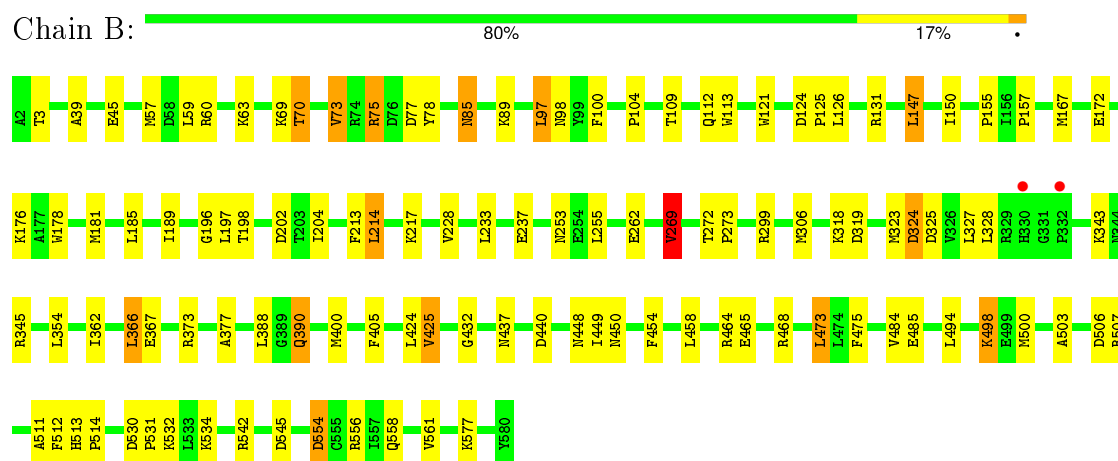
3 Residue-property plots

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.

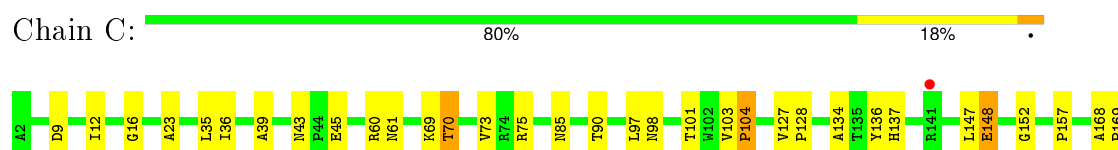
- Molecule 1: Choline dehydrogenase and related flavoproteins

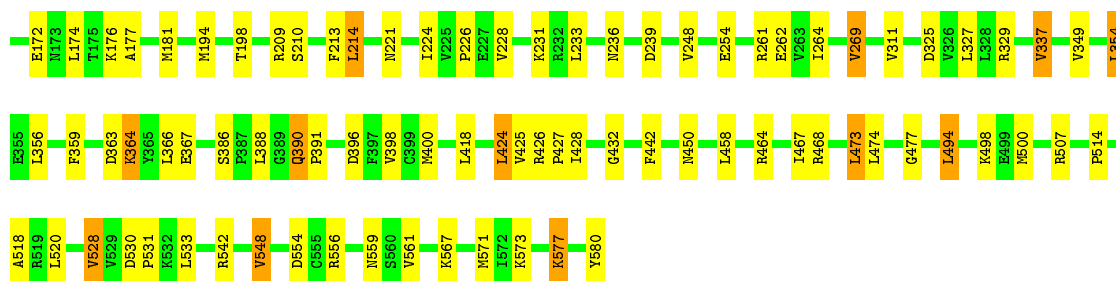


- Molecule 1: Choline dehydrogenase and related flavoproteins



- Molecule 1: Choline dehydrogenase and related flavoproteins





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 0.182 , 0.233	Depositor DCC
R_{free} test set	5334 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.8	EDS
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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
2	B	54	0	29	7	0
2	C	54	0	29	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 9.

All (251) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:MET:HE3	7:A:888:HOH:O	2.07	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	584/577 (101%)	560 (96%)	22 (4%)	2 (0%)	46	51
1	B	582/577 (101%)	551 (95%)	30 (5%)	1 (0%)	52	60
1	C	580/577 (100%)	543 (94%)	36 (6%)	1 (0%)	52	60
All	All	1746/1731 (101%)	1654 (95%)	88 (5%)	4 (0%)	52	60

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%)	22	20
1	B	499/492 (101%)	468 (94%)	31 (6%)	23	21
1	C	497/492 (101%)	463 (93%)	34 (7%)	20	17
All	All	1497/1476 (101%)	1400 (94%)	97 (6%)	24	19

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	559	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	2.04	1 (100%)	0,3,3	0.00	-
3	MRD	A	581	-	6,7,7	0.30	0	7,10,10	0.76	0
3	MRD	A	582	-	6,7,7	0.46	0	7,10,10	0.23	0
2	FAY	A	600	-	49,59,59	1.40	7 (14%)	55,90,90	2.22	12 (21%)
5	PEG	B	1	-	6,6,6	0.59	0	5,5,5	1.04	1 (20%)
2	FAY	B	600	-	49,59,59	1.41	6 (12%)	55,90,90	2.17	11 (20%)
6	MPD	C	1	-	6,7,7	0.27	0	7,10,10	0.42	0
2	FAY	C	600	-	49,59,59	1.36	6 (12%)	55,90,90	2.24	10 (18%)

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	-	-	0/32/52/52	0/6/6/6
5	PEG	B	1	-	-	0/4/4/4	0/0/0/0
2	FAY	B	600	-	-	0/32/52/52	0/6/6/6
6	MPD	C	1	-	-	0/5/5/5	0/0/0/0
2	FAY	C	600	-	-	0/32/52/52	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAY	O2'-C2'	-2.07	1.38	1.43
4	A	1	ACT	CH3-C	2.04	1.51	1.48
2	B	600	FAY	C4-N3	2.17	1.37	1.33
2	B	600	FAY	C2A-N1A	2.29	1.38	1.33
2	C	600	FAY	C5'-C4'	2.29	1.55	1.51
2	A	600	FAY	C5'-C4'	2.36	1.55	1.51
2	A	600	FAY	C4-N3	2.49	1.37	1.33
2	A	600	FAY	C2A-N1A	2.52	1.38	1.33
2	C	600	FAY	C2A-N1A	2.64	1.38	1.33
2	A	600	FAY	C4X-N5	2.73	1.37	1.33
2	B	600	FAY	C4X-N5	2.90	1.37	1.33
2	B	600	FAY	C5'-C4'	3.02	1.56	1.51
2	C	600	FAY	C4-N3	3.16	1.39	1.33
2	C	600	FAY	C4X-N5	3.19	1.38	1.33
2	B	600	FAY	C2A-N3A	3.61	1.38	1.32
2	C	600	FAY	C1'-N10	3.83	1.52	1.48
2	A	600	FAY	C2A-N3A	3.85	1.39	1.32
2	C	600	FAY	C2A-N3A	3.88	1.39	1.32
2	B	600	FAY	C1'-N10	4.79	1.53	1.48
2	A	600	FAY	C1'-N10	4.85	1.53	1.48

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAY	N3A-C2A-N1A	-11.00	120.47	128.89
2	C	600	FAY	N3A-C2A-N1A	-10.64	120.75	128.89
2	B	600	FAY	N3A-C2A-N1A	-10.26	121.04	128.89
2	A	600	FAY	C4X-C4-N3	-4.49	117.45	123.59
2	B	600	FAY	PA-O3P-P	-4.06	121.33	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAY	C4X-C4-N3	-3.77	118.43	123.59
2	C	600	FAY	C2B-C1B-N9A	-3.63	108.74	114.29
2	C	600	FAY	C4X-C4-N3	-3.62	118.63	123.59
2	A	600	FAY	C7-C8-C8M	-3.53	117.63	123.60
2	C	600	FAY	PA-O3P-P	-3.43	123.10	132.73
2	A	600	FAY	PA-O3P-P	-3.12	123.96	132.73
2	B	600	FAY	C7-C8-C8M	-2.85	118.77	123.60
2	B	600	FAY	C4A-C5A-N7A	-2.85	106.86	109.48
2	C	600	FAY	C7-C8-C8M	-2.77	118.92	123.60
2	A	600	FAY	C6-C5X-N5	-2.26	116.05	118.96
2	A	600	FAY	C2B-C1B-N9A	-2.23	110.89	114.29
2	B	600	FAY	O4'-C4'-C3'	-2.20	103.50	109.02
5	B	1	PEG	C3-O2-C2	-2.03	104.58	113.31
2	B	600	FAY	C1'-N10-C9A	2.12	121.24	118.86
2	B	600	FAY	C4X-N5-C5X	2.15	119.23	116.76
2	A	600	FAY	C1'-N10-C9A	2.22	121.36	118.86
2	C	600	FAY	C9-C8-C7	2.58	120.56	118.40
2	A	600	FAY	O3'-C3'-C2'	2.70	115.55	108.75
2	A	600	FAY	C5X-C9A-N10	2.72	119.69	117.62
2	A	600	FAY	C4-C4X-C10	2.74	121.70	119.94
2	C	600	FAY	C5X-C9A-N10	3.07	119.95	117.62
2	B	600	FAY	C5X-C9A-N10	3.13	120.00	117.62
2	C	600	FAY	C1'-C2'-C3'	3.60	120.12	109.82
2	A	600	FAY	C4-N3-C2	3.94	118.65	115.25
2	C	600	FAY	C1'-N10-C9A	4.30	123.69	118.86
2	A	600	FAY	C1'-C2'-C3'	4.41	122.42	109.82
2	B	600	FAY	C4-N3-C2	4.54	119.17	115.25
2	C	600	FAY	C4-N3-C2	4.70	119.31	115.25
2	B	600	FAY	C1'-C2'-C3'	4.72	123.31	109.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	ACT	1	0
3	A	581	MRD	10	0
3	A	582	MRD	2	0
2	A	600	FAY	3	0
5	B	1	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAY	7	0
6	C	1	MPD	3	0
2	C	600	FAY	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.69	0 100 100	15, 22, 36, 57	0
1	B	577/577 (100%)	-0.45	2 (0%) 94 95	16, 29, 49, 79	0
1	C	577/577 (100%)	-0.28	1 (0%) 95 96	19, 36, 54, 81	0
All	All	1731/1731 (100%)	-0.47	3 (0%) 95 96	15, 28, 50, 81	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	HIS	2.9
1	C	141	ARG	2.6
1	B	332	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	ACT	A	1	4/4	0.95	0.25	16.29	28,29,30,36	0
3	MRD	A	582	8/8	0.72	0.28	8.34	24,49,56,57	0
3	MRD	A	581	8/8	0.93	0.14	1.84	27,37,46,46	0
6	MPD	C	1	8/8	0.96	0.18	1.15	29,35,40,42	0
2	FAY	C	600	54/54	0.95	0.12	0.84	21,31,40,42	0
2	FAY	A	600	54/54	0.98	0.10	0.78	14,19,26,28	0
2	FAY	B	600	54/54	0.97	0.12	0.66	15,22,31,35	0
5	PEG	B	1	7/7	0.90	0.17	-0.50	41,45,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.