Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:16 pm BST

PDB ID	:	3HYL
Title	:	Crystal Structure of Transketolase from Bacillus anthracis
Authors	:	Maltseva, N.; Kim, Y.; Kwon, K.; Joachimiak, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2009-06-22
Resolution	:	2.16 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:

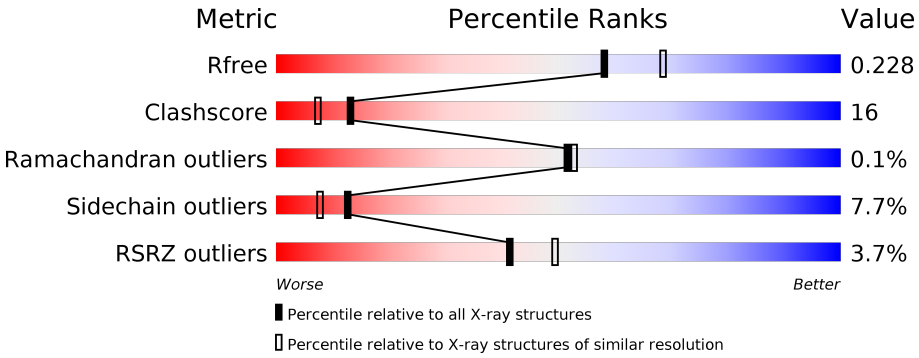
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	690	2% 75% 19%
1	B	690	4% 67% 25%

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	FMT	A	669	-	-	X	-
3	FMT	A	673	-	-	X	-
3	FMT	B	668	-	-	X	-
3	FMT	B	674	-	-	X	-
4	PEG	A	677	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10868 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 Transketolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	Se	0	2	0
			5087	3198	862	1005	1	21			
1	B	663	Total	C	N	O	S	Se	0	3	0
			5096	3205	863	1006	1	21			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	EXPRESSION TAG	UNP C3P4P9
A	-22	HIS	-	EXPRESSION TAG	UNP C3P4P9
A	-21	HIS	-	EXPRESSION TAG	UNP C3P4P9
A	-20	HIS	-	EXPRESSION TAG	UNP C3P4P9
A	-19	HIS	-	EXPRESSION TAG	UNP C3P4P9
A	-18	HIS	-	EXPRESSION TAG	UNP C3P4P9
A	-17	HIS	-	EXPRESSION TAG	UNP C3P4P9
A	-16	SER	-	EXPRESSION TAG	UNP C3P4P9
A	-15	SER	-	EXPRESSION TAG	UNP C3P4P9
A	-14	GLY	-	EXPRESSION TAG	UNP C3P4P9
A	-13	VAL	-	EXPRESSION TAG	UNP C3P4P9
A	-12	ASP	-	EXPRESSION TAG	UNP C3P4P9
A	-11	LEU	-	EXPRESSION TAG	UNP C3P4P9
A	-10	GLY	-	EXPRESSION TAG	UNP C3P4P9
A	-9	THR	-	EXPRESSION TAG	UNP C3P4P9
A	-8	GLU	-	EXPRESSION TAG	UNP C3P4P9
A	-7	ASN	-	EXPRESSION TAG	UNP C3P4P9
A	-6	LEU	-	EXPRESSION TAG	UNP C3P4P9
A	-5	TYR	-	EXPRESSION TAG	UNP C3P4P9
A	-4	PHE	-	EXPRESSION TAG	UNP C3P4P9
A	-3	GLN	-	EXPRESSION TAG	UNP C3P4P9
A	-2	SER	-	EXPRESSION TAG	UNP C3P4P9
A	-1	ASN	-	EXPRESSION TAG	UNP C3P4P9
A	0	ALA	-	EXPRESSION TAG	UNP C3P4P9
B	-23	MSE	-	EXPRESSION TAG	UNP C3P4P9

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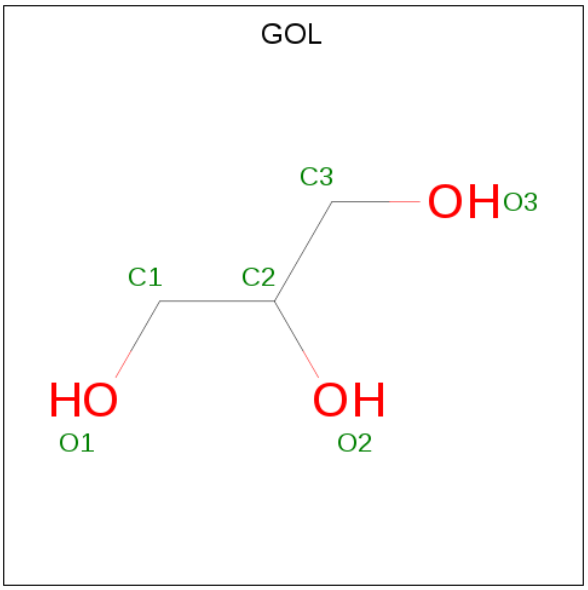
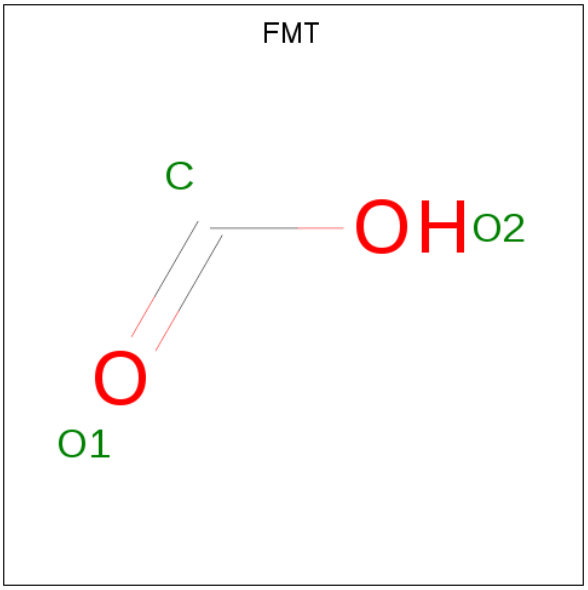
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	EXPRESSION TAG	UNP C3P4P9
B	-21	HIS	-	EXPRESSION TAG	UNP C3P4P9
B	-20	HIS	-	EXPRESSION TAG	UNP C3P4P9
B	-19	HIS	-	EXPRESSION TAG	UNP C3P4P9
B	-18	HIS	-	EXPRESSION TAG	UNP C3P4P9
B	-17	HIS	-	EXPRESSION TAG	UNP C3P4P9
B	-16	SER	-	EXPRESSION TAG	UNP C3P4P9
B	-15	SER	-	EXPRESSION TAG	UNP C3P4P9
B	-14	GLY	-	EXPRESSION TAG	UNP C3P4P9
B	-13	VAL	-	EXPRESSION TAG	UNP C3P4P9
B	-12	ASP	-	EXPRESSION TAG	UNP C3P4P9
B	-11	LEU	-	EXPRESSION TAG	UNP C3P4P9
B	-10	GLY	-	EXPRESSION TAG	UNP C3P4P9
B	-9	THR	-	EXPRESSION TAG	UNP C3P4P9
B	-8	GLU	-	EXPRESSION TAG	UNP C3P4P9
B	-7	ASN	-	EXPRESSION TAG	UNP C3P4P9
B	-6	LEU	-	EXPRESSION TAG	UNP C3P4P9
B	-5	TYR	-	EXPRESSION TAG	UNP C3P4P9
B	-4	PHE	-	EXPRESSION TAG	UNP C3P4P9
B	-3	GLN	-	EXPRESSION TAG	UNP C3P4P9
B	-2	SER	-	EXPRESSION TAG	UNP C3P4P9
B	-1	ASN	-	EXPRESSION TAG	UNP C3P4P9
B	0	ALA	-	EXPRESSION TAG	UNP C3P4P9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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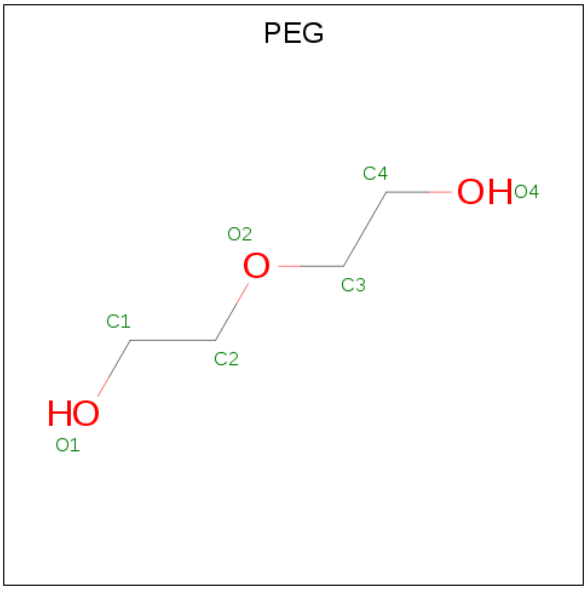
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 1 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

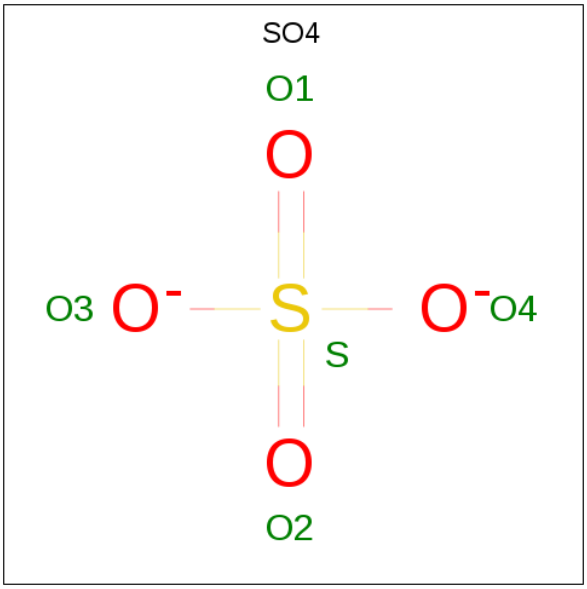
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is water.

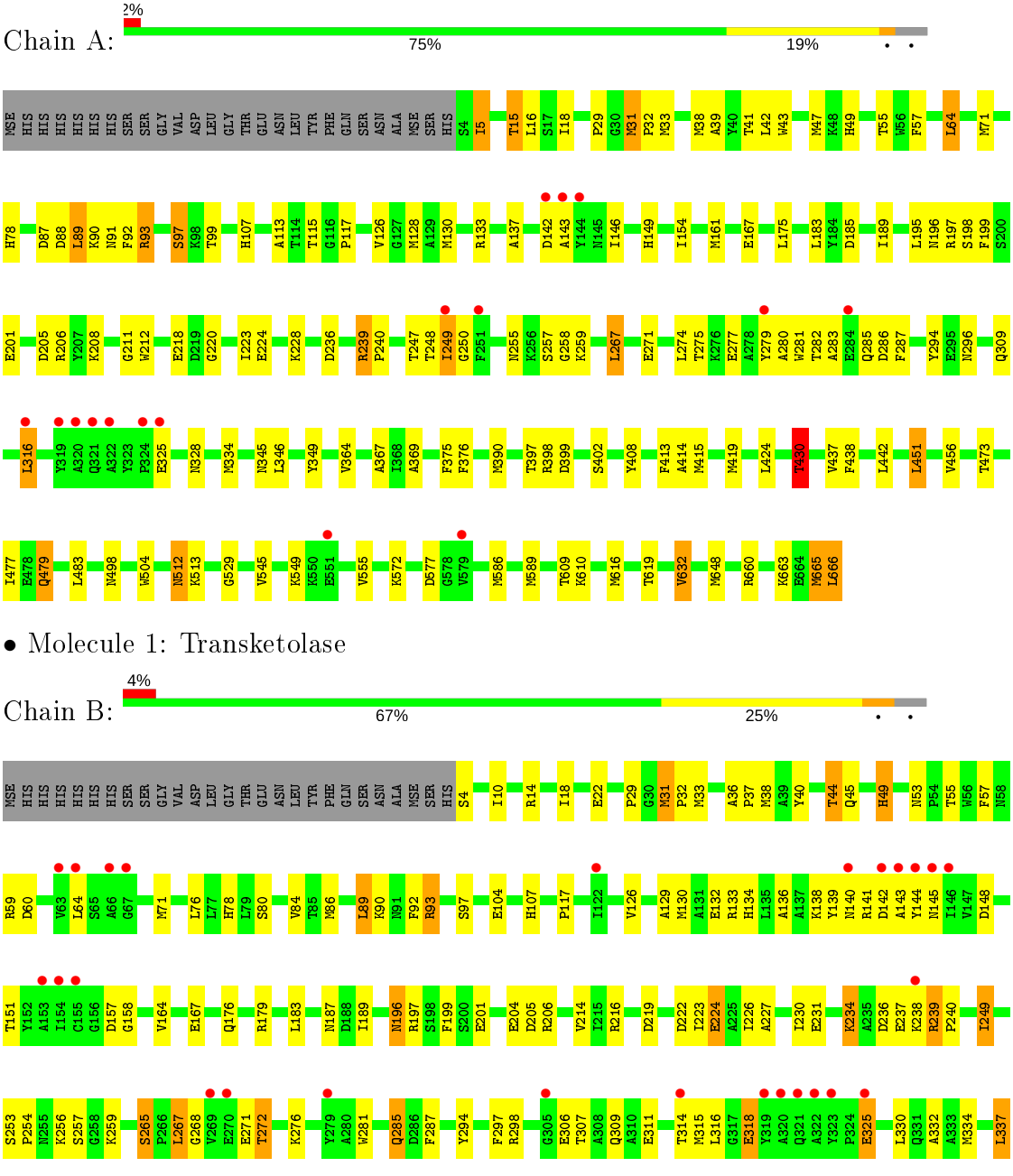
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	343	Total O 343 343	0	0
8	B	261	Total O 261 261	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

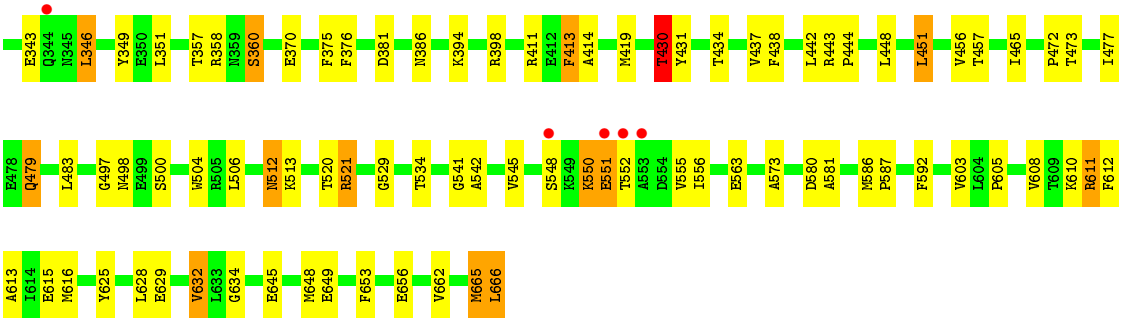
- Molecule 1: Transketolase

Chain A:



- Molecule 1: Transketolase

Chain B:


E343 Q344 N345 L346 Y349 E350 L351 T357 R358 N359 S360 E370 F375 F376 D381 N386 K394 R398 R411 E412 F413 A414 M419 T430 Y431 T434 V437 F438 L442 R443 P444 L448 L451 V456 T457 I465 P472 T473 I477
E478 Q479 L483 G497 N498 E499 S500 W504 R505 L506 N512 K513 T520 R521 G529 T534 G541 A542 V545 S548 K549 K550 E551 T552 A553 D554 V555 I556 E563 A573 D580 A581 M586 P587 F592 V603 L604 P605 V608 T609 K610 R611 F612
A613 I614 E615 M616 Y625 L628 E629 V632 L633 G634 E645 M648 E649 F653 E656 V662 M665 L666

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.80Å 70.97Å 145.79Å 90.00° 117.35° 90.00°	Depositor
Resolution (Å)	36.35 – 2.16 36.35 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.35-2.16) 99.4 (36.35-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.36 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.176 , 0.230 0.172 , 0.228	Depositor DCC
R_{free} test set	3423 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10868	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, MG, CL, FMT, SO4, PEG

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	0/5174	0.77	4/6988 (0.1%)
1	B	0.64	0/5187	0.76	6/7005 (0.1%)
All	All	0.67	0/10361	0.76	10/13993 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ARG	NE-CZ-NH2	-10.79	114.90	120.30
1	A	93	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	B	93	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	665	MSE	CG-SE-CE	-6.16	85.36	98.90
1	B	31	MSE	CG-SE-CE	-5.65	86.46	98.90
1	B	451	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	A	430	THR	CB-CA-C	-5.24	97.44	111.60
1	B	93	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	611	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	430	THR	CB-CA-C	-5.04	97.98	111.60

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	5087	0	4921	134	0
1	B	5096	0	4930	198	0
2	A	12	0	16	2	0
3	A	15	0	5	7	0
3	B	18	0	6	7	0
4	A	21	0	30	7	0
4	B	7	0	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	B	5	0	0	0	0
8	A	343	0	0	5	0
8	B	261	0	0	12	0
All	All	10868	0	9918	329	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 16.

All (329) 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:B:142:ASP:HB2	8:B:866:HOH:O	1.26	1.30
1:B:616:MSE:SE	8:B:741:HOH:O	2.12	1.16
1:B:465:ILE:HD11	1:B:616:MSE:HE2	1.26	1.12
1:B:616:MSE:HE3	1:B:653:PHE:CD2	1.85	1.12
1:A:130:MSE:SE	8:A:927:HOH:O	2.21	1.09
1:B:18:ILE:HG12	1:B:33:MSE:HE2	1.35	1.08
1:A:57:PHE:CD2	1:A:334:MSE:HE2	1.89	1.07
1:A:42:LEU:HG	1:A:47:MSE:HE2	1.37	1.06
1:B:465:ILE:HD11	1:B:616:MSE:CE	1.86	1.06
1:B:332:ALA:HA	1:B:337:LEU:HD12	1.42	1.02
4:A:677:PEG:H21	1:B:205:ASP:HB3	1.41	0.98
1:A:43:TRP:HA	1:A:47:MSE:HE3	1.44	0.98
1:A:397:THR:HG23	1:A:399:ASP:H	1.30	0.97
1:B:126:VAL:HG12	1:B:130:MSE:CE	1.95	0.95
1:A:249:ILE:HD12	1:A:249:ILE:H	1.30	0.95
1:A:29:PRO:HB2	1:A:33:MSE:HE3	1.47	0.94
1:A:31:MSE:HG3	1:A:32:PRO:HD3	1.47	0.94
1:B:44:THR:HG22	1:B:45:GLN:HG3	1.49	0.94
2:A:667:GOL:H31	3:A:669:FMT:O2	1.69	0.91
1:B:38:MSE:HE1	1:B:183:LEU:HB3	1.54	0.90
1:B:129:ALA:HA	1:B:132[B]:GLU:OE2	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASN:OD1	1:B:315:MSE:SE	2.40	0.89
1:B:126:VAL:HG12	1:B:130:MSE:HE2	1.54	0.87
1:A:33:MSE:HE1	1:A:267:LEU:HD13	1.58	0.85
1:B:136:ALA:O	1:B:140:ASN:HB2	1.76	0.85
1:B:18:ILE:CG1	1:B:33:MSE:HE2	2.07	0.84
1:A:349:TYR:H	1:A:498:ASN:HD21	1.23	0.84
1:B:616:MSE:HE3	1:B:653:PHE:CG	2.13	0.84
1:A:161:MSE:HE2	1:B:411:ARG:CZ	2.08	0.83
1:B:268:GLY:O	1:B:272:THR:HG23	1.78	0.83
1:A:126:VAL:CG1	1:A:130:MSE:HE3	2.09	0.83
1:A:29:PRO:HB2	1:A:33:MSE:CE	2.10	0.82
1:B:78:HIS:HE1	1:B:294:TYR:OH	1.61	0.82
1:A:57:PHE:CG	1:A:334:MSE:HE2	2.14	0.82
1:A:126:VAL:HG12	1:A:130:MSE:HE3	1.61	0.81
1:A:451:LEU:HD21	1:B:472:PRO:HB2	1.63	0.81
1:B:57:PHE:CD2	1:B:334:MSE:HE2	2.16	0.80
1:A:249:ILE:HD12	1:A:249:ILE:N	1.96	0.80
1:A:249:ILE:H	1:A:249:ILE:CD1	1.91	0.79
1:B:199:PHE:CZ	1:B:201:GLU:HG2	2.17	0.79
1:A:205:ASP:HB3	4:A:677:PEG:O1	1.82	0.79
1:B:18:ILE:HG12	1:B:33:MSE:CE	2.12	0.79
1:A:239:ARG:HH21	1:A:239:ARG:HG3	1.49	0.78
1:B:92:PHE:CZ	1:B:93:ARG:HD2	2.20	0.77
1:B:479:GLN:H	1:B:479:GLN:HE21	1.30	0.76
1:B:551:GLU:CD	1:B:551:GLU:H	1.88	0.75
1:A:43:TRP:CA	1:A:47:MSE:HE3	2.15	0.75
1:A:42:LEU:CG	1:A:47:MSE:HE2	2.15	0.75
1:A:267:LEU:H	1:A:267:LEU:CD2	2.00	0.75
1:B:254:PRO:HD2	1:B:271:GLU:OE1	1.87	0.74
1:A:479:GLN:H	1:A:479:GLN:HE21	1.34	0.73
1:A:161:MSE:HE2	1:B:411:ARG:NH1	2.03	0.73
1:B:126:VAL:HG12	1:B:130:MSE:HE3	1.70	0.73
1:A:42:LEU:HG	1:A:47:MSE:CE	2.18	0.73
1:B:497:GLY:O	1:B:500:SER:HB3	1.89	0.72
1:A:479:GLN:H	1:A:479:GLN:NE2	1.87	0.72
1:B:97:SER:O	1:B:107[A]:HIS:HE1	1.71	0.72
1:B:249:ILE:N	1:B:249:ILE:HD13	2.05	0.72
1:A:97:SER:HB3	1:A:99:THR:H	1.54	0.71
1:A:18:ILE:HG23	1:A:267:LEU:HD21	1.71	0.71
1:B:332:ALA:CA	1:B:337:LEU:HD12	2.19	0.71
1:A:267:LEU:HD23	1:A:267:LEU:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MSE:HE1	1:A:198:SER:HB2	1.72	0.70
1:A:239:ARG:NH2	1:A:239:ARG:HG3	2.06	0.69
1:B:38:MSE:HE3	1:B:183:LEU:HD23	1.72	0.69
1:A:15:THR:HG21	1:A:281:TRP:CZ2	2.27	0.69
1:B:140:ASN:O	1:B:141:ARG:HG2	1.92	0.69
1:A:92:PHE:CZ	1:A:93:ARG:HD2	2.28	0.69
1:A:397:THR:HG23	1:A:399:ASP:N	2.06	0.68
1:A:236:ASP:OD2	1:A:239:ARG:NH2	2.26	0.68
2:A:667:GOL:H31	3:A:669:FMT:C	2.24	0.68
1:B:249:ILE:H	1:B:249:ILE:HD13	1.59	0.68
1:A:57:PHE:CD2	1:A:334:MSE:CE	2.74	0.67
1:B:332:ALA:HA	1:B:337:LEU:CD1	2.22	0.67
1:A:224:GLU:O	1:A:228:LYS:HG3	1.95	0.67
1:B:134:HIS:NE2	1:B:138:LYS:HD2	2.10	0.67
1:B:133:ARG:NE	1:B:133:ARG:HA	2.10	0.66
1:B:40:TYR:O	1:B:44:THR:HB	1.94	0.66
1:B:18:ILE:CD1	1:B:33:MSE:HE2	2.25	0.66
1:B:222:ASP:O	1:B:226:ILE:HG13	1.96	0.65
1:A:142:ASP:O	1:A:143:ALA:HB3	1.96	0.65
1:A:161:MSE:HE1	1:A:198:SER:CB	2.27	0.65
1:B:550:LYS:HD2	1:B:580:ASP:OD2	1.96	0.65
1:B:465:ILE:CD1	1:B:616:MSE:HE2	2.16	0.64
1:B:59:ARG:HG3	1:B:60:ASP:O	1.98	0.64
1:A:208:LYS:O	4:A:677:PEG:H42	1.99	0.63
1:B:204:GLU:HG3	1:B:214:VAL:HG11	1.81	0.63
1:B:343:GLU:HB2	1:B:346:LEU:HD22	1.80	0.63
1:B:187:ASN:ND2	1:B:249:ILE:HG23	2.13	0.62
1:A:71:MSE:HE1	1:A:89:LEU:HG	1.80	0.62
1:A:267:LEU:HD23	1:A:267:LEU:N	2.13	0.62
1:A:126:VAL:HG12	1:A:130:MSE:CE	2.30	0.61
1:B:357:THR:HA	1:B:360:SER:HB2	1.83	0.61
1:B:616:MSE:CE	1:B:653:PHE:CD2	2.75	0.61
1:A:29:PRO:O	1:A:33:MSE:HG3	2.00	0.61
1:B:92:PHE:CE2	1:B:93:ARG:CD	2.84	0.61
1:B:92:PHE:CE2	1:B:93:ARG:HD2	2.36	0.61
1:A:43:TRP:HE3	1:A:47:MSE:HE1	1.66	0.61
1:A:199:PHE:CZ	1:A:201:GLU:HG2	2.36	0.60
1:B:140:ASN:C	1:B:141:ARG:HG2	2.21	0.60
1:B:157:ASP:N	3:B:668:FMT:H	2.16	0.60
1:B:148:ASP:OD1	1:B:179:ARG:NH2	2.34	0.60
3:A:672:FMT:H	8:B:712:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASP:H	3:B:668:FMT:H	1.67	0.60
1:A:5:ILE:CD1	1:A:296:ASN:HB2	2.31	0.60
1:B:307:THR:O	1:B:311:GLU:HG3	1.99	0.60
1:B:325[A]:GLU:H	1:B:325[A]:GLU:CD	2.03	0.60
1:A:275:THR:HG22	1:A:279:TYR:CE2	2.37	0.59
1:B:86:MSE:HE1	1:B:287:PHE:CD1	2.38	0.59
1:A:663:LYS:HA	1:A:666:LEU:HD11	1.84	0.59
1:B:325[B]:GLU:CD	1:B:325[B]:GLU:H	2.06	0.58
1:A:345:ASN:ND2	1:A:367:ALA:O	2.36	0.58
1:A:97:SER:HB2	3:A:673:FMT:C	2.32	0.58
1:A:161:MSE:HE2	1:B:411:ARG:NH2	2.18	0.58
1:B:542:ALA:HB2	1:B:586:MSE:HG2	1.85	0.58
1:B:130:MSE:SE	8:B:935:HOH:O	2.71	0.58
1:B:249:ILE:H	1:B:249:ILE:CD1	2.15	0.58
1:B:573:ALA:HB2	8:B:877:HOH:O	2.03	0.58
1:A:477:ILE:H	1:A:479:GLN:HE22	1.52	0.58
1:B:479:GLN:N	1:B:479:GLN:HE21	1.98	0.57
1:B:268:GLY:O	1:B:272:THR:CG2	2.51	0.57
1:B:645:GLU:O	1:B:649:GLU:HG3	2.05	0.57
1:A:161:MSE:HE3	1:A:199:PHE:HD2	1.69	0.57
1:B:276:LYS:HD3	1:B:281:TRP:CD1	2.40	0.57
1:A:126:VAL:CG1	1:A:130:MSE:CE	2.83	0.56
1:A:195:LEU:HG	1:A:199:PHE:HB3	1.87	0.56
1:B:520:THR:HG23	3:B:674:FMT:C	2.35	0.56
1:A:616:MSE:SE	1:A:648:MSE:HG2	2.56	0.56
1:B:78:HIS:CE1	1:B:294:TYR:OH	2.52	0.56
1:A:31:MSE:HG3	1:A:32:PRO:CD	2.28	0.56
1:B:14:ARG:O	1:B:18:ILE:HG13	2.06	0.56
1:B:256:LYS:HA	1:B:259:LYS:HD2	1.88	0.56
1:B:541:GLY:O	1:B:587:PRO:HD2	2.06	0.55
1:A:43:TRP:CE3	1:A:47:MSE:HE1	2.42	0.55
1:A:619:THR:HG22	1:A:632:VAL:HG22	1.89	0.55
4:A:677:PEG:H31	1:B:205:ASP:OD2	2.05	0.55
1:B:586:MSE:HE1	1:B:625:TYR:CE1	2.41	0.55
1:A:325:GLU:CD	1:A:325:GLU:H	2.09	0.55
1:B:498:ASN:C	1:B:534:THR:HG21	2.27	0.55
1:B:179:ARG:HD2	1:B:237:GLU:OE1	2.06	0.55
1:A:78:HIS:HE1	1:A:294:TYR:OH	1.89	0.55
1:B:512:ASN:HD22	1:B:512:ASN:C	2.10	0.55
1:B:358:ARG:HD3	1:B:521:ARG:HA	1.88	0.55
1:A:199:PHE:CZ	1:A:201:GLU:CG	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:TYR:CD2	1:B:330:LEU:HD13	2.41	0.54
1:B:187:ASN:ND2	1:B:249:ILE:CG2	2.69	0.54
1:B:236:ASP:OD2	1:B:239:ARG:NH2	2.41	0.54
1:B:44:THR:HG22	1:B:45:GLN:CG	2.33	0.54
1:A:206:ARG:HG3	1:B:206:ARG:HG3	1.90	0.54
1:B:376:PHE:O	1:B:430:THR:HG22	2.07	0.54
1:B:349:TYR:H	1:B:498:ASN:HD21	1.54	0.54
1:A:161:MSE:HE3	1:A:199:PHE:CD2	2.43	0.54
1:A:91:ASN:O	1:A:97:SER:OG	2.24	0.54
1:B:126:VAL:CG1	1:B:130:MSE:HE2	2.34	0.54
1:B:140:ASN:O	1:B:141:ARG:CG	2.55	0.54
1:B:176:GLN:NE2	1:B:398:ARG:HD2	2.23	0.54
1:A:376:PHE:O	1:A:430:THR:HG22	2.08	0.54
1:A:255:ASN:HB2	1:A:271:GLU:OE1	2.08	0.53
1:A:196[B]:ASN:OD1	1:A:199:PHE:O	2.27	0.53
1:B:33:MSE:HE1	1:B:267:LEU:HD22	1.89	0.53
1:B:92:PHE:CE2	1:B:93:ARG:HD3	2.43	0.53
1:B:71:MSE:HE1	1:B:89:LEU:HG	1.91	0.53
1:A:126:VAL:HG13	1:A:130:MSE:HE3	1.89	0.53
1:A:33:MSE:CE	1:A:267:LEU:HD13	2.35	0.53
1:B:249:ILE:N	1:B:249:ILE:CD1	2.71	0.53
1:B:29:PRO:HB3	1:B:33:MSE:CE	2.39	0.52
1:B:437:VAL:HG13	1:B:438:PHE:CD1	2.44	0.52
1:B:204:GLU:OE2	3:B:672:FMT:C	2.57	0.52
1:B:612:PHE:HD2	1:B:665:MSE:HE3	1.74	0.52
1:B:196:ASN:HD22	1:B:196:ASN:C	2.12	0.52
1:B:479:GLN:H	1:B:479:GLN:NE2	2.04	0.52
1:B:49:HIS:CD2	1:B:49:HIS:N	2.77	0.52
1:B:133:ARG:HA	1:B:133:ARG:HE	1.74	0.52
1:B:86:MSE:HE3	1:B:90:LYS:HG3	1.92	0.52
1:A:369:ALA:HB2	1:A:390:MSE:SE	2.60	0.51
8:A:909:HOH:O	1:B:197:ARG:HD2	2.09	0.51
1:A:408:TYR:CE2	1:A:415:MSE:HG3	2.46	0.51
1:B:520:THR:CG2	3:B:674:FMT:C	2.89	0.51
1:A:199:PHE:CE2	1:A:201:GLU:HG2	2.46	0.51
1:B:285:GLN:HA	1:B:285:GLN:OE1	2.11	0.51
1:B:86:MSE:CE	1:B:90:LYS:HG3	2.40	0.51
1:B:314:THR:O	1:B:318:GLU:HG2	2.10	0.51
1:B:465:ILE:HD11	1:B:616:MSE:HE1	1.85	0.51
1:B:199:PHE:CZ	1:B:201:GLU:CG	2.94	0.50
1:B:529:GLY:HA3	1:B:545:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLY:HA3	1:A:545:VAL:O	2.11	0.50
1:B:555:VAL:O	1:B:581:ALA:HA	2.12	0.50
1:A:117:PRO:HD3	1:B:473:THR:HB	1.93	0.50
1:A:239:ARG:HH21	1:A:239:ARG:CG	2.21	0.50
1:A:267:LEU:N	1:A:267:LEU:CD2	2.68	0.50
1:A:92:PHE:CE2	1:A:93:ARG:HD3	2.47	0.50
1:B:134:HIS:NE2	1:B:138:LYS:CD	2.75	0.50
1:A:33:MSE:SE	1:A:250:GLY:HA2	2.61	0.50
1:A:41:THR:OG1	1:A:223:ILE:HG13	2.13	0.49
1:A:479:GLN:NE2	1:A:479:GLN:N	2.60	0.49
1:A:78:HIS:CE1	1:A:294:TYR:OH	2.66	0.49
1:A:130:MSE:HE2	1:A:175:LEU:HD12	1.94	0.49
1:A:473:THR:HB	1:B:117:PRO:HD3	1.95	0.48
1:A:149:HIS:HE1	8:A:800:HOH:O	1.96	0.48
1:A:142:ASP:O	1:A:143:ALA:CB	2.61	0.48
1:A:167:GLU:HB2	1:A:414:ALA:HB2	1.95	0.48
1:A:577:ASP:HB3	1:A:663:LYS:HZ3	1.79	0.48
1:A:64:LEU:O	1:A:115:THR:HG21	2.14	0.48
1:A:274:LEU:O	1:A:277:GLU:HB2	2.14	0.47
1:A:38:MSE:HG3	1:A:39:ALA:N	2.28	0.47
1:B:140:ASN:O	1:B:141:ARG:HD3	2.14	0.47
1:B:29:PRO:HG2	1:B:265:SER:O	2.14	0.47
1:B:31:MSE:HB3	1:B:32:PRO:HD3	1.96	0.47
1:B:57:PHE:CG	1:B:334:MSE:HE2	2.48	0.47
1:B:29:PRO:HB3	1:B:33:MSE:HE3	1.96	0.47
1:A:92:PHE:CE2	1:A:93:ARG:CD	2.97	0.47
1:B:351:LEU:H	1:B:351:LEU:HD22	1.79	0.47
1:A:236:ASP:OD2	1:A:239:ARG:HG3	2.14	0.47
1:B:223:ILE:HB	8:B:754:HOH:O	2.14	0.47
1:B:613:ALA:HB3	1:B:632:VAL:HB	1.96	0.47
1:B:4:SER:N	8:B:851:HOH:O	2.47	0.47
1:A:282:THR:O	1:A:283:ALA:C	2.53	0.47
1:A:286:ASP:O	1:A:287:PHE:HB2	2.15	0.47
1:A:255:ASN:O	1:A:259:LYS:HE3	2.15	0.47
1:B:142:ASP:O	1:B:143:ALA:HB3	2.14	0.47
1:A:161:MSE:HE3	1:A:199:PHE:HB2	1.96	0.46
1:A:512:ASN:C	1:A:512:ASN:HD22	2.17	0.46
1:B:234:LYS:HE3	1:B:234:LYS:HB3	1.53	0.46
1:A:97:SER:HB2	3:A:673:FMT:O2	2.15	0.46
1:B:542:ALA:CB	1:B:586:MSE:HG2	2.45	0.46
1:A:437:VAL:HG13	1:A:438:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:SER:CB	3:A:673:FMT:H	2.46	0.46
1:B:196:ASN:HA	1:B:199:PHE:O	2.16	0.46
1:B:38:MSE:CE	1:B:183:LEU:HB3	2.37	0.46
1:B:662:VAL:O	1:B:665:MSE:HG3	2.15	0.46
1:A:555:VAL:HG23	1:A:610:LYS:O	2.16	0.45
1:B:104:GLU:HB3	1:B:107[B]:HIS:HD2	1.82	0.45
1:B:132[B]:GLU:OE2	1:B:151:THR:OG1	2.32	0.45
1:B:608:VAL:O	1:B:611:ARG:HD2	2.17	0.45
1:B:431:TYR:HA	1:B:457:THR:O	2.16	0.45
1:A:239:ARG:HE	4:A:678:PEG:H41	1.80	0.45
1:A:212:TRP:CE3	1:A:240:PRO:HB2	2.51	0.45
1:B:253:SER:O	1:B:257:SER:HB3	2.16	0.45
1:B:479:GLN:N	1:B:479:GLN:NE2	2.62	0.45
1:A:586:MSE:SE	1:A:589:MSE:HG2	2.67	0.45
1:B:176:GLN:HB3	1:B:238:LYS:O	2.17	0.45
1:B:33:MSE:HE1	1:B:267:LEU:CD2	2.46	0.45
1:B:615:GLU:O	1:B:634:GLY:HA2	2.17	0.45
1:A:5:ILE:HD11	1:A:296:ASN:HB2	1.99	0.45
1:B:556:ILE:HD11	1:B:605:PRO:HD2	1.98	0.45
1:B:158:GLY:H	3:B:668:FMT:C	2.30	0.45
1:B:148:ASP:HA	1:B:179:ARG:NH2	2.31	0.45
1:B:563:GLU:CD	1:B:616:MSE:HG3	2.37	0.45
1:A:128:MSE:HE2	1:A:424:LEU:HD13	1.99	0.44
1:A:133:ARG:HA	1:A:133:ARG:NE	2.33	0.44
1:A:38:MSE:HE1	1:A:185:ASP:HA	1.98	0.44
1:B:148:ASP:HA	1:B:179:ARG:HH22	1.82	0.44
1:B:239:ARG:HB2	1:B:240:PRO:CD	2.47	0.44
1:A:239:ARG:HE	4:A:678:PEG:C4	2.30	0.44
1:A:408:TYR:CD2	1:A:415:MSE:HG3	2.52	0.44
1:B:4:SER:N	8:B:849:HOH:O	2.50	0.44
1:B:134:HIS:CE1	1:B:138:LYS:HD2	2.52	0.44
1:B:164:VAL:HB	1:B:413:PHE:CD2	2.52	0.44
1:B:267:LEU:HB3	1:B:272:THR:HG22	1.99	0.44
1:B:142:ASP:C	1:B:144:TYR:H	2.21	0.44
1:A:477:ILE:H	1:A:479:GLN:NE2	2.14	0.44
1:B:204:GLU:HG3	1:B:214:VAL:CG1	2.46	0.44
1:B:219:ASP:OD2	1:B:219:ASP:C	2.56	0.44
1:B:573:ALA:N	8:B:877:HOH:O	2.50	0.44
1:B:612:PHE:CD2	1:B:665:MSE:HE3	2.53	0.44
1:A:107:HIS:HB3	8:A:844:HOH:O	2.17	0.44
1:A:218:GLU:HA	1:A:218:GLU:OE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASN:HD22	1:B:197:ARG:N	2.16	0.43
1:A:113:ALA:HB2	1:A:128:MSE:HE1	2.00	0.43
1:A:212:TRP:CD2	1:A:240:PRO:HB2	2.53	0.43
1:B:419:MSE:HE2	1:B:456:VAL:HB	2.00	0.43
1:B:224:GLU:OE2	1:B:224:GLU:HA	2.18	0.43
1:B:189:ILE:HG13	1:B:249:ILE:HD11	1.99	0.43
1:B:448:LEU:HA	1:B:448:LEU:HD23	1.71	0.43
1:B:616:MSE:HE1	1:B:648:MSE:HA	1.98	0.43
1:B:443:ARG:HB3	1:B:444:PRO:HD3	2.00	0.43
1:A:279:TYR:O	1:A:280:ALA:HB3	2.18	0.43
1:A:87[B]:ASP:O	1:A:88:ASP:C	2.57	0.43
1:B:612:PHE:HB2	1:B:665:MSE:HE3	2.00	0.43
1:A:87[B]:ASP:O	1:A:90:LYS:N	2.50	0.43
1:B:477:ILE:H	1:B:479:GLN:HE22	1.66	0.43
1:B:506:LEU:HA	1:B:506:LEU:HD23	1.89	0.43
1:B:611:ARG:O	1:B:665:MSE:HE1	2.18	0.43
1:A:146:ILE:HD12	1:A:316:LEU:HD23	2.00	0.43
1:B:78:HIS:HD2	1:B:84:VAL:O	2.02	0.43
1:B:38:MSE:HG2	8:B:752:HOH:O	2.18	0.42
1:B:603:VAL:HG22	8:B:729:HOH:O	2.18	0.42
1:A:211:GLY:HA2	4:A:678:PEG:H22	2.00	0.42
1:A:257:SER:O	1:A:259:LYS:N	2.52	0.42
1:A:419:MSE:CE	1:A:456:VAL:HB	2.48	0.42
1:B:227:ALA:O	1:B:231:GLU:HG3	2.19	0.42
1:B:542:ALA:HB3	1:B:592:PHE:CD1	2.55	0.42
1:B:216:ARG:NH2	3:B:675:FMT:O1	2.52	0.42
1:A:42:LEU:CD2	1:A:47:MSE:HE2	2.49	0.42
1:B:555:VAL:HG12	1:B:666:LEU:HD11	2.02	0.42
1:A:154:ILE:HA	1:A:183:LEU:O	2.19	0.42
1:B:10:ILE:CD1	1:B:223:ILE:HD11	2.50	0.42
1:B:610:LYS:NZ	1:B:629:GLU:HG2	2.34	0.42
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.92	0.42
1:A:137:ALA:HB1	1:A:402:SER:HB3	2.02	0.42
1:B:140:ASN:O	1:B:141:ARG:CD	2.68	0.42
1:B:145:ASN:H	1:B:315:MSE:SE	2.53	0.42
1:B:53:ASN:HD22	1:B:309:GLN:HE22	1.67	0.42
1:B:53:ASN:ND2	1:B:309:GLN:HE22	2.18	0.42
1:B:230:ILE:O	1:B:234:LYS:HG3	2.20	0.42
1:A:249:ILE:CD1	1:A:249:ILE:N	2.61	0.41
1:B:38:MSE:HA	1:B:226:ILE:HD13	2.01	0.41
1:B:22:GLU:CD	1:B:272:THR:HG21	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PRO:CB	1:B:33:MSE:HE3	2.50	0.41
1:B:512:ASN:ND2	1:B:512:ASN:C	2.72	0.41
1:A:189:ILE:HG13	1:A:249:ILE:HG12	2.01	0.41
1:B:22:GLU:CG	1:B:272:THR:HG21	2.50	0.41
1:B:318:GLU:H	1:B:318:GLU:HG2	1.64	0.41
1:B:145:ASN:ND2	8:B:902:HOH:O	2.53	0.41
1:B:167:GLU:HB2	1:B:414:ALA:HB2	2.02	0.41
1:B:253:SER:HA	1:B:254:PRO:HD3	1.74	0.41
1:A:364:VAL:HG11	1:A:504:TRP:CG	2.55	0.41
1:B:80:SER:HA	1:B:297:PHE:HB3	2.02	0.41
1:B:386:ASN:HD21	1:B:434:THR:HA	1.86	0.41
1:A:220:GLY:HA3	1:A:247:THR:HG22	2.03	0.41
3:A:669:FMT:C	8:A:871:HOH:O	2.69	0.41
1:B:38:MSE:HB2	1:B:38:MSE:HE3	1.93	0.40
1:B:29:PRO:CB	1:B:33:MSE:CE	2.98	0.40
1:A:376:PHE:O	1:A:430:THR:HA	2.22	0.40
1:A:577:ASP:HB3	1:A:663:LYS:NZ	2.36	0.40
1:B:236:ASP:OD1	1:B:238:LYS:HB2	2.21	0.40
1:B:36:ALA:HB3	1:B:37:PRO:HD3	2.03	0.40
1:B:189:ILE:HG13	1:B:249:ILE:CD1	2.52	0.40
1:B:38:MSE:HE1	1:B:183:LEU:CB	2.38	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	663/690 (96%)	637 (96%)	25 (4%)	1 (0%)	47 46
1	B	664/690 (96%)	634 (96%)	30 (4%)	0	100 100
All	All	1327/1380 (96%)	1271 (96%)	55 (4%)	1 (0%)	51 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLY

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	528/527 (100%)	492 (93%)	36 (7%)	16 10
1	B	529/527 (100%)	483 (91%)	46 (9%)	10 6
All	All	1057/1054 (100%)	975 (92%)	82 (8%)	13 7

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	15	THR
1	A	16	LEU
1	A	31	MSE
1	A	49	HIS
1	A	55	THR
1	A	64	LEU
1	A	89	LEU
1	A	97	SER
1	A	197	ARG
1	A	239	ARG
1	A	248	THR
1	A	249	ILE
1	A	267	LEU
1	A	285	GLN
1	A	309	GLN
1	A	316	LEU
1	A	328	ASN
1	A	346	LEU
1	A	375	PHE
1	A	398	ARG
1	A	413	PHE

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Mol	Chain	Res	Type
1	A	430	THR
1	A	442	LEU
1	A	451	LEU
1	A	479	GLN
1	A	483	LEU
1	A	512	ASN
1	A	513	LYS
1	A	549	LYS
1	A	572	LYS
1	A	609	THR
1	A	632	VAL
1	A	660	ARG
1	A	665	MSE
1	A	666	LEU
1	B	44	THR
1	B	49	HIS
1	B	55	THR
1	B	64	LEU
1	B	89	LEU
1	B	196	ASN
1	B	224	GLU
1	B	234	LYS
1	B	239	ARG
1	B	249	ILE
1	B	265	SER
1	B	267	LEU
1	B	272	THR
1	B	285	GLN
1	B	298	ARG
1	B	306	GLU
1	B	316	LEU
1	B	318	GLU
1	B	325[A]	GLU
1	B	325[B]	GLU
1	B	337	LEU
1	B	346	LEU
1	B	360	SER
1	B	370	GLU
1	B	375	PHE
1	B	381	ASP
1	B	394	LYS
1	B	413	PHE

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Mol	Chain	Res	Type
1	B	430	THR
1	B	442	LEU
1	B	451	LEU
1	B	479	GLN
1	B	483	LEU
1	B	504	TRP
1	B	512	ASN
1	B	513	LYS
1	B	521	ARG
1	B	548	SER
1	B	550	LYS
1	B	551	GLU
1	B	552	THR
1	B	628	LEU
1	B	632	VAL
1	B	656	GLU
1	B	665	MSE
1	B	666	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	91	ASN
1	A	255	ASN
1	A	285	GLN
1	A	386	ASN
1	A	453	GLN
1	A	479	GLN
1	A	488	ASN
1	A	498	ASN
1	A	512	ASN
1	B	53	ASN
1	B	78	HIS
1	B	91	ASN
1	B	196	ASN
1	B	313	ASN
1	B	386	ASN
1	B	453	GLN
1	B	479	GLN
1	B	488	ASN
1	B	498	ASN

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Mol	Chain	Res	Type
1	B	512	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

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PEG	A	674	-	6,6,6	0.52	0	5,5,5	1.66	1 (20%)
3	FMT	B	668	5	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	667	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	669	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	673	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	A	667	-	5,5,5	0.39	0	5,5,5	0.55	0
3	FMT	B	673	-	0,2,2	0.00	-	0,1,1	0.00	-
4	PEG	B	669	-	6,6,6	0.58	0	5,5,5	2.32	3 (60%)
3	FMT	B	672	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	670	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	A	668	-	5,5,5	0.38	0	5,5,5	0.51	0
4	PEG	A	678	-	6,6,6	0.50	0	5,5,5	1.88	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FMT	A	671	-	0,2,2	0.00	-	0,1,1	0.00	-
4	PEG	A	677	-	6,6,6	0.51	0	5,5,5	1.50	1 (20%)
3	FMT	B	675	-	0,2,2	0.00	-	0,1,1	0.00	-
7	SO4	B	671	-	4,4,4	0.15	0	6,6,6	0.19	0
3	FMT	A	672	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	674	-	0,2,2	0.00	-	0,1,1	0.00	-

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	PEG	A	674	-	-	3/4/4/4	-
2	GOL	A	668	-	-	2/4/4/4	-
4	PEG	A	677	-	-	2/4/4/4	-
4	PEG	B	669	-	-	2/4/4/4	-
2	GOL	A	667	-	-	0/4/4/4	-
4	PEG	A	678	-	-	1/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	669	PEG	O2-C3-C4	3.21	124.18	110.07
4	A	677	PEG	O2-C3-C4	2.45	120.84	110.07
4	B	669	PEG	C3-O2-C2	2.37	123.56	113.29
4	B	669	PEG	O2-C2-C1	2.29	120.14	110.07
4	A	678	PEG	O2-C2-C1	2.28	120.07	110.07
4	A	678	PEG	O2-C3-C4	2.21	119.77	110.07
4	A	674	PEG	O2-C2-C1	2.17	119.62	110.07

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	669	PEG	C4-C3-O2-C2
4	B	669	PEG	O2-C3-C4-O4
4	A	677	PEG	O1-C1-C2-O2
2	A	668	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	668	GOL	O1-C1-C2-O2
4	A	677	PEG	O2-C3-C4-O4
4	A	674	PEG	O1-C1-C2-O2
4	A	674	PEG	O2-C3-C4-O4
4	A	678	PEG	O1-C1-C2-O2
4	A	674	PEG	C4-C3-O2-C2

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	668	FMT	3	0
3	A	669	FMT	3	0
3	A	673	FMT	3	0
2	A	667	GOL	2	0
3	B	672	FMT	1	0
4	A	678	PEG	3	0
4	A	677	PEG	4	0
3	B	675	FMT	1	0
3	A	672	FMT	1	0
3	B	674	FMT	2	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, 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	642/690 (93%)	-0.12	16 (2%)	57	65	17, 42, 77, 120	0
1	B	642/690 (93%)	0.22	31 (4%)	30	39	19, 53, 91, 126	0
All	All	1284/1380 (93%)	0.05	47 (3%)	41	49	17, 47, 87, 126	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	TYR	5.1
1	B	142	ASP	5.0
1	A	142	ASP	4.3
1	B	269	VAL	3.9
1	A	144	TYR	3.8
1	B	552	THR	3.4
1	B	344	GLN	3.3
1	B	321	GLN	3.3
1	B	319	TYR	3.3
1	B	548	SER	3.3
1	B	270	GLU	3.2
1	A	279	TYR	3.2
1	A	551	GLU	3.2
1	B	146	ILE	3.1
1	A	321	GLN	3.1
1	A	316	LEU	3.0
1	B	279	TYR	2.9
1	B	143	ALA	2.8
1	B	323	TYR	2.8
1	B	325[A]	GLU	2.8
1	A	319	TYR	2.8
1	A	320	ALA	2.8
1	B	238	LYS	2.8
1	B	551	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	64	LEU	2.7
1	A	143	ALA	2.7
1	B	314	THR	2.7
1	B	145	ASN	2.6
1	B	154	ILE	2.6
1	B	322	ALA	2.6
1	B	155	CYS	2.6
1	A	284	GLU	2.5
1	B	140	ASN	2.5
1	B	320	ALA	2.5
1	B	153	ALA	2.5
1	B	122	ILE	2.5
1	A	251	PHE	2.4
1	B	66	ALA	2.3
1	B	553	ALA	2.3
1	A	322	ALA	2.2
1	A	324	PRO	2.2
1	A	325	GLU	2.1
1	A	579	VAL	2.1
1	A	249	ILE	2.1
1	B	305	GLY	2.1
1	B	63	VAL	2.1
1	B	67	GLY	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 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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	A	678	7/7	0.36	0.25	76,78,82,83	0
4	PEG	A	674	7/7	0.53	0.35	78,80,80,81	0
3	FMT	B	672	3/3	0.70	0.17	60,60,65,66	0
4	PEG	B	669	7/7	0.77	0.26	50,58,66,67	0
3	FMT	B	674	3/3	0.77	0.17	46,46,47,50	0
3	FMT	A	673	3/3	0.79	0.19	45,45,47,49	0
7	SO4	B	671	5/5	0.84	0.37	121,121,122,124	0
3	FMT	B	673	3/3	0.84	0.21	65,65,70,71	0
2	GOL	A	667	6/6	0.85	0.19	43,53,58,58	0
2	GOL	A	668	6/6	0.86	0.15	64,68,72,74	0
3	FMT	B	675	3/3	0.88	0.12	65,65,66,67	0
3	FMT	A	672	3/3	0.89	0.16	54,54,58,61	0
3	FMT	A	669	3/3	0.90	0.16	48,48,51,53	0
4	PEG	A	677	7/7	0.90	0.36	68,71,73,74	0
3	FMT	A	671	3/3	0.92	0.11	53,53,57,59	0
3	FMT	B	667	3/3	0.92	0.19	41,41,47,49	0
5	MG	A	675	1/1	0.94	0.10	43,43,43,43	0
5	MG	B	670	1/1	0.94	0.09	42,42,42,42	0
3	FMT	A	670	3/3	0.95	0.09	44,44,45,47	0
3	FMT	B	668	3/3	0.96	0.12	43,43,45,47	0
6	CL	A	676	1/1	0.97	0.08	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.