Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 10:02 AM EDT

PDB ID	:	3LXV
Title	:	Tyrosine 447 of Protocatechuate 3,4-Dioxygenase Controls Efficient Progress Through Catalysis
Authors	:	Purpero, V.M.; Lipscomb, J.D.
Deposited on	:	2010-02-25
Resolution	:	1.90 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:

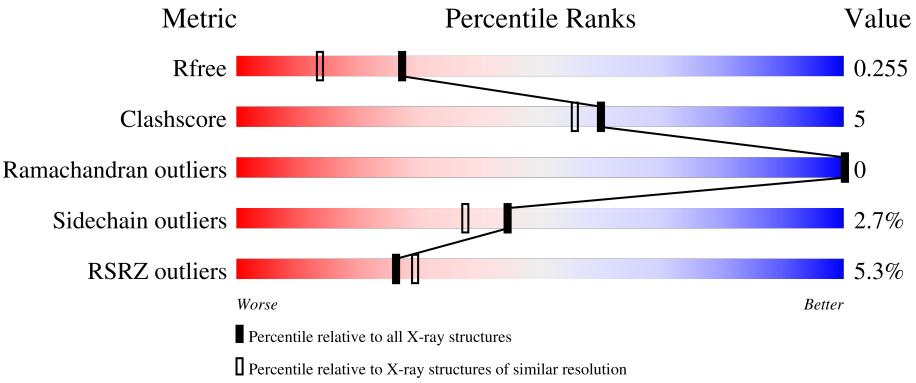
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	200	7% 84% 16%
1	B	200	2% 94% 6%
1	C	200	14% 92% 7%
2	M	238	3% 95% 5%
2	N	238	2% 91% 8%

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Mol	Chain	Length	Quality of chain
2	O	238	6% 93% 7%

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
4	GOL	A	202	-	-	X	-
5	BME	A	204	-	-	X	X
7	CO3	M	33	-	-	-	X
9	4NC	O	3	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11718 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 Protocatechuate 3,4-dioxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	3	0
			1589	1005	277	304	3			
1	B	200	Total	C	N	O	S	0	1	0
			1578	998	277	300	3			
1	C	200	Total	C	N	O	S	0	1	0
			1578	998	277	300	3			

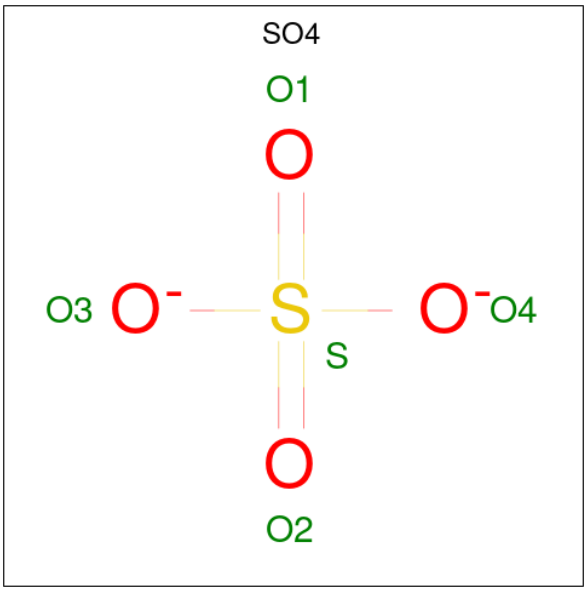
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	238	Total	C	N	O	S	0	2	0
			1893	1198	348	339	8			
2	N	238	Total	C	N	O	S	0	2	0
			1890	1197	347	338	8			
2	O	238	Total	C	N	O	S	0	2	0
			1891	1196	347	340	8			

There are 3 discrepancies between the modelled and reference sequences:

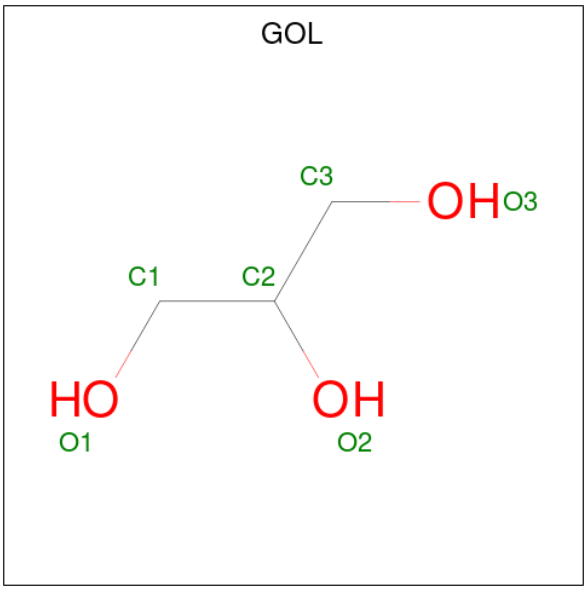
Chain	Residue	Modelled	Actual	Comment	Reference
M	447	HIS	TYR	engineered mutation	UNP P00437
N	447	HIS	TYR	engineered mutation	UNP P00437
O	447	HIS	TYR	engineered mutation	UNP P00437

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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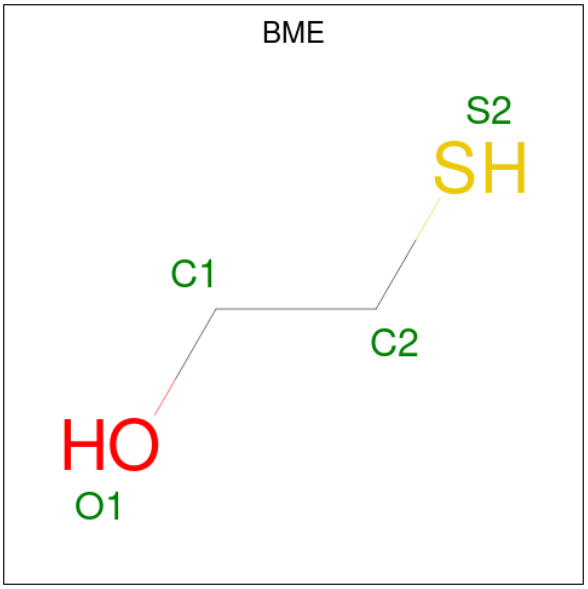
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

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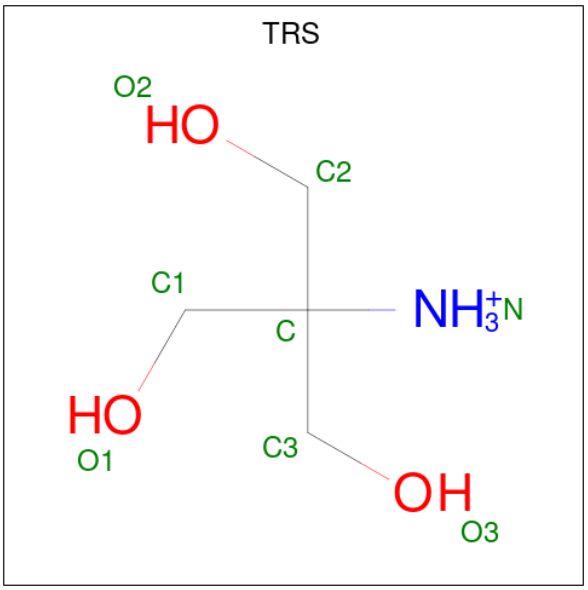
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O S 4 2 1 1	0	0
5	N	1	Total C O S 4 2 1 1	0	0
5	N	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4 2 1 1	0	0
5	O	1	Total C O S 8 4 2 2	0	1
5	O	1	Total C O S 4 2 1 1	0	0
5	O	1	Total C O S 4 2 1 1	0	0
5	O	1	Total C O S 4 2 1 1	0	0
5	O	1	Total C O S 4 2 1 1	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 8 4 1 3	0	0

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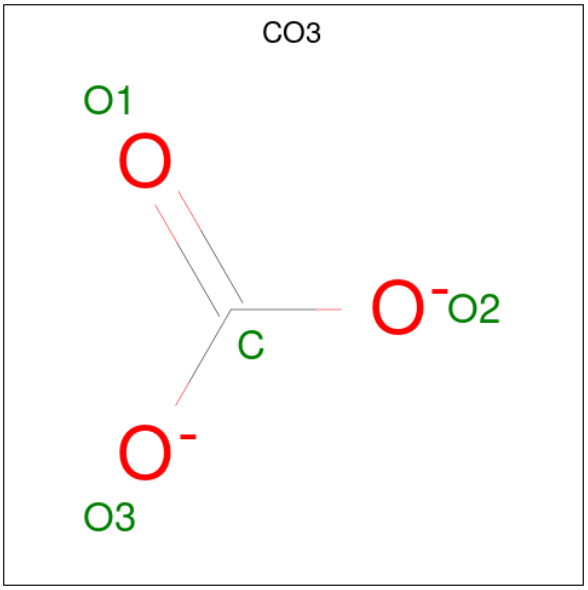
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 8 4 1 3	0	0
6	O	1	Total C N O 8 4 1 3	0	0

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 1 3	0	0
7	M	1	Total C O 4 1 3	0	0
7	M	1	Total C O 4 1 3	0	0
7	N	1	Total C O 4 1 3	0	0
7	C	1	Total C O 4 1 3	0	0

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total Fe 1 1	0	0
8	N	1	Total Fe 1 1	0	0

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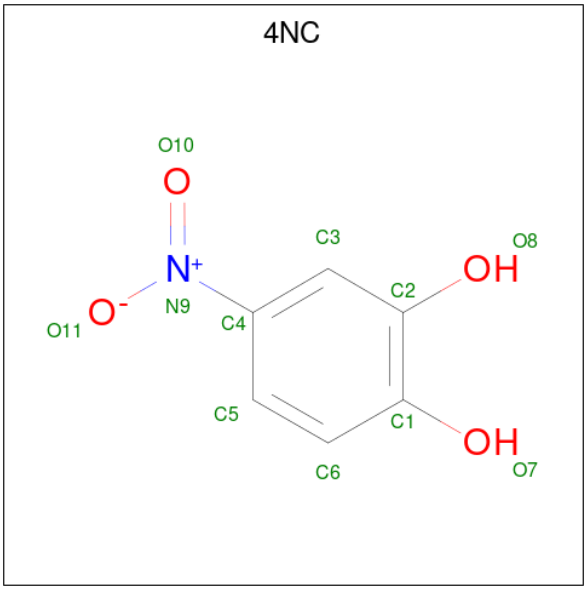
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	O	1	Total Fe 1 1	0	0

- Molecule 9 is 4-NITROCATECHOL (three-letter code: 4NC) (formula: $C_6H_5NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C N O 11 6 1 4	0	0
9	N	1	Total C N O 11 6 1 4	0	0
9	O	1	Total C N O 22 12 2 8	0	1
9	O	1	Total C N O 11 6 1 4	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cl 1 1	0	0
10	N	1	Total Cl 1 1	0	0
10	O	1	Total Cl 1 1	0	0

- Molecule 11 is water.

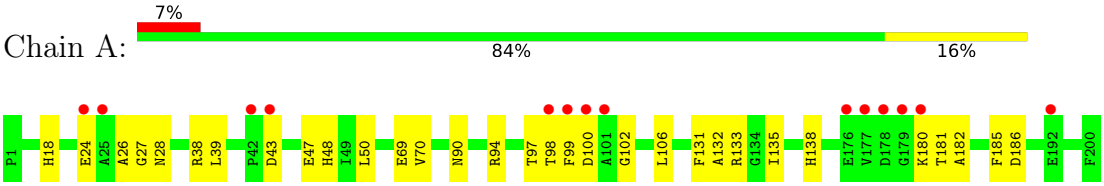
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	164	Total O 168 168	0	4
11	M	210	Total O 211 211	0	1
11	B	156	Total O 157 157	0	1
11	N	208	Total O 210 210	0	2
11	C	124	Total O 125 125	0	1
11	O	200	Total O 202 202	0	2

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.

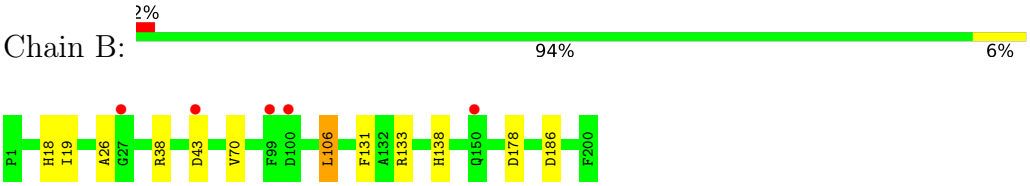
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain A:



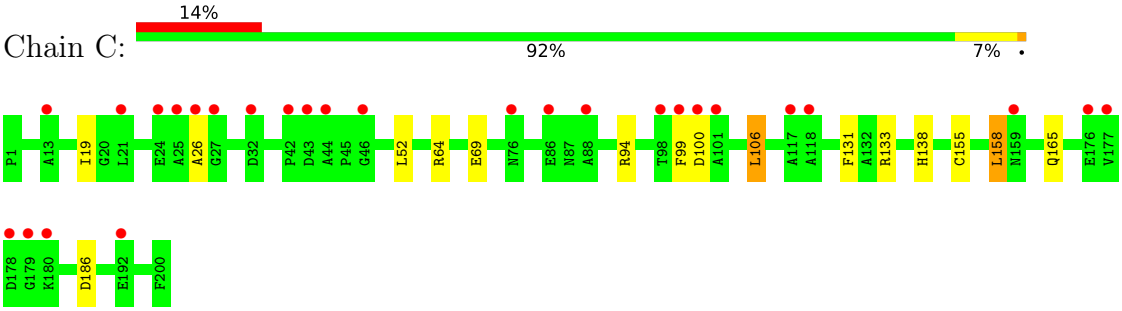
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain B:



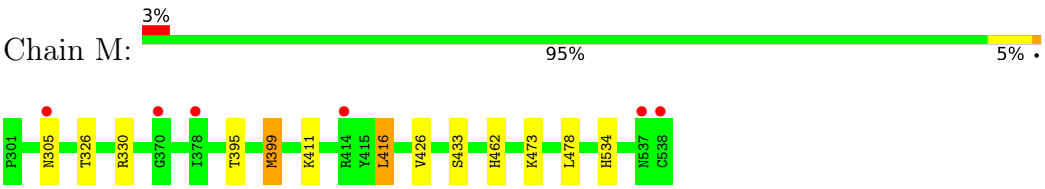
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain C:



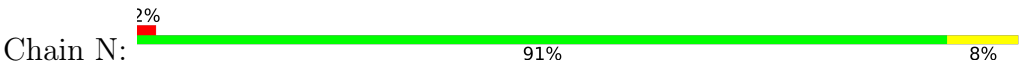
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

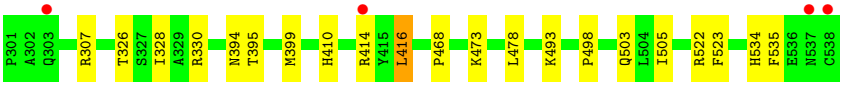
Chain M:



• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

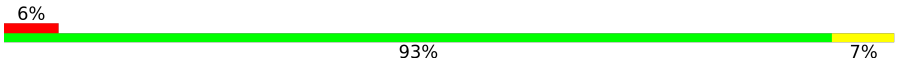
Chain N:

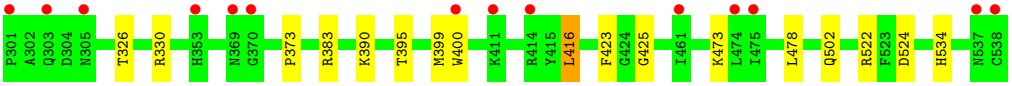




• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain O:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	128.11Å 140.59Å 167.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.99 – 1.90 41.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.99-1.90) 99.5 (41.44-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.246 0.210 , 0.255	Depositor DCC
R_{free} test set	5928 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11718	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, CL, BME, FE, 4NC, CO3, TRS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.68	0/1638	0.70	0/2230
1	B	0.67	0/1621	0.73	1/2207 (0.0%)
1	C	0.63	0/1621	0.69	1/2207 (0.0%)
2	M	0.71	0/1955	0.72	1/2659 (0.0%)
2	N	0.69	0/1953	0.71	1/2657 (0.0%)
2	O	0.67	0/1950	0.69	1/2653 (0.0%)
All	All	0.68	0/10738	0.71	5/14613 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	106	LEU	CA-CB-CG	7.18	131.83	115.30
1	C	106	LEU	CA-CB-CG	6.64	130.57	115.30
2	N	416	LEU	CA-CB-CG	6.26	129.70	115.30
2	M	416	LEU	CA-CB-CG	6.02	129.15	115.30
2	O	416	LEU	CA-CB-CG	6.01	129.13	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1589	0	1525	34	0
1	B	1578	0	1515	8	0
1	C	1578	0	1515	11	0
2	M	1893	0	1852	9	0
2	N	1890	0	1849	16	0
2	O	1891	0	1847	10	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	6	0	8	7	0
4	C	6	0	8	2	0
4	M	12	0	16	0	0
4	N	18	0	24	3	0
5	A	8	0	12	5	0
5	B	4	0	6	0	0
5	C	8	0	12	1	0
5	M	12	0	18	3	0
5	N	8	0	12	4	0
5	O	24	0	36	4	0
6	A	8	0	12	5	0
6	B	8	0	12	1	0
6	O	8	0	12	4	0
7	A	4	0	0	0	0
7	C	4	0	0	1	0
7	M	8	0	0	0	0
7	N	4	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
9	M	11	0	3	2	0
9	N	11	0	3	0	0
9	O	33	0	9	5	0
10	B	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
11	A	168	0	0	14	0
11	B	157	0	0	2	0
11	C	125	0	0	2	0
11	M	211	0	0	2	0
11	N	210	0	0	4	0
11	O	202	0	0	8	0
All	All	11718	0	10306	97	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 5.

All (97) 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)
9:O:3:4NC:H3	11:O:955:HOH:O	1.23	1.29
9:M:1:4NC:H3	11:M:964:HOH:O	0.89	1.07
2:O:524:ASP:H	6:O:27:TRS:H11	1.18	1.06
9:O:3:4NC:C3	11:O:955:HOH:O	1.87	1.03
1:A:26:ALA:O	11:A:1042:HOH:O	1.76	1.03
2:O:383:ARG:HH22	5:O:20:BME:H21	1.24	1.00
2:N:493:LYS:HE2	11:N:979:HOH:O	1.62	0.96
1:B:178:ASP:OD2	11:B:871:HOH:O	1.86	0.93
1:C:99:PHE:HB3	11:C:1041:HOH:O	1.68	0.93
2:O:502:GLN:OE1	9:O:37[B]:4NC:O8	1.93	0.87
1:B:70:VAL:HG11	1:B:106:LEU:HD21	1.57	0.86
1:B:186:ASP:H	6:B:203:TRS:H12	1.40	0.85
1:A:186:ASP:H	6:A:205:TRS:H12	1.42	0.84
9:O:3:4NC:O8	11:O:955:HOH:O	1.95	0.84
1:A:38:ARG:O	4:A:202:GOL:H32	1.77	0.82
5:A:204:BME:H21	2:M:426:VAL:HG12	1.60	0.81
1:A:98:THR:HA	11:A:864:HOH:O	1.81	0.81
6:O:27:TRS:H21	11:O:1005:HOH:O	1.80	0.80
1:C:186:ASP:H	4:C:202:GOL:H31	1.48	0.77
2:N:535:PHE:H	5:N:12:BME:H21	1.51	0.75
1:A:27:GLY:N	11:A:1036:HOH:O	1.69	0.74
2:O:524:ASP:H	6:O:27:TRS:C1	2.00	0.73
2:O:524:ASP:N	6:O:27:TRS:H11	2.00	0.72
2:M:433:SER:N	5:M:16:BME:H22	2.05	0.71
1:C:19:ILE:HG22	1:C:26:ALA:HB1	1.72	0.70
5:A:204:BME:H21	2:M:426:VAL:CG1	2.20	0.70
9:M:1:4NC:C3	11:M:964:HOH:O	1.69	0.70
1:A:186:ASP:H	6:A:205:TRS:C1	2.05	0.69
2:N:394[A]:ASN:OD1	11:N:569[A]:HOH:O	2.11	0.67
1:A:47[A]:GLU:HG2	11:A:867:HOH:O	1.94	0.67
1:A:97:THR:O	11:A:734:HOH:O	2.13	0.65
5:O:19:BME:H21	11:O:1062:HOH:O	1.95	0.65
2:N:307:ARG:HD2	5:N:22:BME:H11	1.78	0.65
5:A:204:BME:H11	11:A:705:HOH:O	1.99	0.62
1:A:27:GLY:CA	11:A:1036:HOH:O	2.33	0.62
1:B:38:ARG:HD3	11:B:901:HOH:O	1.99	0.62
2:N:505:ILE:CD1	4:N:10:GOL:H11	2.29	0.62
1:C:133:ARG:HG2	2:O:326[A]:THR:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:ND2	4:A:202:GOL:H2	2.17	0.60
2:O:326[A]:THR:HG22	2:O:330:ARG:HD2	1.86	0.58
1:C:155:CYS:HB3	1:C:158:LEU:HB2	1.87	0.56
1:B:19:ILE:HD11	2:N:410:HIS:HB2	1.87	0.56
1:A:98:THR:O	1:A:102:GLY:HA2	2.07	0.55
1:A:180:LYS:HG2	1:A:181:THR:N	2.21	0.55
1:A:90:ASN:HD22	4:A:202:GOL:C3	2.20	0.55
1:C:19:ILE:HG22	1:C:26:ALA:CB	2.38	0.54
2:N:307:ARG:HD2	5:N:22:BME:C1	2.38	0.54
1:C:131:PHE:CE2	1:C:138:HIS:HB3	2.43	0.53
1:A:186:ASP:N	6:A:205:TRS:H12	2.19	0.53
2:M:433:SER:H	5:M:16:BME:H22	1.71	0.53
1:A:99:PHE:HB2	11:A:897:HOH:O	2.07	0.52
1:A:133:ARG:HG2	2:M:326:THR:HG21	1.91	0.52
1:C:186:ASP:H	4:C:202:GOL:C3	2.18	0.52
1:A:18:HIS:ND1	11:A:802:HOH:O	2.34	0.51
6:A:205:TRS:O2	6:A:205:TRS:O1	2.20	0.51
1:A:18:HIS:CG	11:A:802:HOH:O	2.64	0.49
1:A:38:ARG:O	4:A:202:GOL:C3	2.54	0.49
1:C:69:GLU:HG2	1:C:94:ARG:HG2	1.95	0.48
2:M:326:THR:HG22	2:M:330:ARG:HD2	1.95	0.48
2:O:400:TRP:HA	2:O:425:GLY:O	2.13	0.47
1:C:64:ARG:HD3	1:C:99:PHE:O	2.15	0.47
1:A:39:LEU:O	4:A:202:GOL:H31	2.15	0.47
2:N:505:ILE:HD12	4:N:10:GOL:H11	1.95	0.47
5:C:204:BME:H22	11:O:811:HOH:O	2.14	0.47
9:O:3:4NC:C2	11:O:955:HOH:O	2.20	0.47
1:A:70:VAL:HG11	1:A:106:LEU:HD11	1.97	0.46
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.51	0.46
1:A:18:HIS:CE1	11:A:734:HOH:O	2.68	0.46
1:A:90:ASN:HD22	4:A:202:GOL:H2	1.81	0.46
2:N:523:PHE:HA	4:N:6:GOL:H2	1.98	0.46
1:A:18:HIS:HE1	11:A:734:HOH:O	1.97	0.46
1:A:90:ASN:HD22	4:A:202:GOL:C2	2.28	0.46
2:M:433:SER:H	5:M:16:BME:C2	2.29	0.45
2:O:478:LEU:C	2:O:478:LEU:HD23	2.38	0.45
2:N:326:THR:HG22	2:N:330:ARG:HD2	2.00	0.44
1:A:50:LEU:O	1:A:182:ALA:HA	2.18	0.44
2:N:498:PRO:HB3	11:N:1057:HOH:O	2.18	0.43
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.52	0.43
2:M:478:LEU:HD23	2:M:478:LEU:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:535:PHE:N	5:N:12:BME:H21	2.25	0.43
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.53	0.43
1:A:24:GLU:C	11:A:1036:HOH:O	2.58	0.42
2:N:328:ILE:HD13	5:O:21:BME:H21	2.00	0.42
1:A:132:ALA:HB3	1:A:135:ILE:HD12	2.01	0.42
2:M:399:MET:HA	2:M:462:HIS:O	2.19	0.42
1:A:185:PHE:HA	6:A:205:TRS:H11	2.00	0.42
1:B:18:HIS:HB2	1:B:26:ALA:HB2	2.02	0.42
2:O:373:PRO:HB3	2:O:423:PHE:HB2	2.02	0.42
5:O:19:BME:C2	11:O:1062:HOH:O	2.62	0.41
1:A:69:GLU:HG2	1:A:94:ARG:HG2	2.02	0.41
7:C:205:CO3:C	11:C:1055:HOH:O	2.69	0.41
1:A:28:ASN:HB3	5:A:204:BME:O1	2.21	0.41
1:A:48:HIS:CG	5:A:203:BME:H21	2.55	0.41
1:B:133:ARG:HG2	2:N:326:THR:HG21	2.03	0.41
2:N:503:GLN:HG2	11:N:180:HOH:O	2.21	0.41
2:N:478:LEU:C	2:N:478:LEU:HD23	2.42	0.40
1:A:99:PHE:N	11:A:864:HOH:O	2.45	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	201/200 (100%)	197 (98%)	4 (2%)	0	100	100
1	B	199/200 (100%)	197 (99%)	2 (1%)	0	100	100
1	C	199/200 (100%)	194 (98%)	5 (2%)	0	100	100
2	M	238/238 (100%)	230 (97%)	8 (3%)	0	100	100
2	N	238/238 (100%)	232 (98%)	6 (2%)	0	100	100
2	O	238/238 (100%)	233 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1313/1314 (100%)	1283 (98%)	30 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	166/163 (102%)	164 (99%)	2 (1%)	71 70
1	B	164/163 (101%)	163 (99%)	1 (1%)	86 87
1	C	164/163 (101%)	159 (97%)	5 (3%)	41 33
2	M	204/202 (101%)	197 (97%)	7 (3%)	37 28
2	N	204/202 (101%)	196 (96%)	8 (4%)	32 23
2	O	204/202 (101%)	197 (97%)	7 (3%)	37 28
All	All	1106/1095 (101%)	1076 (97%)	30 (3%)	44 38

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	100	ASP
2	M	305	ASN
2	M	395	THR
2	M	399	MET
2	M	411	LYS
2	M	416	LEU
2	M	473	LYS
2	M	534	HIS
1	B	43	ASP
2	N	395	THR
2	N	399	MET
2	N	414	ARG
2	N	416	LEU

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Mol	Chain	Res	Type
2	N	468	PRO
2	N	473	LYS
2	N	522	ARG
2	N	534	HIS
1	C	52	LEU
1	C	100	ASP
1	C	106	LEU
1	C	158	LEU
1	C	165	GLN
2	O	390	LYS
2	O	395	THR
2	O	399	MET
2	O	416	LEU
2	O	473	LYS
2	O	522	ARG
2	O	534	HIS

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

Mol	Chain	Res	Type
2	M	305	ASN
2	N	502	GLN
2	O	502	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 6 are monoatomic - leaving 39 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	CO3	M	29	-	0,3,3	-	-	0,3,3	-	-
5	BME	C	203	-	3,3,3	0.40	0	1,2,2	0.30	0
5	BME	C	204	-	3,3,3	0.26	0	1,2,2	1.24	0
6	TRS	B	203	-	7,7,7	0.32	0	9,9,9	0.56	0
7	CO3	C	205	-	0,3,3	-	-	0,3,3	-	-
5	BME	O	20	-	3,3,3	0.29	0	1,2,2	0.19	0
7	CO3	A	206	-	0,3,3	-	-	0,3,3	-	-
5	BME	N	22	-	3,3,3	0.49	0	1,2,2	0.68	0
5	BME	O	19	-	3,3,3	0.46	0	1,2,2	1.37	0
3	SO4	B	201	-	4,4,4	0.17	0	6,6,6	0.25	0
6	TRS	O	27	-	7,7,7	0.77	0	9,9,9	1.19	1 (11%)
4	GOL	N	9	-	5,5,5	0.44	0	5,5,5	0.73	0
9	4NC	O	37[A]	-	10,11,11	1.71	1 (10%)	13,15,15	1.39	2 (15%)
4	GOL	M	5	-	5,5,5	0.34	0	5,5,5	0.62	0
5	BME	M	18	-	3,3,3	0.27	0	1,2,2	0.52	0
9	4NC	M	1	8	10,11,11	1.37	1 (10%)	13,15,15	0.90	0
5	BME	O	14[A]	-	3,3,3	0.30	0	1,2,2	0.80	0
4	GOL	A	202	-	5,5,5	0.45	0	5,5,5	1.07	0
5	BME	O	17	-	3,3,3	0.34	0	1,2,2	0.71	0
4	GOL	C	202	-	5,5,5	0.39	0	5,5,5	0.54	0
4	GOL	N	6	-	5,5,5	0.61	0	5,5,5	0.55	0
9	4NC	O	3	8	10,11,11	1.78	2 (20%)	13,15,15	2.23	3 (23%)
3	SO4	A	201	-	4,4,4	0.19	0	6,6,6	0.33	0
5	BME	O	21	-	3,3,3	0.51	0	1,2,2	1.20	0
9	4NC	N	2	8	10,11,11	1.45	1 (10%)	13,15,15	1.36	3 (23%)
5	BME	M	16	-	3,3,3	0.40	0	1,2,2	1.44	0
9	4NC	O	37[B]	-	10,11,11	1.74	1 (10%)	13,15,15	1.52	3 (23%)
6	TRS	A	205	-	7,7,7	0.39	0	9,9,9	0.61	0
4	GOL	M	7	-	5,5,5	0.54	0	5,5,5	0.43	0
7	CO3	N	31	-	0,3,3	-	-	0,3,3	-	-
5	BME	A	204	-	3,3,3	0.27	0	1,2,2	0.65	0
5	BME	B	202	-	3,3,3	0.44	0	1,2,2	0.52	0
5	BME	O	14[B]	-	3,3,3	0.32	0	1,2,2	0.02	0
4	GOL	N	10	-	5,5,5	0.37	0	5,5,5	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	C	201	-	4,4,4	0.68	0	6,6,6	0.63	0
5	BME	M	15	-	3,3,3	0.19	0	1,2,2	0.79	0
5	BME	A	203	-	3,3,3	0.27	0	1,2,2	0.17	0
7	CO3	M	33	-	0,3,3	-	-	0,3,3	-	-
5	BME	N	12	-	3,3,3	0.34	0	1,2,2	0.56	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
5	BME	C	203	-	-	1/1/1/1	-
5	BME	C	204	-	-	1/1/1/1	-
6	TRS	B	203	-	-	5/9/9/9	-
5	BME	O	20	-	-	1/1/1/1	-
5	BME	N	22	-	-	0/1/1/1	-
5	BME	O	19	-	-	1/1/1/1	-
6	TRS	O	27	-	-	3/9/9/9	-
4	GOL	N	9	-	-	2/4/4/4	-
9	4NC	O	37[A]	-	-	0/2/4/4	0/1/1/1
4	GOL	M	5	-	-	2/4/4/4	-
5	BME	M	18	-	-	1/1/1/1	-
9	4NC	M	1	8	-	0/2/4/4	0/1/1/1
5	BME	O	14[A]	-	-	0/1/1/1	-
4	GOL	A	202	-	-	0/4/4/4	-
5	BME	O	17	-	-	1/1/1/1	-
4	GOL	C	202	-	-	4/4/4/4	-
4	GOL	N	6	-	-	4/4/4/4	-
9	4NC	O	3	8	-	0/2/4/4	0/1/1/1
5	BME	O	21	-	-	0/1/1/1	-
9	4NC	N	2	8	-	0/2/4/4	0/1/1/1
5	BME	M	16	-	-	1/1/1/1	-
9	4NC	O	37[B]	-	-	0/2/4/4	0/1/1/1
6	TRS	A	205	-	-	6/9/9/9	-
4	GOL	M	7	-	-	3/4/4/4	-
5	BME	A	204	-	-	1/1/1/1	-
5	BME	B	202	-	-	1/1/1/1	-
5	BME	O	14[B]	-	-	0/1/1/1	-
4	GOL	N	10	-	-	2/4/4/4	-
5	BME	M	15	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BME	A	203	-	-	1/1/1/1	-
5	BME	N	12	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	37[B]	4NC	C2-C1	4.85	1.47	1.40
9	O	37[A]	4NC	C2-C1	4.45	1.47	1.40
9	O	3	4NC	C2-C1	4.09	1.46	1.40
9	N	2	4NC	C2-C1	3.75	1.46	1.40
9	M	1	4NC	C2-C1	3.29	1.45	1.40
9	O	3	4NC	C4-N9	-2.40	1.39	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	3	4NC	C5-C4-N9	5.22	123.31	119.38
9	O	3	4NC	C3-C4-N9	-3.85	115.35	118.75
9	O	3	4NC	O10-N9-C4	3.73	124.08	118.80
9	O	37[B]	4NC	C5-C6-C1	-3.09	117.33	120.50
9	O	37[B]	4NC	C6-C5-C4	3.03	124.30	120.08
9	N	2	4NC	C5-C4-N9	2.77	121.46	119.38
9	O	37[A]	4NC	C5-C6-C1	-2.67	117.75	120.50
9	O	37[A]	4NC	C4-C3-C2	2.36	120.77	118.75
9	O	37[B]	4NC	C3-C4-N9	2.31	120.78	118.75
9	N	2	4NC	O10-N9-C4	2.23	121.96	118.80
6	O	27	TRS	C2-C-C1	-2.10	104.31	110.81
9	N	2	4NC	C4-C3-C2	2.01	120.47	118.75

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	6	GOL	C1-C2-C3-O3
4	N	10	GOL	C1-C2-C3-O3
4	C	202	GOL	C1-C2-C3-O3
5	A	204	BME	O1-C1-C2-S2
5	M	15	BME	O1-C1-C2-S2
5	M	18	BME	O1-C1-C2-S2
5	B	202	BME	O1-C1-C2-S2
5	N	12	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
5	C	203	BME	O1-C1-C2-S2
5	C	204	BME	O1-C1-C2-S2
5	O	19	BME	O1-C1-C2-S2
6	A	205	TRS	C1-C-C2-O2
6	A	205	TRS	C3-C-C2-O2
6	A	205	TRS	N-C-C2-O2
6	B	203	TRS	N-C-C3-O3
6	O	27	TRS	C2-C-C1-O1
6	O	27	TRS	C3-C-C1-O1
6	O	27	TRS	N-C-C1-O1
4	C	202	GOL	O1-C1-C2-O2
4	C	202	GOL	O2-C2-C3-O3
4	M	7	GOL	O1-C1-C2-C3
4	N	6	GOL	O1-C1-C2-C3
4	N	9	GOL	O1-C1-C2-C3
4	C	202	GOL	O1-C1-C2-C3
4	N	6	GOL	O2-C2-C3-O3
4	N	10	GOL	O2-C2-C3-O3
5	A	203	BME	O1-C1-C2-S2
5	M	16	BME	O1-C1-C2-S2
6	A	205	TRS	C2-C-C1-O1
6	B	203	TRS	C2-C-C1-O1
4	M	5	GOL	O1-C1-C2-O2
4	M	7	GOL	O2-C2-C3-O3
5	O	20	BME	O1-C1-C2-S2
4	N	6	GOL	O1-C1-C2-O2
6	A	205	TRS	N-C-C1-O1
6	B	203	TRS	N-C-C1-O1
4	N	9	GOL	O1-C1-C2-O2
6	A	205	TRS	C3-C-C1-O1
6	B	203	TRS	C3-C-C1-O1
4	M	5	GOL	O1-C1-C2-C3
5	O	17	BME	O1-C1-C2-S2
6	B	203	TRS	C3-C-C2-O2
4	M	7	GOL	O1-C1-C2-O2

There are no ring outliers.

20 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	204	BME	1	0
6	B	203	TRS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	205	CO3	1	0
5	O	20	BME	1	0
5	N	22	BME	2	0
5	O	19	BME	2	0
6	O	27	TRS	4	0
9	M	1	4NC	2	0
4	A	202	GOL	7	0
4	C	202	GOL	2	0
4	N	6	GOL	1	0
9	O	3	4NC	4	0
5	O	21	BME	1	0
5	M	16	BME	3	0
9	O	37[B]	4NC	1	0
6	A	205	TRS	5	0
5	A	204	BME	4	0
4	N	10	GOL	2	0
5	A	203	BME	1	0
5	N	12	BME	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	200/200 (100%)	0.36	14 (7%) 16 18	23, 30, 47, 56	0
1	B	200/200 (100%)	0.24	5 (2%) 57 60	24, 30, 41, 50	3 (1%)
1	C	200/200 (100%)	0.85	27 (13%) 3 3	25, 36, 51, 60	1 (0%)
2	M	238/238 (100%)	0.28	6 (2%) 57 60	23, 28, 38, 51	1 (0%)
2	N	238/238 (100%)	0.14	4 (1%) 70 72	24, 28, 37, 48	0
2	O	238/238 (100%)	0.46	14 (5%) 22 25	24, 30, 40, 54	0
All	All	1314/1314 (100%)	0.38	70 (5%) 26 29	23, 30, 44, 60	5 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	VAL	7.4
1	A	99	PHE	6.1
1	C	101	ALA	5.8
1	C	178	ASP	5.7
1	A	101	ALA	5.6
1	A	178	ASP	5.4
1	C	99	PHE	5.1
1	A	100	ASP	5.0
1	C	100	ASP	5.0
1	C	179	GLY	4.6
1	C	43	ASP	4.5
2	M	538	CYS	4.4
1	C	26	ALA	4.1
2	O	538	CYS	4.0
2	O	301	PRO	4.0
1	C	180	LYS	4.0
1	C	176	GLU	3.8
2	O	305	ASN	3.7
1	A	176	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	THR	3.6
1	A	180	LYS	3.5
1	A	179	GLY	3.5
1	A	43	ASP	3.2
2	O	303	GLN	3.2
2	O	461	ILE	3.2
2	N	414	ARG	3.2
1	C	98	THR	3.1
1	C	159	ASN	3.1
2	O	370	GLY	3.0
2	O	353	HIS	3.0
1	C	24	GLU	3.0
1	C	86	GLU	3.0
1	C	42	PRO	3.0
1	A	24	GLU	3.0
2	M	370	GLY	2.9
2	N	538	CYS	2.9
1	C	46	GLY	2.9
2	O	475	ILE	2.8
1	B	99	PHE	2.8
2	O	369	ASN	2.8
2	O	474	LEU	2.7
2	M	414	ARG	2.7
1	C	25	ALA	2.7
2	O	400	TRP	2.7
2	O	414	ARG	2.7
1	C	192	GLU	2.7
1	C	44	ALA	2.6
1	A	177	VAL	2.6
2	O	537	ASN	2.6
1	C	88	ALA	2.6
1	B	150	GLN	2.6
2	M	537	ASN	2.6
2	M	305	ASN	2.6
1	B	27	GLY	2.6
1	C	27	GLY	2.5
2	N	303	GLN	2.5
1	B	100	ASP	2.5
1	A	42	PRO	2.5
1	B	43	ASP	2.5
1	A	192	GLU	2.4
1	C	32	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	378	ILE	2.3
2	N	537	ASN	2.2
1	C	76	ASN	2.1
1	A	25	ALA	2.1
1	C	13	ALA	2.1
1	C	117	ALA	2.1
1	C	118	ALA	2.1
1	C	21	LEU	2.0
2	O	411	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BME	B	202	4/4	0.41	0.40	39,41,42,45	0
5	BME	A	204	4/4	0.56	0.59	20,20,20,20	0
5	BME	C	203	4/4	0.60	0.25	65,67,68,70	0
4	GOL	N	9	6/6	0.61	0.24	57,58,59,59	0
4	GOL	N	10	6/6	0.64	0.23	47,48,50,51	0
5	BME	O	21	4/4	0.68	0.19	57,59,59,62	0
9	4NC	O	37[A]	11/11	0.68	0.27	52,54,56,56	11
9	4NC	O	37[B]	11/11	0.68	0.27	61,63,64,64	11
7	CO3	A	206	4/4	0.69	0.24	61,61,61,61	0
7	CO3	M	33	4/4	0.69	0.50	20,20,20,20	0
5	BME	O	17	4/4	0.71	0.22	68,69,69,69	0
6	TRS	O	27	8/8	0.71	0.27	61,63,63,63	0
5	BME	O	20	4/4	0.72	0.20	79,80,80,80	0
10	CL	O	36	1/1	0.73	0.20	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	202	6/6	0.75	0.31	49,52,55,55	0
6	TRS	B	203	8/8	0.75	0.30	57,58,59,59	0
4	GOL	N	6	6/6	0.78	0.19	48,51,51,54	0
5	BME	M	16	4/4	0.79	0.16	74,76,76,77	0
5	BME	N	22	4/4	0.80	0.20	55,56,57,60	0
4	GOL	M	5	6/6	0.80	0.19	45,50,51,53	0
5	BME	N	12	4/4	0.80	0.13	70,70,70,72	0
7	CO3	N	31	4/4	0.81	0.17	60,60,61,61	0
5	BME	O	14[B]	4/4	0.81	0.26	20,20,21,22	4
5	BME	O	14[A]	4/4	0.81	0.26	73,75,75,76	4
5	BME	O	19	4/4	0.81	0.17	68,68,68,69	0
7	CO3	C	205	4/4	0.82	0.21	40,40,41,42	4
5	BME	A	203	4/4	0.82	0.61	20,20,20,20	0
4	GOL	C	202	6/6	0.83	0.15	47,49,51,51	0
7	CO3	M	29	4/4	0.83	0.18	60,61,61,61	0
5	BME	M	15	4/4	0.84	0.16	56,58,59,60	0
9	4NC	O	3	11/11	0.84	0.18	38,41,44,45	0
5	BME	C	204	4/4	0.84	0.21	60,61,61,63	0
6	TRS	A	205	8/8	0.87	0.17	48,49,49,52	0
5	BME	M	18	4/4	0.87	0.21	64,65,65,66	0
4	GOL	M	7	6/6	0.87	0.23	50,51,52,52	0
9	4NC	M	1	11/11	0.89	0.18	39,43,44,45	0
9	4NC	N	2	11/11	0.90	0.15	39,41,43,43	0
10	CL	N	34	1/1	0.92	0.20	54,54,54,54	0
10	CL	B	204	1/1	0.93	0.13	52,52,52,52	0
3	SO4	B	201	5/5	0.93	0.12	50,50,52,52	5
3	SO4	C	201	5/5	0.93	0.19	52,53,54,54	5
3	SO4	A	201	5/5	0.94	0.14	49,50,50,51	5
8	FE	O	600	1/1	0.99	0.08	28,28,28,28	0
8	FE	M	600	1/1	0.99	0.06	27,27,27,27	0
8	FE	N	600	1/1	0.99	0.04	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.