



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2021 – 03:16 PM GMT

PDB ID : 6ZT6
Title : X-ray structure of mutated arabinofuranosidase
Authors : Tandrup, T.; Lo Leggio, L.; Zhao, J.; Bissaro, B.; Barbe, S.; Andre, I.; Dumon, C.; O'Donohue, M.J.; Faure, R.
Deposited on : 2020-07-17
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

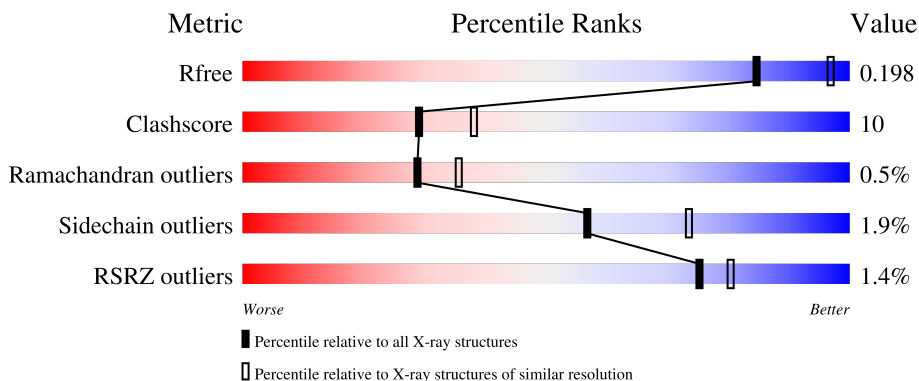
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

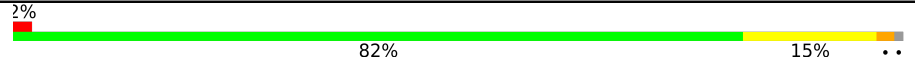
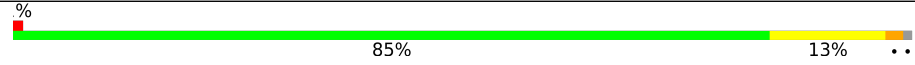

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	496	
1	B	496	
1	C	496	

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
2	MPD	A	501	-	-	X	-
2	MPD	A	502	-	-	-	X
2	MPD	A	503	-	-	X	-
2	MPD	A	505	-	-	-	X
2	MPD	A	506	-	-	-	X
2	MPD	B	501	-	-	-	X
2	MPD	B	505	-	-	-	X
2	MPD	C	502	-	-	X	X
2	MPD	C	504	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13421 atoms, of which 210 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 Alpha-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3934	2492	689	729	24	0	5	0
1	B	490	3943	2496	691	732	24	0	6	0
1	C	490	3933	2490	690	729	24	0	4	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	HIS	ARG	engineered mutation	UNP O69262
A	274	GLU	ARG	conflict	UNP O69262
A	352	MET	LEU	engineered mutation	UNP O69262
B	69	HIS	ARG	engineered mutation	UNP O69262
B	274	GLU	ARG	conflict	UNP O69262
B	352	MET	LEU	engineered mutation	UNP O69262
C	69	HIS	ARG	engineered mutation	UNP O69262
C	274	GLU	ARG	conflict	UNP O69262
C	352	MET	LEU	engineered mutation	UNP O69262

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



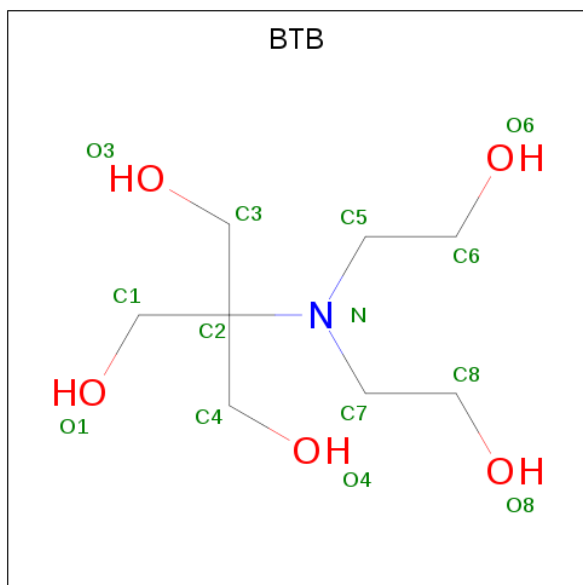
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	22	6	14	2	0	0
2	A	1	22	6	14	2	0	0
2	A	1	22	6	14	2	0	0
2	A	1	22	6	14	2	0	0
2	A	1	22	6	14	2	0	0
2	A	1	22	6	14	2	0	0
2	A	1	22	6	14	2	0	0
2	B	1	22	6	14	2	0	0
2	B	1	22	6	14	2	0	0
2	B	1	22	6	14	2	0	0
2	B	1	22	6	14	2	0	0
2	B	1	22	6	14	2	0	0
2	C	1	22	6	14	2	0	0
2	C	1	22	6	14	2	0	0
2	C	1	22	6	14	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

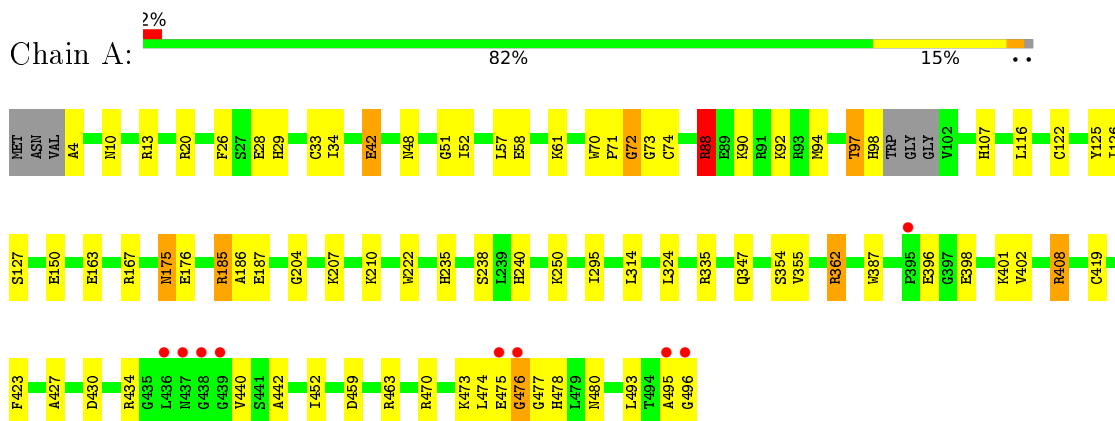
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	460	Total	O	0	0
			460	460		
4	B	419	Total	O	0	0
			419	419		
4	C	388	Total	O	0	0
			388	388		

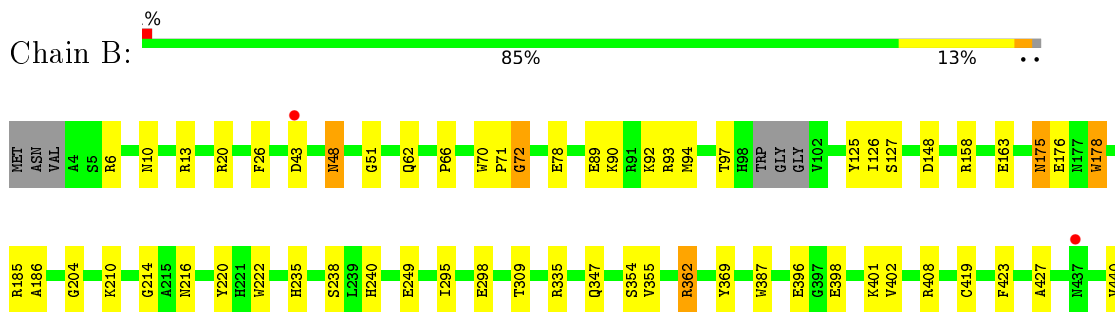
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

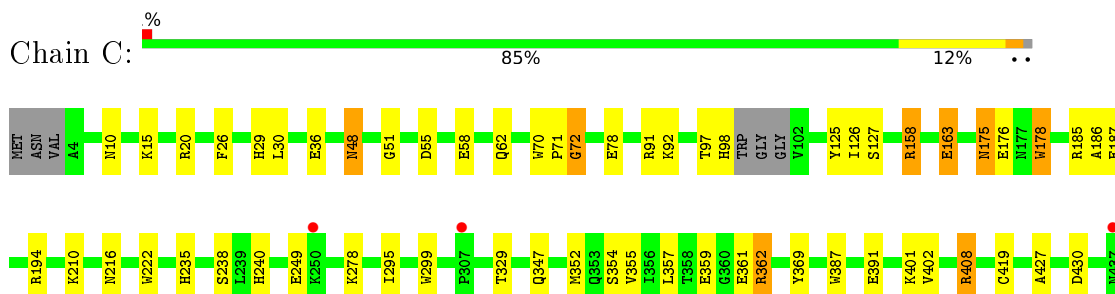
- Molecule 1: Alpha-L-arabinofuranosidase

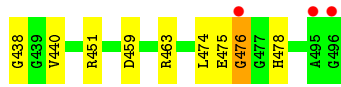


- Molecule 1: Alpha-L-arabinofuranosidase



- Molecule 1: Alpha-L-arabinofuranosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.14Å 156.14Å 377.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.00 – 2.30 48.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-2.30) 100.0 (48.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.156 , 0.189 0.168 , 0.198	Depositor DCC
R_{free} test set	1189 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtrriage
Anisotropy	0.080	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13421	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BTB

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	0.70	2/4055 (0.0%)	0.79	2/5503 (0.0%)
1	B	0.67	1/4064 (0.0%)	0.76	0/5514
1	C	0.70	2/4048 (0.0%)	0.78	2/5492 (0.0%)
All	All	0.69	5/12167 (0.0%)	0.78	4/16509 (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	5
1	B	0	4
1	C	0	4
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	GLU	CD-OE1	6.56	1.32	1.25
1	C	185	ARG	NE-CZ	5.64	1.40	1.33
1	A	185	ARG	NE-CZ	5.58	1.40	1.33
1	A	42	GLU	CD-OE2	5.36	1.31	1.25
1	B	185	ARG	NE-CZ	5.24	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	434	ARG	NE-CZ-NH2	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	194	ARG	NE-CZ-NH2	-5.26	117.67	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	408	ARG	Sidechain
1	A	463	ARG	Sidechain
1	A	88	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	451	ARG	Sidechain
1	B	463	ARG	Sidechain
1	B	6	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	408	ARG	Sidechain
1	C	451	ARG	Sidechain
1	C	463	ARG	Sidechain

5.2 Too-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 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	3934	0	3791	89	0
1	B	3943	0	3796	68	0
1	C	3933	0	3786	60	1
2	A	48	84	84	21	0
2	B	40	70	70	7	0
2	C	32	56	56	11	0
3	A	14	0	19	3	0
4	A	460	0	0	44	1
4	B	419	0	0	40	2
4	C	388	0	0	29	0
All	All	13211	210	11602	227	3

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 10.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:CYS:SG	4:A:862:HOH:O	1.94	1.25
1:C:91:ARG:HB2	4:C:607:HOH:O	1.46	1.16
1:B:176:GLU:HG3	4:B:711:HOH:O	1.49	1.12
1:A:398:GLU:HG3	2:A:501:MPD:C5	1.78	1.12
4:A:887:HOH:O	1:C:78:GLU:HG2	1.51	1.08
1:C:20:ARG:HD2	4:C:695:HOH:O	1.54	1.06
1:C:15:LYS:HB3	2:C:503:MPD:HM2	1.36	1.06
1:B:398:GLU:HG3	2:B:502:MPD:H11	1.39	1.05
1:C:352:MET:SD	4:C:858:HOH:O	2.14	1.02
1:C:30:LEU:CD1	2:C:502:MPD:C1	2.38	1.01
1:A:13[B]:ARG:HG2	1:A:13[B]:ARG:HH11	1.26	1.01
1:A:88:ARG:HD3	4:A:703:HOH:O	1.60	1.00
1:B:20:ARG:HD2	4:B:615:HOH:O	1.63	0.99
1:A:20:ARG:HD2	4:A:924:HOH:O	1.64	0.97
1:A:42:GLU:OE1	1:A:88:ARG:NH2	1.98	0.96
1:C:176:GLU:HG3	4:C:697:HOH:O	1.67	0.93
1:A:10:ASN:OD1	4:A:601:HOH:O	1.89	0.91
1:A:398:GLU:HG3	2:A:501:MPD:H53	1.53	0.90
1:C:30:LEU:CD1	2:C:502:MPD:H12	2.01	0.90
1:C:30:LEU:HD12	2:C:502:MPD:H12	1.52	0.90
1:B:176:GLU:OE2	2:B:504:MPD:H13	1.74	0.88
1:C:15:LYS:O	2:C:503:MPD:HM3	1.73	0.87
1:A:387:TRP:CD1	4:A:810:HOH:O	2.29	0.86
1:C:15:LYS:HB3	2:C:503:MPD:CM	2.06	0.86
1:B:10:ASN:OD1	4:B:601:HOH:O	1.93	0.86
1:B:71:PRO:O	4:B:602:HOH:O	1.94	0.85
1:C:30:LEU:HD11	2:C:502:MPD:C1	2.05	0.85
1:A:335:ARG:O	2:A:505:MPD:HM3	1.77	0.84
1:C:408:ARG:HD3	4:C:802:HOH:O	1.78	0.83
1:A:92:LYS:HD3	4:A:964:HOH:O	1.79	0.82
2:B:503:MPD:HM1	4:B:995:HOH:O	1.78	0.82
1:A:398:GLU:HG3	2:A:501:MPD:H51	1.61	0.82
1:A:476:GLY:O	4:A:602:HOH:O	1.96	0.81
1:B:496:GLY:HA2	4:B:950:HOH:O	1.82	0.80
1:A:210:LYS:H	1:A:235:HIS:HD2	1.30	0.79
2:C:501:MPD:H51	4:C:956:HOH:O	1.83	0.79
1:C:91:ARG:CB	4:C:607:HOH:O	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:HD11	2:A:503:MPD:H52	1.63	0.78
1:B:398:GLU:HG3	2:B:502:MPD:C1	2.14	0.77
1:A:240:HIS:CD2	4:A:659:HOH:O	2.37	0.77
1:A:470:ARG:HD3	4:A:616:HOH:O	1.84	0.76
1:A:187[B]:GLU:OE2	4:A:603:HOH:O	2.03	0.76
1:B:210:LYS:H	1:B:235:HIS:HD2	1.35	0.75
1:A:94:MET:HG2	4:A:1004:HOH:O	1.87	0.74
1:A:34:ILE:CD1	4:A:721:HOH:O	2.34	0.74
1:B:94:MET:HB2	4:B:779:HOH:O	1.86	0.74
1:C:210:LYS:H	1:C:235:HIS:HD2	1.34	0.74
1:C:71:PRO:O	4:C:601:HOH:O	2.06	0.73
1:B:309:THR:HG23	4:B:622:HOH:O	1.89	0.72
1:B:408:ARG:HD3	4:B:883:HOH:O	1.90	0.72
1:A:163:GLU:OE1	4:A:604:HOH:O	2.08	0.71
1:B:71:PRO:HB2	4:B:602:HOH:O	1.90	0.71
1:A:88:ARG:NH1	4:A:608:HOH:O	2.23	0.70
1:B:335:ARG:HD3	4:B:822:HOH:O	1.89	0.70
1:A:362:ARG:NH2	1:A:459:ASP:OD1	2.26	0.69
1:B:480[A]:ASN:ND2	4:B:603:HOH:O	2.01	0.69
1:C:357:LEU:HD21	4:C:795:HOH:O	1.92	0.69
1:B:175:ASN:OD1	4:B:604:HOH:O	2.11	0.68
1:A:74:CYS:H	2:A:503:MPD:CM	2.06	0.68
1:B:71:PRO:O	1:B:72:GLY:O	2.12	0.68
1:A:71:PRO:O	1:A:72:GLY:O	2.13	0.67
1:C:362:ARG:NH2	1:C:459:ASP:OD1	2.27	0.67
1:A:335:ARG:O	2:A:505:MPD:CM	2.43	0.67
1:A:250:LYS:HG2	4:A:1055:HOH:O	1.93	0.67
1:C:71:PRO:O	1:C:72:GLY:O	2.12	0.67
1:C:36:GLU:HB2	4:C:641:HOH:O	1.95	0.65
1:A:57[B]:LEU:CD2	1:A:61:LYS:HD2	2.27	0.65
1:A:150:GLU:OE2	4:A:606:HOH:O	2.15	0.64
1:A:28:GLU:O	4:A:605:HOH:O	2.15	0.64
1:C:30:LEU:HD11	2:C:502:MPD:H11	1.77	0.64
1:B:210:LYS:H	1:B:235:HIS:CD2	2.15	0.64
1:C:359:GLU:HB3	4:C:610:HOH:O	1.97	0.64
1:A:408:ARG:HD3	4:A:751:HOH:O	1.99	0.63
1:A:74:CYS:H	2:A:503:MPD:HM2	1.62	0.63
1:B:94:MET:HG2	4:B:980:HOH:O	1.99	0.63
1:A:13[B]:ARG:HH11	1:A:13[B]:ARG:CG	2.03	0.63
1:A:210:LYS:H	1:A:235:HIS:CD2	2.13	0.62
1:C:249:GLU:HB3	4:C:748:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ASP:C	4:C:630:HOH:O	2.38	0.62
1:C:210:LYS:H	1:C:235:HIS:CD2	2.16	0.62
1:C:10:ASN:ND2	1:C:387:TRP:CZ3	2.68	0.62
1:A:398:GLU:CG	2:A:501:MPD:H51	2.30	0.62
1:A:73:GLY:C	4:A:697:HOH:O	2.37	0.61
1:A:10:ASN:ND2	1:A:387:TRP:CZ3	2.69	0.61
1:B:158:ARG:HD2	4:B:848:HOH:O	2.01	0.60
1:A:58:GLU:HG3	4:A:986:HOH:O	2.02	0.60
1:B:176:GLU:CG	4:B:711:HOH:O	2.26	0.60
1:C:98:HIS:HE1	4:C:934:HOH:O	1.82	0.60
1:A:13[B]:ARG:HG2	1:A:13[B]:ARG:NH1	2.05	0.60
1:C:30:LEU:CD1	2:C:502:MPD:H13	2.30	0.60
1:B:71:PRO:CB	4:B:602:HOH:O	2.49	0.59
1:A:28:GLU:HA	4:A:609:HOH:O	2.01	0.59
1:A:98:HIS:HE1	4:A:968:HOH:O	1.86	0.59
1:A:97:THR:O	4:A:607:HOH:O	2.16	0.58
1:B:10:ASN:ND2	1:B:387:TRP:CZ3	2.71	0.58
1:B:440:VAL:HG23	1:B:474:LEU:HD21	1.86	0.58
1:A:204:GLY:HA3	4:A:713:HOH:O	2.04	0.58
1:C:278[B]:LYS:NZ	4:C:612:HOH:O	2.31	0.58
1:C:440:VAL:HG23	1:C:474:LEU:HD21	1.84	0.58
1:B:43[B]:ASP:CG	4:B:636:HOH:O	2.43	0.57
1:B:240:HIS:CD2	4:B:770:HOH:O	2.57	0.57
1:B:204:GLY:HA3	4:B:874:HOH:O	2.04	0.57
1:A:440:VAL:HG23	1:A:474:LEU:HD21	1.86	0.57
1:C:240:HIS:CD2	4:C:744:HOH:O	2.57	0.56
1:A:70:TRP:O	1:A:126:ILE:HA	2.05	0.56
1:C:187[B]:GLU:OE1	4:C:603:HOH:O	2.18	0.56
1:C:362:ARG:HD3	4:C:734:HOH:O	2.05	0.56
1:B:70:TRP:O	1:B:126:ILE:HA	2.06	0.56
1:A:398:GLU:OE2	2:A:501:MPD:H51	2.06	0.55
1:A:122:CYS:O	2:A:504:MPD:HM1	2.07	0.55
1:A:13[B]:ARG:NH1	1:A:13[B]:ARG:CG	2.67	0.55
1:C:70:TRP:O	1:C:126:ILE:HA	2.07	0.55
1:B:92:LYS:HB2	4:B:964:HOH:O	2.06	0.55
1:C:359:GLU:N	4:C:610:HOH:O	2.39	0.55
1:A:207:LYS:HD3	4:A:881:HOH:O	2.07	0.55
1:B:71:PRO:CA	4:B:602:HOH:O	2.55	0.54
1:A:250:LYS:CG	4:A:1055:HOH:O	2.53	0.54
1:B:480[B]:ASN:ND2	4:B:619:HOH:O	2.40	0.54
1:B:13[B]:ARG:NE	4:B:616:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13[A]:ARG:NH1	4:B:617:HOH:O	2.40	0.53
1:B:93:ARG:NH1	4:B:620:HOH:O	2.41	0.53
1:C:158:ARG:HD2	4:C:786:HOH:O	2.09	0.53
1:B:78:GLU:HG2	4:C:895:HOH:O	2.08	0.53
1:A:430:ASP:OD2	1:A:478:HIS:HD2	1.92	0.52
1:A:58:GLU:CG	4:A:986:HOH:O	2.57	0.52
1:A:398:GLU:CG	2:A:501:MPD:C5	2.70	0.52
1:B:238:SER:HA	1:B:295:ILE:O	2.10	0.52
3:A:507:BTB:H72	3:A:507:BTB:O6	2.10	0.52
1:A:176:GLU:HG3	4:A:697:HOH:O	2.11	0.51
1:A:29:HIS:CD2	1:A:70:TRP:HE1	2.29	0.51
1:C:362:ARG:HB2	4:C:610:HOH:O	2.11	0.51
1:C:430:ASP:OD2	1:C:478:HIS:HD2	1.93	0.51
1:C:391:GLU:CG	4:C:684:HOH:O	2.58	0.51
1:C:408:ARG:CD	4:C:802:HOH:O	2.46	0.50
1:A:396:GLU:HG2	4:A:989:HOH:O	2.12	0.50
1:A:496:GLY:CA	4:A:961:HOH:O	2.59	0.50
1:B:92:LYS:HD3	4:B:853:HOH:O	2.10	0.50
1:C:475:GLU:O	1:C:476:GLY:O	2.30	0.50
1:A:48:ASN:HD22	1:A:51:GLY:H	1.60	0.49
1:B:335:ARG:CD	4:B:822:HOH:O	2.56	0.49
1:B:347:GLN:O	1:B:354:SER:HA	2.12	0.49
1:B:97:THR:OG1	4:B:607:HOH:O	2.20	0.49
2:A:501:MPD:HM1	2:A:501:MPD:H52	1.94	0.49
1:B:496:GLY:CA	4:B:950:HOH:O	2.52	0.49
1:A:347:GLN:O	1:A:354:SER:HA	2.13	0.48
1:B:475:GLU:O	1:B:476:GLY:O	2.31	0.48
1:B:148:ASP:OD1	4:B:606:HOH:O	2.19	0.48
1:B:71:PRO:C	4:B:602:HOH:O	2.47	0.47
1:B:249:GLU:HB3	4:B:618:HOH:O	2.14	0.47
1:B:451:ARG:HE	1:B:463:ARG:NH2	2.13	0.47
1:A:57[B]:LEU:CD2	1:A:61:LYS:CD	2.91	0.47
1:A:496:GLY:HA3	4:A:961:HOH:O	2.14	0.47
2:C:504:MPD:H11	4:C:932:HOH:O	2.15	0.47
1:A:74:CYS:SG	2:A:503:MPD:HM1	2.54	0.47
1:A:475:GLU:O	1:A:476:GLY:O	2.32	0.47
1:B:48:ASN:HD22	1:B:51:GLY:H	1.63	0.47
1:A:94:MET:HB2	4:A:964:HOH:O	2.14	0.47
1:C:71:PRO:HB2	4:C:601:HOH:O	2.15	0.46
1:A:423:PHE:HB2	1:A:452[B]:ILE:HG22	1.98	0.46
3:A:507:BTB:C7	3:A:507:BTB:O6	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:HIS:HE1	4:B:975:HOH:O	1.98	0.46
1:A:207:LYS:HB3	4:A:800:HOH:O	2.14	0.46
1:A:238:SER:HA	1:A:295:ILE:O	2.15	0.46
1:C:238:SER:HA	1:C:295:ILE:O	2.14	0.46
1:A:495:ALA:HB1	4:A:845:HOH:O	2.15	0.46
1:B:298:GLU:OE1	2:B:504:MPD:H12	2.16	0.46
2:A:504:MPD:C5	4:A:725:HOH:O	2.63	0.46
1:A:48:ASN:ND2	1:A:51:GLY:H	2.14	0.46
1:A:235:HIS:CE1	2:A:506:MPD:H11	2.51	0.45
1:A:430:ASP:OD1	1:A:480[B]:ASN:OD1	2.35	0.45
1:A:4:ALA:HB3	4:A:979:HOH:O	2.16	0.45
1:A:88:ARG:HD2	1:A:107:HIS:CG	2.52	0.45
1:B:176:GLU:OE2	2:B:504:MPD:C1	2.57	0.45
1:C:127:SER:OG	1:C:175:ASN:ND2	2.49	0.45
1:B:335:ARG:HD2	4:B:830:HOH:O	2.15	0.45
1:A:314:LEU:HD11	2:A:503:MPD:C5	2.42	0.44
1:C:278[B]:LYS:CE	4:C:612:HOH:O	2.65	0.44
1:B:186:ALA:HB2	4:B:872:HOH:O	2.17	0.44
1:B:423:PHE:HB2	1:B:452[A]:ILE:HG22	2.00	0.44
3:A:507:BTB:H51	4:A:865:HOH:O	2.17	0.44
1:A:396:GLU:HB2	1:A:398:GLU:HG2	1.99	0.44
1:C:210:LYS:N	1:C:235:HIS:HD2	2.11	0.44
1:A:402:VAL:HA	1:A:419:CYS:O	2.18	0.44
1:B:175:ASN:HB3	4:B:711:HOH:O	2.18	0.43
1:B:13[A]:ARG:CZ	4:B:617:HOH:O	2.66	0.43
1:B:186:ALA:HB2	1:B:222:TRP:CE3	2.53	0.43
1:B:463:ARG:HG2	4:B:948:HOH:O	2.17	0.43
1:A:235:HIS:HE1	4:A:1000:HOH:O	2.01	0.43
1:A:442:ALA:HB2	1:A:493:LEU:HD22	1.99	0.43
1:B:396:GLU:HB2	1:B:398:GLU:HG2	1.99	0.43
1:B:178:TRP:CZ2	1:B:216:ASN:HB2	2.53	0.43
1:A:52:ILE:HD13	1:A:116:LEU:HD13	2.00	0.43
1:B:127:SER:OG	1:B:175:ASN:ND2	2.52	0.43
1:C:347:GLN:O	1:C:354:SER:HA	2.18	0.42
1:A:355:VAL:HG13	4:A:890:HOH:O	2.18	0.42
1:C:359:GLU:OE1	1:C:362:ARG:NH1	2.52	0.42
1:C:438:GLY:HA3	4:C:787:HOH:O	2.19	0.42
1:B:220:TYR:HB2	2:B:503:MPD:H31	2.01	0.42
1:C:401:LYS:HE3	1:C:427:ALA:HB2	2.02	0.42
1:C:48:ASN:HD22	1:C:51:GLY:H	1.68	0.42
1:A:127:SER:OG	1:A:175:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HG22	1:A:57[A]:LEU:HG	2.02	0.42
1:C:178:TRP:CZ2	1:C:216:ASN:HB2	2.54	0.42
1:B:355:VAL:O	1:B:369:TYR:HB2	2.19	0.42
1:A:477:GLY:HA3	4:A:602:HOH:O	2.19	0.41
1:B:362:ARG:NH1	1:B:458:PHE:O	2.40	0.41
1:C:158:ARG:HG2	1:C:163:GLU:HA	2.02	0.41
1:C:299:TRP:CE3	1:C:329:THR:HG21	2.55	0.41
2:A:504:MPD:H52	4:A:725:HOH:O	2.19	0.41
1:B:398:GLU:HB2	4:B:755:HOH:O	2.19	0.41
1:C:402:VAL:HA	1:C:419:CYS:O	2.20	0.41
1:A:167:ARG:O	2:A:504:MPD:H51	2.20	0.41
1:A:401:LYS:HE3	1:A:427:ALA:HB2	2.02	0.41
1:B:158:ARG:HG2	1:B:163:GLU:HA	2.02	0.41
1:A:186:ALA:HB2	1:A:222:TRP:CE3	2.56	0.41
1:B:401:LYS:HE3	1:B:427:ALA:HB2	2.03	0.41
1:A:74:CYS:N	2:A:503:MPD:HM2	2.34	0.41
1:B:402:VAL:HA	1:B:419:CYS:O	2.21	0.41
2:A:505:MPD:C1	4:A:1039:HOH:O	2.69	0.41
1:C:58:GLU:HG3	4:C:937:HOH:O	2.21	0.41
1:C:186:ALA:HB2	1:C:222:TRP:CE3	2.55	0.40
1:A:324:LEU:HA	1:A:324:LEU:HD13	1.94	0.40
1:A:48:ASN:ND2	4:A:637:HOH:O	2.53	0.40
1:B:214:GLY:HA3	1:B:238:SER:O	2.21	0.40
1:C:355:VAL:O	1:C:369:TYR:HB2	2.20	0.40
1:C:29:HIS:CD2	1:C:70:TRP:HE1	2.39	0.40
1:C:92:LYS:HA	1:C:92:LYS:HD3	1.78	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:617:HOH:O	4:B:617:HOH:O[9_555]	1.97	0.23
1:C:387:TRP:CD1	4:A:766:HOH:O[9_555]	2.10	0.10
4:B:601:HOH:O	4:B:601:HOH:O[9_555]	2.12	0.08

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	491/496 (99%)	468 (95%)	21 (4%)	2 (0%)	34	42
1	B	492/496 (99%)	470 (96%)	19 (4%)	3 (1%)	25	31
1	C	490/496 (99%)	467 (95%)	21 (4%)	2 (0%)	34	42
All	All	1473/1488 (99%)	1405 (95%)	61 (4%)	7 (0%)	29	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	GLY
1	B	476	GLY
1	C	476	GLY
1	A	72	GLY
1	B	72	GLY
1	C	72	GLY
1	B	66	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/419 (100%)	413 (98%)	7 (2%)	60	76
1	B	421/419 (100%)	412 (98%)	9 (2%)	53	70
1	C	419/419 (100%)	411 (98%)	8 (2%)	57	73
All	All	1260/1257 (100%)	1236 (98%)	24 (2%)	57	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	88	ARG
1	A	90	LYS
1	A	97	THR
1	A	125	TYR
1	A	175	ASN
1	A	473	LYS
1	B	26	PHE
1	B	48	ASN
1	B	62	GLN
1	B	89	GLU
1	B	90	LYS
1	B	125	TYR
1	B	175	ASN
1	B	178	TRP
1	B	473	LYS
1	C	26	PHE
1	C	48	ASN
1	C	62	GLN
1	C	97	THR
1	C	125	TYR
1	C	175	ASN
1	C	178	TRP
1	C	361	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	98	HIS
1	A	175	ASN
1	A	183	ASN
1	A	235	HIS
1	A	240	HIS
1	A	478	HIS
1	B	48	ASN
1	B	175	ASN
1	B	183	ASN
1	B	235	HIS
1	B	240	HIS
1	B	478	HIS

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Mol	Chain	Res	Type
1	C	48	ASN
1	C	175	ASN
1	C	235	HIS
1	C	240	HIS
1	C	478	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
2	MPD	A	506	-	7,7,7	0.15	0	9,10,10	0.32	0
2	MPD	C	503	-	7,7,7	0.16	0	9,10,10	0.23	0
2	MPD	B	501	-	7,7,7	0.15	0	9,10,10	0.29	0
3	BTB	A	507	-	13,13,13	1.30	2 (15%)	7,16,16	1.60	1 (14%)
2	MPD	B	505	-	7,7,7	0.11	0	9,10,10	0.52	0
2	MPD	A	504	-	7,7,7	0.16	0	9,10,10	0.78	0
2	MPD	B	504	-	7,7,7	0.12	0	9,10,10	0.38	0
2	MPD	B	503	-	7,7,7	0.15	0	9,10,10	0.29	0
2	MPD	C	501	-	7,7,7	0.17	0	9,10,10	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	C	504	-	7,7,7	0.16	0	9,10,10	0.31	0
2	MPD	A	501	-	7,7,7	0.11	0	9,10,10	0.63	0
2	MPD	A	505	-	7,7,7	0.15	0	9,10,10	0.34	0
2	MPD	C	502	-	7,7,7	0.15	0	9,10,10	0.35	0
2	MPD	B	502	-	7,7,7	0.11	0	9,10,10	0.30	0
2	MPD	A	502	-	7,7,7	0.14	0	9,10,10	0.47	0
2	MPD	A	503	-	7,7,7	0.11	0	9,10,10	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	A	506	-	-	0/5/5/5	-
2	MPD	C	503	-	-	0/5/5/5	-
2	MPD	B	501	-	-	1/5/5/5	-
3	BTB	A	507	-	-	7/21/21/21	-
2	MPD	B	505	-	-	2/5/5/5	-
2	MPD	A	504	-	-	1/5/5/5	-
2	MPD	B	504	-	-	0/5/5/5	-
2	MPD	B	503	-	-	1/5/5/5	-
2	MPD	C	501	-	-	0/5/5/5	-
2	MPD	C	504	-	-	0/5/5/5	-
2	MPD	A	501	-	-	1/5/5/5	-
2	MPD	A	505	-	-	1/5/5/5	-
2	MPD	C	502	-	-	1/5/5/5	-
2	MPD	B	502	-	-	0/5/5/5	-
2	MPD	A	502	-	-	2/5/5/5	-
2	MPD	A	503	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	BTB	C2-N	3.08	1.54	1.48
3	A	507	BTB	C3-C2	2.33	1.56	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	507	BTB	O8-C8-C7	-2.49	100.85	111.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	507	BTB	C1-C2-N-C7
3	A	507	BTB	C4-C2-N-C5
3	A	507	BTB	C4-C2-N-C7
2	B	505	MPD	C2-C3-C4-O4
2	B	505	MPD	C2-C3-C4-C5
2	A	501	MPD	C2-C3-C4-O4
3	A	507	BTB	N-C7-C8-O8
2	A	502	MPD	C2-C3-C4-C5
2	A	502	MPD	C2-C3-C4-O4
2	B	501	MPD	C1-C2-C3-C4
3	A	507	BTB	C1-C2-N-C5
3	A	507	BTB	C3-C2-N-C7
2	A	505	MPD	C1-C2-C3-C4
2	C	502	MPD	C1-C2-C3-C4
3	A	507	BTB	N-C5-C6-O6
2	B	503	MPD	O2-C2-C3-C4
2	A	504	MPD	C2-C3-C4-C5

There are no ring outliers.

13 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	506	MPD	1	0
2	C	503	MPD	3	0
3	A	507	BTB	3	0
2	A	504	MPD	4	0
2	B	504	MPD	3	0
2	B	503	MPD	2	0
2	C	501	MPD	1	0
2	C	504	MPD	1	0
2	A	501	MPD	7	0
2	A	505	MPD	3	0
2	C	502	MPD	6	0
2	B	502	MPD	2	0
2	A	503	MPD	6	0

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	490/496 (98%)	-0.55	9 (1%) 68 74	19, 30, 60, 109	0
1	B	490/496 (98%)	-0.45	5 (1%) 82 86	18, 33, 64, 113	0
1	C	490/496 (98%)	-0.41	6 (1%) 79 83	19, 35, 64, 116	0
All	All	1470/1488 (98%)	-0.47	20 (1%) 75 80	18, 32, 63, 116	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	GLY	8.4
1	B	496	GLY	4.9
1	C	496	GLY	4.7
1	C	437	ASN	3.9
1	A	437	ASN	3.4
1	A	476	GLY	3.0
1	B	43[A]	ASP	3.0
1	C	495	ALA	2.8
1	B	495	ALA	2.8
1	A	395	PRO	2.8
1	A	438	GLY	2.7
1	A	495	ALA	2.7
1	B	437	ASN	2.6
1	C	476	GLY	2.3
1	C	250	LYS	2.2
1	A	475	GLU	2.2
1	C	307	PRO	2.2
1	A	439	GLY	2.1
1	B	475	GLU	2.0
1	A	436	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MPD	C	502	8/8	0.62	0.51	20,20,20,20	0
2	MPD	B	505	8/8	0.67	0.49	20,20,20,20	0
2	MPD	A	502	8/8	0.72	0.42	20,20,20,20	0
2	MPD	B	501	8/8	0.73	0.41	20,20,20,20	0
2	MPD	A	506	8/8	0.76	0.51	20,20,20,20	0
2	MPD	A	505	8/8	0.76	0.44	20,20,20,20	0
2	MPD	C	504	8/8	0.79	0.72	20,20,20,20	0
2	MPD	A	503	8/8	0.80	0.50	20,20,20,20	0
2	MPD	A	501	8/8	0.81	0.63	20,20,20,20	0
2	MPD	B	502	8/8	0.81	0.67	20,20,20,20	0
2	MPD	B	504	8/8	0.82	0.43	20,20,20,20	0
2	MPD	C	501	8/8	0.83	0.43	20,20,20,20	0
2	MPD	A	504	8/8	0.83	0.49	20,20,20,20	0
2	MPD	B	503	8/8	0.86	0.43	20,20,20,20	0
2	MPD	C	503	8/8	0.89	0.42	20,20,20,20	0
3	BTB	A	507	14/14	0.89	0.22	48,72,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.