WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:33 am BST

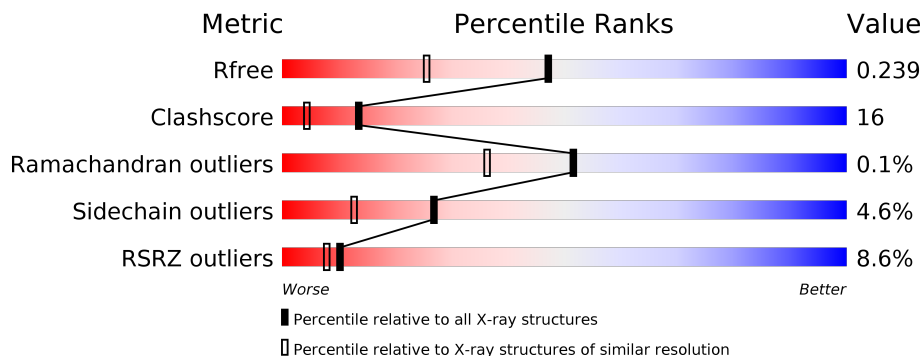|		
PDB ID	:	5JX5
Title	:	GH6 Orpinomyces sp. Y102 enzyme
Authors	:	Tsai, L.C.; Huang, H.C.
Deposited on	:	2016-05-12
Resolution	:	1.80 Å(reported)

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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 1.80 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		16
Ramachandran outliers		0.1%
Sidechain outliers		4.6%
RSRZ outliers		8.6%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	322	8% — 82% — 15% •
1	B	322	9% — 85% — 13% •
1	C	322	9% — 77% — 18% • •
1	D	322	8% — 84% — 13% •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	501	-	-	X	-
3	GOL	C	502	-	-	X	-
4	EDO	A	507	-	-	X	-
4	EDO	A	510	-	-	X	-
4	EDO	B	502	-	-	X	-
4	EDO	B	507	-	-	X	-
7	PEG	C	506	-	-	X	-
7	PEG	C	507	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11278 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 Glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	5	0
			2507	1560	449	488	10			
1	B	322	Total	C	N	O	S	0	3	0
			2503	1559	448	486	10			
1	C	322	Total	C	N	O	S	0	3	0
			2501	1558	446	486	11			
1	D	322	Total	C	N	O	S	0	6	0
			2509	1562	448	489	10			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
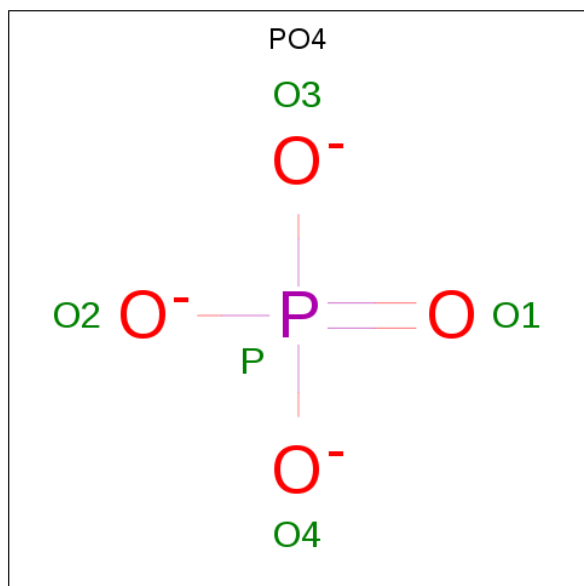
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1

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

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

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).
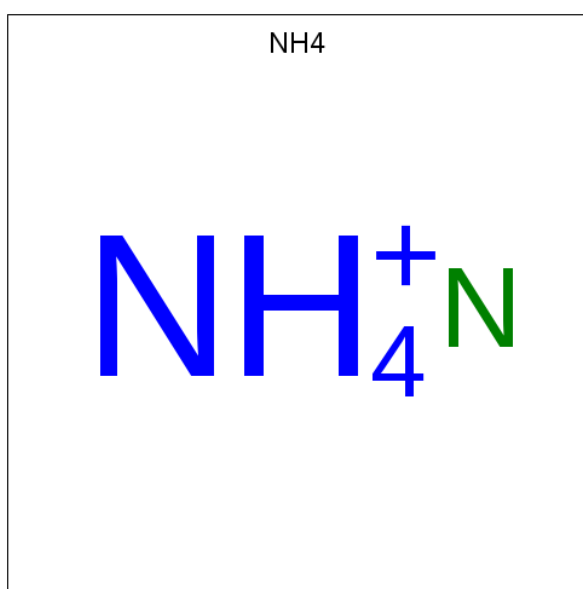
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	N	0	0
			1	1		
5	A	1	Total	N	0	0
			1	1		
5	A	1	Total	N	0	0
			1	1		
5	A	1	Total	N	0	0
			1	1		
5	B	1	Total	N	0	0
			1	1		
5	B	1	Total	N	0	0
			1	1		
5	C	1	Total	N	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	N 1	0	0
5	C	1	Total 1	N 1	0	0
5	C	1	Total 1	N 1	0	0
5	C	1	Total 1	N 1	0	0
5	D	1	Total 1	N 1	0	0
5	D	1	Total 1	N 1	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
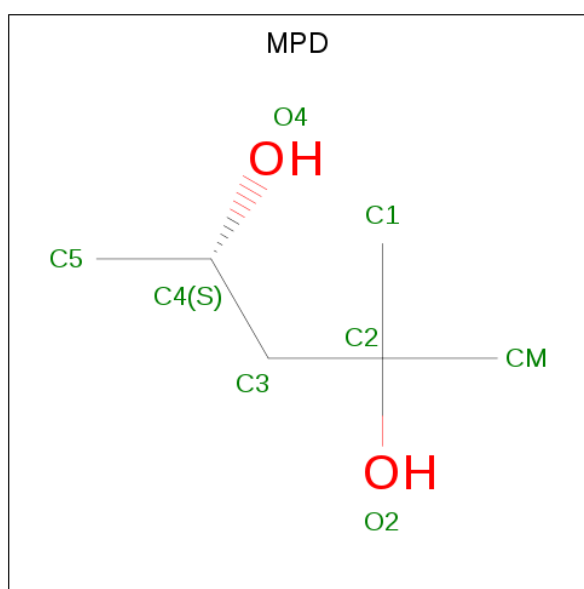
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 8	C 6	O 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG
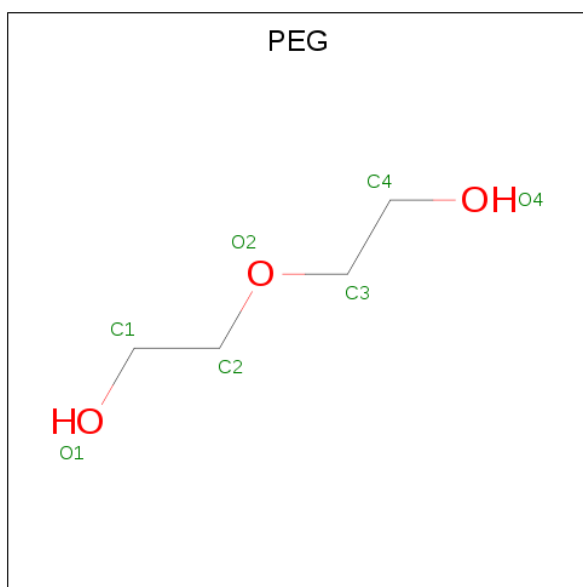
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total 7	C 4	O 3		0	0
7	C	1	Total 7	C 4	O 3		0	0
7	D	1	Total 7	C 4	O 3		0	0

• Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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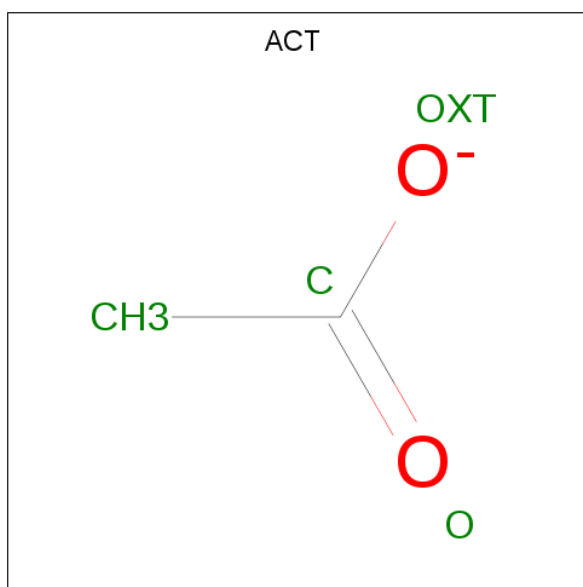
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total 4	C 2	O 2	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	275	Total O 275 275	0	0
9	B	274	Total O 274 274	0	0
9	C	273	Total O 273 273	0	0
9	D	271	Total O 271 271	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: Glucanase

Chain A:

- Molecule 1: Glucanase

Chain B:

- Molecule 1: Glucanase

Chain C:

- Molecule 1: Glucanase

Chain D:
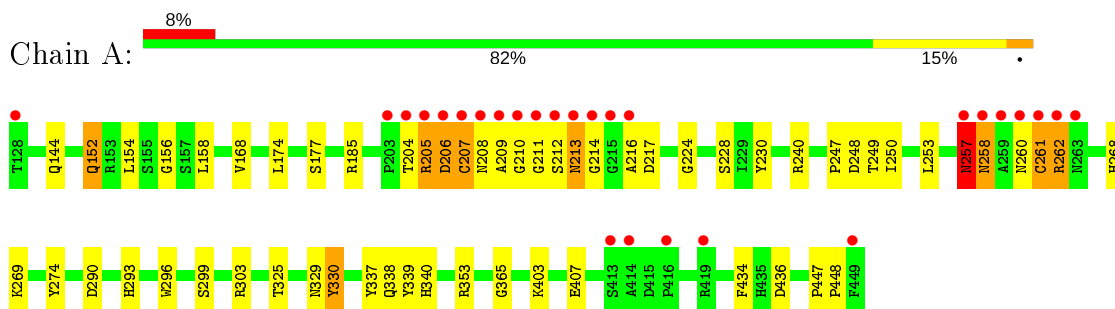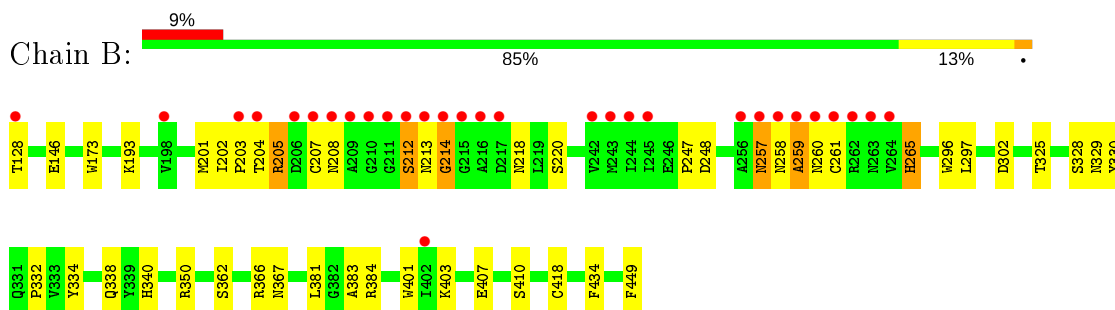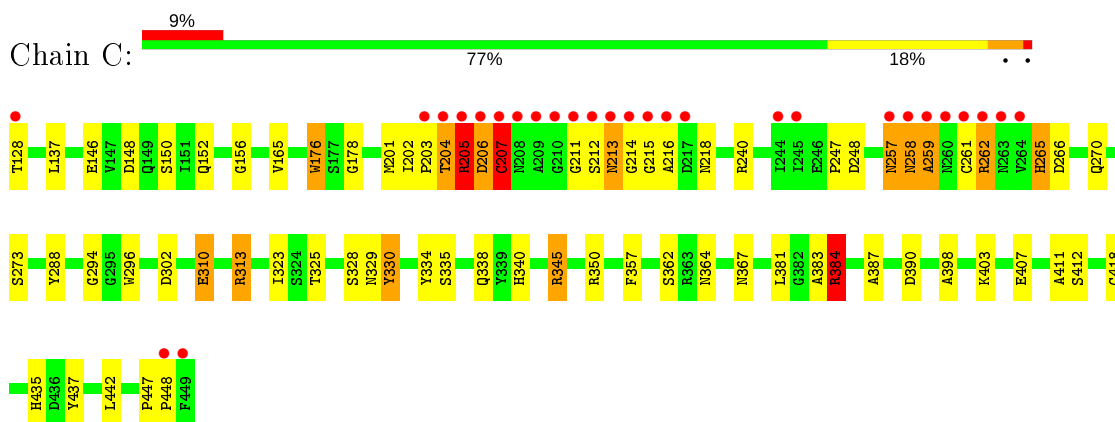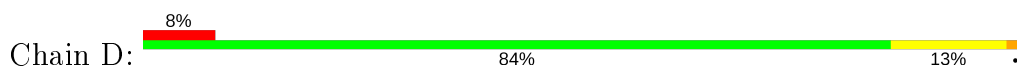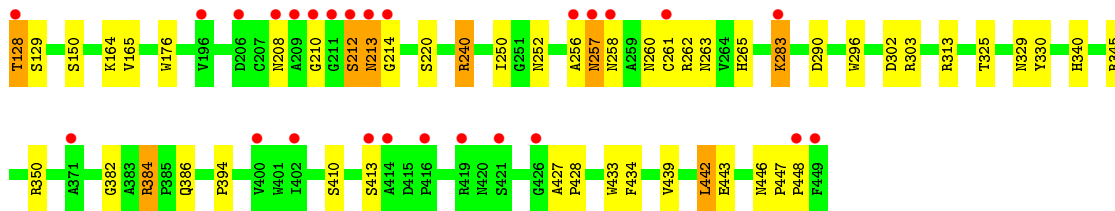
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	309.86Å 87.35Å 82.55Å 90.00° 93.95° 90.00°	Depositor
Resolution (Å)	27.76 – 1.80 27.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (27.76-1.80) 98.3 (27.76-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.69 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.239 0.209 , 0.239	Depositor DCC
R_{free} test set	10048 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.0	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11278	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MPD, PO4, EDO, NH4, ACT, 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	1.34	6/2592 (0.2%)	1.10	5/3523 (0.1%)
1	B	1.30	3/2577 (0.1%)	1.10	4/3503 (0.1%)
1	C	1.25	5/2574 (0.2%)	1.07	7/3498 (0.2%)
1	D	1.25	4/2598 (0.2%)	1.06	1/3532 (0.0%)
All	All	1.29	18/10341 (0.2%)	1.09	17/14056 (0.1%)

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	2
1	C	0	1
All	All	0	3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	TRP	CD2-CE2	5.96	1.48	1.41
1	C	176	TRP	CD2-CE2	5.95	1.48	1.41
1	C	296	TRP	CD2-CE2	5.75	1.48	1.41
1	C	330	TYR	CG-CD2	5.74	1.46	1.39
1	A	337	TYR	CE1-CZ	5.66	1.46	1.38
1	D	296	TRP	CD2-CE2	5.66	1.48	1.41
1	D	382	GLY	C-O	5.62	1.32	1.23
1	C	437	TYR	CE1-CZ	5.55	1.45	1.38
1	B	366	ARG	N-CA	5.47	1.57	1.46
1	D	394	PRO	N-CA	-5.38	1.38	1.47
1	B	401	TRP	NE1-CE2	-5.31	1.30	1.37
1	D	176	TRP	CD2-CE2	5.13	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	GLY	N-CA	5.10	1.53	1.46
1	A	230	TYR	CE1-CZ	5.07	1.45	1.38
1	A	299[A]	SER	CB-OG	-5.05	1.35	1.42
1	A	299[B]	SER	CB-OG	-5.05	1.35	1.42
1	C	288	TYR	CG-CD1	5.05	1.45	1.39
1	A	230	TYR	CG-CD2	5.04	1.45	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	LEU	CB-CG-CD1	5.97	121.15	111.00
1	B	214	GLY	N-CA-C	5.76	127.51	113.10
1	A	330	TYR	N-CA-CB	-5.73	100.29	110.60
1	C	390	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	C	384	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	193	LYS	CD-CE-NZ	-5.57	98.89	111.70
1	C	398	ALA	CB-CA-C	-5.55	101.78	110.10
1	C	216	ALA	CB-CA-C	-5.43	101.95	110.10
1	C	411	ALA	N-CA-C	-5.29	96.70	111.00
1	B	297	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	B	259	ALA	CB-CA-C	-5.19	102.31	110.10
1	A	339	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	C	259	ALA	CB-CA-C	-5.12	102.42	110.10
1	A	168	VAL	CG1-CB-CG2	-5.10	102.74	110.90
1	C	258	ASN	CB-CA-C	-5.09	100.22	110.40
1	A	217	ASP	N-CA-CB	5.05	119.68	110.60
1	D	442	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	ALA	Peptide
1	A	257	ASN	Peptide
1	C	207	CYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2507	0	2391	99	0
1	B	2503	0	2390	80	0
1	C	2501	0	2396	75	0
1	D	2509	0	2400	52	0
2	A	5	0	0	1	0
3	A	12	0	16	4	0
3	B	6	0	8	2	0
3	C	12	0	16	13	0
3	D	12	0	16	3	0
4	A	40	0	60	36	0
4	B	12	0	18	19	0
4	C	12	0	18	3	0
4	D	8	0	12	2	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	5	0	0	0	0
5	D	2	0	0	0	0
6	B	8	0	14	2	0
7	C	14	0	20	11	0
7	D	7	0	10	2	0
8	C	4	0	3	1	0
9	A	275	0	0	16	0
9	B	274	0	0	12	0
9	C	273	0	0	11	0
9	D	271	0	0	5	0
All	All	11278	0	9788	320	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 (320) 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:204:THR:HG22	1:B:213:ASN:CB	1.65	1.23
1:A:211:GLY:CA	1:A:214:GLY:HA2	1.70	1.22
1:A:211:GLY:HA2	1:A:213:ASN:HA	1.25	1.18
1:A:248:ASP:HA	9:A:665:HOH:O	1.47	1.15
1:D:240:ARG:HG3	1:D:240:ARG:HH11	1.12	1.13
1:B:204:THR:HG22	1:B:213:ASN:HB3	1.24	1.11
1:A:250:ILE:H	4:A:507:EDO:C1	1.64	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:501:GOL:H31	9:C:769:HOH:O	1.54	1.05
1:D:208:ASN:O	1:D:210:GLY:HA3	1.58	1.04
1:A:211:GLY:HA2	1:A:214:GLY:HA2	1.06	1.03
1:A:211:GLY:HA2	1:A:214:GLY:CA	1.90	1.01
1:A:212:SER:HA	1:A:213:ASN:HD22	1.25	0.99
1:B:257:ASN:ND2	1:B:258:ASN:N	2.11	0.98
1:A:250:ILE:H	4:A:507:EDO:H12	1.29	0.97
1:B:407:GLU:OE1	3:B:501:GOL:H11	1.65	0.95
1:B:338:GLN:CB	4:B:507:EDO:H12	1.97	0.95
1:B:257:ASN:ND2	1:B:259:ALA:H	1.64	0.94
1:A:211:GLY:HA3	1:A:213:ASN:HD22	1.31	0.93
1:B:257:ASN:HD22	1:B:259:ALA:H	1.13	0.93
1:B:204:THR:CG2	1:B:213:ASN:HB3	1.99	0.93
1:B:257:ASN:HD22	1:B:258:ASN:N	1.68	0.92
4:B:502:EDO:H22	9:B:699:HOH:O	1.70	0.90
1:C:205:ARG:HG3	1:C:205:ARG:HH11	1.37	0.89
1:A:248:ASP:N	4:A:507:EDO:H21	1.88	0.88
1:B:204:THR:HG22	1:B:213:ASN:HB2	1.53	0.88
7:D:505:PEG:H41	9:D:614:HOH:O	1.72	0.88
1:D:252:ASN:O	1:D:256:ALA:HB2	1.72	0.88
1:D:220[A]:SER:OG	3:D:501:GOL:C3	2.21	0.88
1:B:204:THR:CG2	1:B:213:ASN:CB	2.51	0.88
1:B:201:MET:HG2	9:B:841:HOH:O	1.71	0.87
1:A:250:ILE:H	4:A:507:EDO:H11	1.39	0.86
1:C:387:ALA:H	7:C:506:PEG:C4	1.89	0.85
4:B:507:EDO:H11	1:C:335:SER:HB2	1.57	0.85
1:A:211:GLY:HA3	1:A:213:ASN:ND2	1.90	0.84
1:B:205:ARG:HD2	9:B:673:HOH:O	1.75	0.84
1:A:224:GLY:HA2	4:A:512:EDO:H22	1.59	0.84
1:A:211:GLY:CA	1:A:213:ASN:HD22	1.91	0.84
1:B:384:ARG:HB3	4:B:503:EDO:H21	1.60	0.84
1:A:211:GLY:CA	1:A:213:ASN:HA	2.06	0.84
1:A:212:SER:HA	1:A:213:ASN:ND2	1.92	0.84
1:C:257:ASN:HD22	1:C:258:ASN:N	1.76	0.84
1:D:220[A]:SER:OG	3:D:501:GOL:H31	1.77	0.83
1:A:211:GLY:CA	1:A:214:GLY:CA	2.52	0.83
4:A:505:EDO:H11	1:C:156:GLY:HA3	1.61	0.82
1:D:427:ALA:HB2	1:D:434:PHE:CE2	2.14	0.82
9:B:790:HOH:O	1:C:345:ARG:HD2	1.78	0.82
1:A:290:ASP:OD2	4:A:507:EDO:H22	1.79	0.82
1:B:329:ASN:HD22	1:B:330:TYR:H	1.25	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLN:HB2	4:B:507:EDO:H12	1.61	0.81
1:A:144:GLN:OE1	3:A:503:GOL:H31	1.82	0.80
1:D:208:ASN:O	1:D:210:GLY:CA	2.29	0.80
1:C:137:LEU:HG	7:C:506:PEG:H11	1.64	0.80
1:C:273:SER:HB2	4:C:504:EDO:H21	1.64	0.80
1:B:204:THR:CG2	1:B:214:GLY:H	1.96	0.79
1:A:208:ASN:O	1:A:210:GLY:HA3	1.82	0.79
1:B:205:ARG:HB2	1:B:205:ARG:NH1	1.98	0.79
1:B:329:ASN:ND2	1:B:330:TYR:H	1.79	0.79
1:D:384:ARG:N	1:D:384:ARG:HD3	1.97	0.77
1:A:250:ILE:HB	4:A:507:EDO:H11	1.64	0.77
1:A:262:ARG:HE	1:A:262:ARG:HA	1.50	0.77
1:B:334:TYR:HB3	3:C:502:GOL:H11	1.67	0.77
1:A:329:ASN:HD22	1:A:330:TYR:H	1.31	0.77
1:C:205:ARG:CG	1:C:205:ARG:HH11	1.96	0.77
1:A:338:GLN:CD	9:A:644:HOH:O	2.24	0.76
1:A:224:GLY:CA	4:A:512:EDO:H22	2.15	0.76
7:C:506:PEG:H12	9:C:640:HOH:O	1.86	0.76
1:A:329:ASN:ND2	1:A:330:TYR:H	1.84	0.74
1:A:204:THR:O	1:A:268:HIS:HE1	1.70	0.73
1:C:257:ASN:HD22	1:C:259:ALA:H	1.36	0.73
1:B:338:GLN:HG3	4:B:507:EDO:O2	1.89	0.73
1:A:338:GLN:NE2	9:A:601:HOH:O	2.20	0.73
1:A:211:GLY:HA2	1:A:213:ASN:CA	2.13	0.73
1:C:329:ASN:HD22	1:C:330:TYR:H	1.37	0.72
7:C:507:PEG:H11	9:C:677:HOH:O	1.88	0.72
1:B:204:THR:HG22	1:B:214:GLY:N	2.05	0.72
1:C:387:ALA:H	7:C:506:PEG:H41	1.55	0.72
1:C:364:ASN:O	3:C:501:GOL:H11	1.90	0.71
1:B:205:ARG:H	1:B:205:ARG:NH1	1.88	0.71
1:C:212:SER:HB2	1:C:213:ASN:HB3	1.72	0.71
1:C:329:ASN:ND2	1:C:330:TYR:H	1.88	0.71
1:B:257:ASN:HD22	1:B:257:ASN:C	1.93	0.71
4:B:503:EDO:H11	9:B:836:HOH:O	1.91	0.71
1:B:204:THR:CG2	1:B:213:ASN:HB2	2.20	0.71
1:B:257:ASN:HD22	1:B:259:ALA:N	1.87	0.70
1:A:250:ILE:CB	4:A:507:EDO:H11	2.20	0.70
1:C:310:GLU:HG2	1:C:313:ARG:NH1	2.06	0.70
1:C:302:ASP:HB3	1:C:350:ARG:NH2	2.07	0.70
1:B:257:ASN:ND2	1:B:259:ALA:N	2.39	0.70
1:B:204:THR:HG22	1:B:214:GLY:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ARG:CG	1:D:240:ARG:HH11	2.00	0.69
1:A:250:ILE:N	4:A:507:EDO:H12	2.05	0.69
1:C:384:ARG:HD3	1:C:384:ARG:N	2.06	0.69
1:D:220[A]:SER:OG	3:D:501:GOL:H32	1.92	0.69
1:C:212:SER:HA	1:C:213:ASN:CB	2.23	0.69
1:B:302:ASP:HB3	1:B:350:ARG:NH2	2.08	0.69
4:A:505:EDO:H11	1:C:156:GLY:CA	2.22	0.69
1:B:383:ALA:HB1	4:B:502:EDO:H21	1.74	0.69
1:B:204:THR:HA	1:B:213:ASN:CG	2.13	0.68
1:C:206:ASP:OD1	1:C:206:ASP:C	2.31	0.68
1:D:212:SER:HA	1:D:214:GLY:H	1.57	0.68
1:B:205:ARG:N	1:B:205:ARG:HH11	1.91	0.68
6:B:504:MPD:C5	9:B:834:HOH:O	2.42	0.67
1:A:248:ASP:H	4:A:507:EDO:H21	1.58	0.67
1:C:257:ASN:ND2	1:C:258:ASN:N	2.42	0.66
1:C:212:SER:CB	1:C:213:ASN:HB3	2.24	0.66
1:C:213:ASN:OD1	1:C:213:ASN:C	2.33	0.66
1:A:247:PRO:O	1:A:248:ASP:HB2	1.96	0.66
1:A:290:ASP:HB3	4:A:507:EDO:H22	1.78	0.66
1:D:329:ASN:ND2	1:D:330:TYR:H	1.92	0.65
1:B:204:THR:CG2	1:B:214:GLY:N	2.59	0.65
1:B:257:ASN:ND2	1:B:258:ASN:H	1.92	0.64
1:D:256:ALA:HB1	1:D:265:HIS:HE1	1.62	0.64
4:A:509:EDO:H11	9:A:677:HOH:O	1.97	0.64
1:D:213:ASN:O	1:D:213:ASN:ND2	2.30	0.64
1:A:325:THR:OG1	1:A:340:HIS:HE1	1.80	0.64
1:B:384:ARG:CB	4:B:503:EDO:H21	2.28	0.64
1:B:260:ASN:O	1:B:260:ASN:OD1	2.16	0.64
1:A:403:LYS:NZ	3:A:502:GOL:H31	2.13	0.64
1:D:164:LYS:HE3	9:D:828:HOH:O	1.98	0.63
1:A:154:LEU:HD23	4:A:510:EDO:H11	1.78	0.63
1:D:240:ARG:HG3	1:D:240:ARG:NH1	1.91	0.63
1:C:257:ASN:O	1:C:258:ASN:CB	2.47	0.62
1:A:211:GLY:C	1:A:214:GLY:HA2	2.18	0.62
1:C:205:ARG:CG	1:C:205:ARG:NH1	2.61	0.62
1:B:338:GLN:NE2	9:B:602:HOH:O	2.31	0.62
1:A:257:ASN:HA	1:A:258:ASN:OD1	1.99	0.62
1:C:257:ASN:O	1:C:258:ASN:HB2	1.98	0.62
1:B:204:THR:CB	1:B:213:ASN:HB2	2.30	0.62
1:D:303:ARG:HG3	1:D:303:ARG:HH11	1.64	0.61
1:B:204:THR:HA	1:B:213:ASN:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HB2	1:B:205:ARG:CZ	2.30	0.61
1:C:334:TYR:HB3	3:C:502:GOL:H31	1.82	0.61
1:A:353:ARG:HD2	9:A:652:HOH:O	2.00	0.61
1:B:338:GLN:HB3	4:B:507:EDO:H12	1.81	0.61
1:A:403:LYS:HZ2	3:A:502:GOL:H31	1.66	0.60
1:D:252:ASN:O	1:D:256:ALA:CB	2.49	0.60
1:A:250:ILE:N	4:A:507:EDO:H11	2.13	0.60
1:A:152[A]:GLN:NE2	9:A:606:HOH:O	2.33	0.60
1:D:329:ASN:HD22	1:D:330:TYR:H	1.48	0.60
1:B:204:THR:CA	1:B:213:ASN:CB	2.79	0.60
1:C:261:CYS:SG	1:C:265:HIS:CE1	2.95	0.59
1:C:383:ALA:HB1	7:C:507:PEG:H12	1.85	0.59
1:A:211:GLY:H	1:A:214:GLY:HA3	1.67	0.58
1:B:258:ASN:HA	1:B:261:CYS:HB2	1.85	0.58
1:B:214:GLY:C	1:B:218:ASN:HD21	2.07	0.58
1:D:302:ASP:CG	1:D:350:ARG:HH21	2.07	0.58
1:C:334:TYR:CB	3:C:502:GOL:H31	2.34	0.57
1:C:150:SER:OG	1:C:435:HIS:HD2	1.87	0.57
1:D:128:THR:CG2	1:D:129:SER:N	2.68	0.57
1:A:407:GLU:OE1	3:A:502:GOL:H32	2.05	0.57
7:C:507:PEG:C1	9:C:677:HOH:O	2.50	0.57
1:A:154:LEU:HD23	4:A:510:EDO:C1	2.34	0.57
1:B:205:ARG:H	1:B:205:ARG:HH11	1.51	0.57
1:D:256:ALA:CB	1:D:265:HIS:HE1	2.18	0.57
1:B:203:PRO:O	1:B:204:THR:OG1	2.22	0.56
1:C:435:HIS:HE1	9:C:828:HOH:O	1.86	0.56
1:B:260:ASN:O	1:B:260:ASN:CG	2.44	0.56
1:A:290:ASP:OD2	4:A:507:EDO:C2	2.52	0.56
1:B:338:GLN:CG	4:B:507:EDO:O2	2.52	0.56
1:C:387:ALA:CB	7:C:506:PEG:H41	2.36	0.56
3:C:501:GOL:C3	9:C:769:HOH:O	2.30	0.56
1:B:449:PHE:C	9:B:820:HOH:O	2.45	0.56
1:D:164:LYS:HA	1:D:164:LYS:HE2	1.88	0.56
1:A:253:LEU:HD22	1:A:269[B]:LYS:HE3	1.88	0.56
1:B:204:THR:HG21	1:B:214:GLY:H	1.70	0.56
1:B:332:PRO:CB	3:C:502:GOL:H2	2.36	0.56
1:A:268:HIS:HD2	9:A:788:HOH:O	1.89	0.55
1:C:165:VAL:HG21	1:C:442:LEU:HD11	1.88	0.55
1:A:436:ASP:HB3	4:A:505:EDO:H22	1.88	0.55
1:C:310:GLU:HG2	1:C:313:ARG:HH11	1.71	0.55
1:B:367:ASN:HD21	3:C:502:GOL:C3	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:SER:CA	1:C:213:ASN:HB3	2.36	0.54
1:C:325:THR:OG1	1:C:340:HIS:HE1	1.89	0.54
1:D:302:ASP:OD2	1:D:350:ARG:NH2	2.40	0.54
1:A:290:ASP:CB	4:A:507:EDO:H22	2.37	0.54
1:A:250:ILE:N	4:A:507:EDO:C1	2.50	0.54
1:B:204:THR:CA	1:B:213:ASN:HB2	2.37	0.54
1:B:367:ASN:HD21	3:C:502:GOL:H32	1.73	0.54
1:C:212:SER:CA	1:C:213:ASN:CB	2.86	0.54
1:C:257:ASN:ND2	1:C:258:ASN:H	2.05	0.54
1:A:269[A]:LYS:HE2	9:A:840:HOH:O	2.08	0.53
1:A:274:TYR:HA	4:A:504:EDO:H11	1.91	0.53
1:C:447:PRO:HG2	7:C:507:PEG:H21	1.91	0.53
1:D:256:ALA:CB	1:D:265:HIS:CE1	2.91	0.52
1:B:257:ASN:O	1:B:258:ASN:CB	2.58	0.52
1:D:165:VAL:HG21	1:D:442:LEU:CD1	2.39	0.52
1:D:263:ASN:HD21	4:D:503:EDO:H21	1.74	0.52
1:A:249:THR:H	4:A:507:EDO:H21	1.75	0.52
1:C:364:ASN:O	3:C:501:GOL:C1	2.56	0.52
1:D:263:ASN:HD21	4:D:503:EDO:C2	2.23	0.52
1:A:211:GLY:N	1:A:214:GLY:CA	2.74	0.51
4:B:507:EDO:H22	1:C:294:GLY:HA3	1.92	0.51
1:D:212:SER:HA	1:D:214:GLY:N	2.25	0.51
1:B:296:TRP:HZ3	9:B:823:HOH:O	1.91	0.51
1:B:325:THR:OG1	1:B:340:HIS:HE1	1.94	0.51
1:C:211:GLY:HA2	1:C:212:SER:HB3	1.93	0.51
1:A:208:ASN:O	1:A:208:ASN:OD1	2.29	0.51
1:B:261:CYS:HB3	1:B:265[B]:HIS:CE1	2.45	0.51
1:A:250:ILE:CG1	4:A:507:EDO:H11	2.41	0.50
6:B:504:MPD:H52	9:B:834:HOH:O	2.08	0.50
1:C:262:ARG:O	1:C:266:ASP:OD2	2.29	0.50
1:C:206:ASP:OD1	1:C:207:CYS:N	2.45	0.50
1:A:156:GLY:HA3	9:C:669:HOH:O	2.11	0.50
1:A:262:ARG:NE	1:A:262:ARG:HA	2.24	0.50
1:A:258:ASN:ND2	1:A:262:ARG:NH2	2.59	0.50
1:C:257:ASN:ND2	1:C:259:ALA:H	2.06	0.50
1:D:303:ARG:HH11	1:D:303:ARG:CG	2.25	0.50
1:B:205:ARG:HG2	9:B:613:HOH:O	2.12	0.50
1:C:165:VAL:HG21	1:C:442:LEU:CD1	2.41	0.50
1:A:249:THR:HB	4:A:507:EDO:H12	1.94	0.49
1:D:250[A]:ILE:HD12	1:D:290:ASP:O	2.13	0.49
1:C:148:ASP:O	1:C:152:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:TRP:CZ2	1:C:178:GLY:HA3	2.47	0.49
1:B:367:ASN:ND2	3:C:502:GOL:H32	2.27	0.49
1:C:362:SER:O	1:C:381:LEU:HA	2.12	0.49
1:C:204:THR:C	1:C:206:ASP:H	2.17	0.49
1:D:262:ARG:NH2	9:D:605:HOH:O	2.40	0.48
1:B:247:PRO:O	1:B:248:ASP:HB2	2.14	0.48
1:B:338:GLN:HE21	4:B:507:EDO:H21	1.78	0.48
1:D:257:ASN:H	1:D:257:ASN:ND2	2.11	0.48
1:A:293:HIS:CE1	1:A:296:TRP:N	2.81	0.48
1:B:204:THR:OG1	1:B:204:THR:O	2.31	0.48
1:A:338:GLN:CG	9:A:644:HOH:O	2.60	0.48
1:A:248:ASP:H	4:A:507:EDO:C2	2.26	0.48
1:D:258:ASN:O	1:D:261:CYS:N	2.47	0.48
1:D:325:THR:OG1	1:D:340:HIS:HE1	1.97	0.47
1:D:448[A]:PRO:HB3	9:D:823:HOH:O	2.12	0.47
1:A:207:CYS:HB3	1:A:261:CYS:CA	2.44	0.47
1:C:257:ASN:HD22	1:C:259:ALA:N	2.07	0.47
1:B:338:GLN:NE2	4:B:507:EDO:O2	2.47	0.47
1:A:204:THR:O	1:A:268:HIS:CE1	2.60	0.47
1:C:338:GLN:NE2	9:C:603:HOH:O	2.30	0.47
1:D:128:THR:HG22	1:D:129:SER:N	2.30	0.47
1:D:428:PRO:HG3	1:D:433:TRP:O	2.14	0.47
1:D:303:ARG:NH1	1:D:303:ARG:CG	2.77	0.47
1:A:205:ARG:HG3	1:A:205:ARG:HH11	1.79	0.47
1:B:384:ARG:H	4:B:502:EDO:C2	2.28	0.47
1:A:211:GLY:H	1:A:214:GLY:CA	2.28	0.47
1:A:447:PRO:HA	1:A:448:PRO:HD3	1.77	0.47
1:A:258:ASN:O	1:A:262:ARG:HB2	2.15	0.46
1:A:258:ASN:CB	1:A:262:ARG:HH21	2.28	0.46
1:A:338:GLN:HG3	9:A:644:HOH:O	2.14	0.46
1:B:383:ALA:CB	4:B:502:EDO:H21	2.43	0.46
1:A:211:GLY:N	1:A:214:GLY:HA3	2.30	0.46
1:B:212:SER:C	1:B:213:ASN:HD22	2.19	0.46
1:C:302:ASP:HB3	9:C:605:HOH:O	2.15	0.46
1:A:257:ASN:ND2	1:A:257:ASN:H	2.13	0.46
1:C:202:ILE:CG2	1:C:202:ILE:O	2.62	0.46
1:A:249:THR:H	4:A:507:EDO:H12	1.81	0.46
1:A:154:LEU:CD2	4:A:510:EDO:C1	2.93	0.46
1:C:350:ARG:NH2	9:C:605:HOH:O	2.38	0.46
4:A:509:EDO:H21	9:A:677:HOH:O	2.16	0.45
1:A:205:ARG:CG	1:A:205:ARG:HH11	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:HA	1:B:213:ASN:HB2	1.97	0.45
1:D:257:ASN:ND2	1:D:257:ASN:O	2.49	0.45
1:D:439:VAL:O	1:D:443:GLU:HG3	2.17	0.45
1:C:176:TRP:CH2	1:C:178:GLY:HA3	2.50	0.45
1:A:158:LEU:HA	1:A:158:LEU:HD23	1.88	0.45
1:C:137:LEU:CG	7:C:506:PEG:H11	2.42	0.45
1:D:384:ARG:H	1:D:384:ARG:HD3	1.75	0.45
1:D:427:ALA:CB	1:D:434:PHE:CE2	2.92	0.45
1:C:248:ASP:OD2	8:C:513:ACT:OXT	2.34	0.45
1:A:209:ALA:HB1	1:A:214:GLY:HA3	1.99	0.44
1:B:338:GLN:HE21	4:B:507:EDO:C2	2.30	0.44
1:C:334:TYR:HB3	3:C:502:GOL:O1	2.18	0.44
1:A:154:LEU:HD21	4:A:510:EDO:H12	1.99	0.44
1:A:250:ILE:HG12	4:A:507:EDO:H11	1.98	0.44
1:B:403:LYS:NZ	3:B:501:GOL:H12	2.32	0.44
1:D:257:ASN:HD22	1:D:257:ASN:C	2.20	0.44
1:D:257:ASN:ND2	1:D:257:ASN:N	2.66	0.44
1:D:165:VAL:HG21	1:D:442:LEU:HD11	2.00	0.43
1:A:249:THR:N	4:A:507:EDO:H12	2.33	0.43
1:B:329:ASN:HD22	1:B:330:TYR:N	2.04	0.43
1:D:447:PRO:HG2	7:D:505:PEG:O2	2.17	0.43
1:A:158:LEU:HB2	9:A:604:HOH:O	2.18	0.43
1:C:146:GLU:OE2	1:C:407:GLU:OE2	2.36	0.43
1:A:258:ASN:OD1	1:A:258:ASN:N	2.50	0.43
1:C:247:PRO:O	1:C:248:ASP:HB2	2.19	0.43
1:C:367:ASN:OD1	3:C:501:GOL:O1	2.37	0.43
1:A:154:LEU:CD2	4:A:510:EDO:H12	2.49	0.42
1:A:290:ASP:CG	4:A:507:EDO:H22	2.37	0.42
1:A:185:ARG:HB3	9:A:622:HOH:O	2.19	0.42
1:A:211:GLY:HA2	1:A:213:ASN:HD22	1.80	0.42
7:C:506:PEG:C1	9:C:640:HOH:O	2.57	0.42
1:A:207:CYS:HB3	1:A:261:CYS:HA	2.00	0.42
1:B:205:ARG:NH1	1:B:205:ARG:CB	2.76	0.42
1:A:213:ASN:HD22	1:A:213:ASN:HA	1.51	0.42
1:C:203:PRO:CB	1:C:218:ASN:HB3	2.49	0.42
1:A:240:ARG:NH2	9:A:617:HOH:O	2.52	0.42
1:B:410[A]:SER:HB3	1:B:418:CYS:SG	2.60	0.42
1:C:148:ASP:OD1	4:C:505:EDO:C2	2.68	0.42
1:D:258:ASN:O	1:D:261:CYS:HB2	2.20	0.42
1:A:303:ARG:HH22	2:A:501:PO4:P	2.43	0.41
1:A:207:CYS:O	1:A:208:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:LYS:NZ	1:D:283:LYS:H	2.18	0.41
1:D:446:ASN:HA	1:D:447:PRO:C	2.40	0.41
1:A:205:ARG:O	9:A:602:HOH:O	2.22	0.41
4:B:502:EDO:C2	9:B:699:HOH:O	2.46	0.41
9:A:768:HOH:O	1:D:345:ARG:HG2	2.20	0.41
1:B:362:SER:O	1:B:381:LEU:HA	2.20	0.41
1:C:202:ILE:HA	1:C:203:PRO:HD3	1.90	0.41
1:C:412:SER:HA	1:C:418:CYS:HB3	2.01	0.41
1:C:266:ASP:O	1:C:270:GLN:HG3	2.20	0.41
1:A:228:SER:HA	4:A:511:EDO:H21	2.03	0.41
1:B:328:SER:HA	1:B:403:LYS:HB2	2.03	0.41
1:C:214:GLY:HA3	1:C:215:GLY:HA2	1.88	0.41
1:C:323:ILE:HB	1:C:357:PHE:CD2	2.55	0.41
1:B:302:ASP:CB	1:B:350:ARG:NH2	2.82	0.40
1:B:146:GLU:OE2	1:B:407:GLU:OE2	2.38	0.40
1:C:273:SER:CB	4:C:504:EDO:H21	2.43	0.40
1:D:386:GLN:NE2	9:D:614:HOH:O	2.52	0.40
1:C:328:SER:HA	1:C:403:LYS:HB2	2.04	0.40
1:C:447:PRO:HA	1:C:448:PRO:HD3	1.96	0.40
1:A:206:ASP:OD1	1:A:206:ASP:N	2.54	0.40
1:B:205:ARG:CB	1:B:205:ARG:HH11	2.34	0.40
1:B:383:ALA:CA	4:B:502:EDO:H21	2.51	0.40
1:C:218:ASN:HA	1:C:218:ASN:HD22	1.67	0.40
1:A:207:CYS:O	1:A:208:ASN:CB	2.70	0.40
1:A:262:ARG:NE	1:A:262:ARG:CA	2.84	0.40
1:B:204:THR:HA	1:B:213:ASN:OD1	2.22	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	325/322 (101%)	313 (96%)	12 (4%)	0	100	100
1	B	323/322 (100%)	306 (95%)	17 (5%)	0	100	100
1	C	323/322 (100%)	309 (96%)	13 (4%)	1 (0%)	41	27
1	D	326/322 (101%)	315 (97%)	11 (3%)	0	100	100
All	All	1297/1288 (101%)	1243 (96%)	53 (4%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	205	ARG

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	271/266 (102%)	258 (95%)	13 (5%)	25	11
1	B	269/266 (101%)	258 (96%)	11 (4%)	30	16
1	C	269/266 (101%)	253 (94%)	16 (6%)	19	7
1	D	272/266 (102%)	259 (95%)	13 (5%)	25	11
All	All	1081/1064 (102%)	1028 (95%)	53 (5%)	27	11

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152[A]	GLN
1	A	152[B]	GLN
1	A	177	SER
1	A	205	ARG
1	A	206	ASP
1	A	207	CYS
1	A	213	ASN
1	A	257	ASN
1	A	258	ASN
1	A	260	ASN

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Mol	Chain	Res	Type
1	A	261	CYS
1	A	262	ARG
1	A	434	PHE
1	B	128	THR
1	B	202	ILE
1	B	205	ARG
1	B	207	CYS
1	B	208	ASN
1	B	212	SER
1	B	220	SER
1	B	257	ASN
1	B	265[A]	HIS
1	B	265[B]	HIS
1	B	434	PHE
1	C	128	THR
1	C	201[A]	MET
1	C	201[B]	MET
1	C	204	THR
1	C	205	ARG
1	C	206	ASP
1	C	207	CYS
1	C	213	ASN
1	C	240	ARG
1	C	257	ASN
1	C	262	ARG
1	C	265	HIS
1	C	310	GLU
1	C	313	ARG
1	C	345	ARG
1	C	384	ARG
1	D	128	THR
1	D	150	SER
1	D	212	SER
1	D	213	ASN
1	D	240	ARG
1	D	257	ASN
1	D	260	ASN
1	D	283	LYS
1	D	313[A]	ARG
1	D	313[B]	ARG
1	D	384	ARG
1	D	410	SER

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Mol	Chain	Res	Type
1	D	413	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	A	213	ASN
1	A	218	ASN
1	A	257	ASN
1	A	268	HIS
1	A	329	ASN
1	A	331	GLN
1	A	338	GLN
1	A	340	HIS
1	A	386	GLN
1	A	420	ASN
1	B	218	ASN
1	B	257	ASN
1	B	258	ASN
1	B	329	ASN
1	B	331	GLN
1	B	338	GLN
1	B	340	HIS
1	B	367	ASN
1	B	386	GLN
1	B	420	ASN
1	C	218	ASN
1	C	235	GLN
1	C	257	ASN
1	C	265	HIS
1	C	329	ASN
1	C	331	GLN
1	C	340	HIS
1	C	386	GLN
1	C	420	ASN
1	C	435	HIS
1	D	213	ASN
1	D	218	ASN
1	D	223	GLN
1	D	257	ASN
1	D	263	ASN
1	D	329	ASN

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Mol	Chain	Res	Type
1	D	331	GLN
1	D	340	HIS
1	D	386	GLN
1	D	392	ASN
1	D	420	ASN

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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 44 ligands modelled in this entry, 13 are modelled with single atom - leaving 31 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	EDO	B	507	-	3,3,3	0.58	0	2,2,2	0.87	0
3	GOL	D	501	-	5,5,5	0.54	0	5,5,5	1.25	0
4	EDO	D	503	-	3,3,3	0.56	0	2,2,2	0.54	0
3	GOL	A	503	-	5,5,5	0.78	0	5,5,5	1.49	1 (20%)
4	EDO	A	510	-	3,3,3	0.42	0	2,2,2	0.41	0
7	PEG	D	505	-	6,6,6	0.94	0	5,5,5	1.65	2 (40%)
4	EDO	D	502	-	3,3,3	0.93	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	PO4	A	501	-	4,4,4	0.38	0	6,6,6	1.26	0
4	EDO	A	506	-	3,3,3	0.67	0	2,2,2	0.64	0
8	ACT	C	513	-	1,3,3	1.75	0	0,3,3	0.00	-
4	EDO	A	512	-	3,3,3	0.28	0	2,2,2	1.56	1 (50%)
4	EDO	A	508	-	3,3,3	0.56	0	2,2,2	0.18	0
4	EDO	A	517	-	3,3,3	0.57	0	2,2,2	1.23	0
6	MPD	B	504	-	7,7,7	1.53	1 (14%)	9,10,10	1.82	3 (33%)
4	EDO	C	503	-	3,3,3	0.79	0	2,2,2	0.10	0
4	EDO	A	509	-	3,3,3	0.68	0	2,2,2	1.45	0
3	GOL	B	501	-	5,5,5	0.58	0	5,5,5	0.93	0
4	EDO	A	507	-	3,3,3	1.39	1 (33%)	2,2,2	1.33	0
7	PEG	C	506	-	6,6,6	0.63	0	5,5,5	0.81	0
7	PEG	C	507	-	6,6,6	1.23	0	5,5,5	1.87	1 (20%)
3	GOL	C	502	-	5,5,5	0.45	0	5,5,5	0.68	0
4	EDO	A	511	-	3,3,3	0.37	0	2,2,2	1.36	0
4	EDO	B	502	-	3,3,3	0.73	0	2,2,2	0.78	0
4	EDO	C	505	-	3,3,3	0.47	0	2,2,2	0.62	0
4	EDO	B	503	-	3,3,3	0.60	0	2,2,2	0.50	0
4	EDO	A	505	-	3,3,3	0.29	0	2,2,2	0.52	0
3	GOL	C	501	-	5,5,5	0.45	0	5,5,5	0.59	0
4	EDO	A	504	-	3,3,3	0.71	0	2,2,2	0.64	0
4	EDO	C	504	-	3,3,3	0.47	0	2,2,2	0.60	0
3	GOL	D	504	-	5,5,5	0.52	0	5,5,5	0.65	0
3	GOL	A	502	-	5,5,5	0.70	0	5,5,5	0.59	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
4	EDO	B	507	-	-	0/1/1/1	-
3	GOL	D	501	-	-	2/4/4/4	-
4	EDO	D	503	-	-	1/1/1/1	-
3	GOL	A	503	-	-	3/4/4/4	-
4	EDO	A	510	-	-	1/1/1/1	-
7	PEG	D	505	-	-	2/4/4/4	-
3	GOL	C	501	-	-	3/4/4/4	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	A	512	-	-	1/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	517	-	-	1/1/1/1	-
4	EDO	D	502	-	-	0/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
6	MPD	B	504	-	-	2/5/5/5	-
4	EDO	A	509	-	-	1/1/1/1	-
3	GOL	B	501	-	-	0/4/4/4	-
4	EDO	A	507	-	-	1/1/1/1	-
7	PEG	C	506	-	-	3/4/4/4	-
7	PEG	C	507	-	-	3/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	B	502	-	-	1/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	C	504	-	-	1/1/1/1	-
3	GOL	D	504	-	-	2/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	MPD	O2-C2	3.40	1.53	1.44
4	A	507	EDO	O2-C2	2.39	1.54	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	504	MPD	CM-C2-C1	-3.65	102.98	110.57
7	C	507	PEG	O2-C2-C1	3.45	125.21	110.07
6	B	504	MPD	O4-C4-C3	2.84	122.83	111.36
3	A	503	GOL	O1-C1-C2	2.40	121.69	110.20
7	D	505	PEG	O2-C3-C4	2.36	120.45	110.07
6	B	504	MPD	O2-C2-CM	2.26	115.32	108.08
4	A	512	EDO	O1-C1-C2	-2.12	96.62	111.91
7	D	505	PEG	O4-C4-C3	2.08	123.88	111.81

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-C3
3	C	501	GOL	O1-C1-C2-O2
3	C	501	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	D	501	GOL	O1-C1-C2-O2
3	A	502	GOL	O2-C2-C3-O3
7	D	505	PEG	O2-C3-C4-O4
7	C	506	PEG	O2-C3-C4-O4
7	C	507	PEG	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
7	C	506	PEG	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2
4	A	517	EDO	O1-C1-C2-O2
4	B	502	EDO	O1-C1-C2-O2
4	A	505	EDO	O1-C1-C2-O2
4	A	504	EDO	O1-C1-C2-O2
4	C	504	EDO	O1-C1-C2-O2
7	C	507	PEG	O2-C3-C4-O4
4	C	505	EDO	O1-C1-C2-O2
3	C	501	GOL	C1-C2-C3-O3
4	A	508	EDO	O1-C1-C2-O2
4	A	507	EDO	O1-C1-C2-O2
7	D	505	PEG	C1-C2-O2-C3
7	C	506	PEG	C4-C3-O2-C2
7	C	507	PEG	C1-C2-O2-C3
3	A	503	GOL	C1-C2-C3-O3
4	A	506	EDO	O1-C1-C2-O2
4	A	512	EDO	O1-C1-C2-O2
4	A	510	EDO	O1-C1-C2-O2
3	D	504	GOL	O1-C1-C2-O2
6	B	504	MPD	O2-C2-C3-C4
4	A	509	EDO	O1-C1-C2-O2
3	D	504	GOL	O1-C1-C2-C3
6	B	504	MPD	C2-C3-C4-O4

There are no ring outliers.

25 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	507	EDO	10	0
3	D	501	GOL	3	0
4	D	503	EDO	2	0
3	A	503	GOL	1	0
4	A	510	EDO	5	0
7	D	505	PEG	2	0
2	A	501	PO4	1	0
8	C	513	ACT	1	0
4	A	512	EDO	2	0
6	B	504	MPD	2	0
4	A	509	EDO	2	0
3	B	501	GOL	2	0
4	A	507	EDO	22	0
7	C	506	PEG	7	0
7	C	507	PEG	4	0
3	C	502	GOL	8	0
4	A	511	EDO	1	0
4	B	502	EDO	6	0
4	C	505	EDO	1	0
4	B	503	EDO	3	0
4	A	505	EDO	3	0
3	C	501	GOL	5	0
4	A	504	EDO	1	0
4	C	504	EDO	2	0
3	A	502	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	322/322 (100%)	0.30	27 (8%)	11	8	17, 26, 61, 86	13 (4%)
1	B	322/322 (100%)	0.44	30 (9%)	8	6	16, 26, 66, 80	17 (5%)
1	C	322/322 (100%)	0.55	28 (8%)	10	8	17, 28, 70, 86	16 (4%)
1	D	322/322 (100%)	0.25	26 (8%)	12	9	17, 28, 57, 85	8 (2%)
All	All	1288/1288 (100%)	0.39	111 (8%)	10	8	16, 27, 66, 86	54 (4%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	211	GLY	18.6
1	B	209	ALA	17.3
1	C	214	GLY	17.2
1	C	209	ALA	16.6
1	C	216	ALA	15.6
1	C	213	ASN	14.4
1	B	212	SER	13.6
1	B	211	GLY	12.6
1	C	212	SER	12.3
1	C	215	GLY	12.0
1	B	210	GLY	11.5
1	B	216	ALA	10.7
1	A	214	GLY	10.3
1	A	211	GLY	10.2
1	A	212	SER	9.9
1	D	257	ASN	9.3
1	C	210	GLY	8.9
1	B	207	CYS	8.7
1	A	210	GLY	8.7
1	C	259	ALA	8.7
1	B	213	ASN	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	209	ALA	8.5
1	C	207	CYS	8.5
1	B	215	GLY	8.2
1	A	259	ALA	8.1
1	A	216	ALA	7.9
1	B	214	GLY	7.8
1	D	210	GLY	7.6
1	B	206	ASP	7.3
1	D	128	THR	7.1
1	D	214	GLY	7.1
1	D	213	ASN	7.0
1	A	208	ASN	7.0
1	C	260	ASN	6.8
1	D	212	SER	6.7
1	C	208	ASN	6.6
1	D	209	ALA	6.4
1	D	211	GLY	6.2
1	A	261	CYS	6.1
1	C	206	ASP	6.1
1	B	258	ASN	6.0
1	A	213	ASN	5.9
1	A	260	ASN	5.9
1	C	204	THR	5.9
1	B	128	THR	5.8
1	B	208	ASN	5.8
1	A	206	ASP	5.7
1	A	257	ASN	5.7
1	B	260	ASN	5.6
1	C	261	CYS	5.4
1	A	207	CYS	5.4
1	B	261	CYS	5.4
1	C	128	THR	5.1
1	B	217	ASP	5.1
1	C	257	ASN	5.0
1	A	128	THR	4.9
1	A	258	ASN	4.9
1	C	258	ASN	4.8
1	D	426	GLY	4.6
1	C	203	PRO	4.5
1	B	257	ASN	4.4
1	C	263	ASN	4.4
1	B	259	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	256	ALA	4.2
1	B	262	ARG	4.0
1	A	263	ASN	4.0
1	D	258	ASN	3.9
1	B	263	ASN	3.8
1	B	244	ILE	3.7
1	A	215	GLY	3.7
1	D	419	ARG	3.4
1	D	208	ASN	3.4
1	C	262	ARG	3.3
1	A	203	PRO	3.2
1	C	217	ASP	3.2
1	C	264	VAL	3.2
1	A	262	ARG	3.0
1	D	421	SER	2.9
1	B	198	VAL	2.9
1	B	402	ILE	2.9
1	B	204	THR	2.9
1	D	449	PHE	2.9
1	D	413	SER	2.9
1	D	414	ALA	2.8
1	B	264	VAL	2.8
1	D	196	VAL	2.7
1	A	419	ARG	2.7
1	A	413	SER	2.7
1	D	371	ALA	2.6
1	C	244	ILE	2.6
1	D	416	PRO	2.6
1	C	449	PHE	2.5
1	A	449	PHE	2.5
1	A	414	ALA	2.4
1	D	402	ILE	2.4
1	A	416	PRO	2.4
1	D	261	CYS	2.4
1	B	203	PRO	2.3
1	A	204	THR	2.3
1	B	242	VAL	2.3
1	D	206	ASP	2.3
1	C	245	ILE	2.3
1	D	283	LYS	2.3
1	A	205	ARG	2.3
1	B	256	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	245	ILE	2.2
1	D	400	VAL	2.2
1	D	448[A]	PRO	2.2
1	B	243	MET	2.2
1	C	205	ARG	2.1
1	C	448	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($Å^2$)	Q<0.9
6	MPD	B	504	8/8	0.70	0.23	28,43,49,50	0
4	EDO	A	517	4/4	0.71	0.16	47,51,57,59	0
8	ACT	C	513	4/4	0.79	0.21	39,46,51,53	0
7	PEG	C	507	7/7	0.80	0.36	35,36,49,51	0
4	EDO	D	503	4/4	0.81	0.53	46,50,51,52	0
4	EDO	A	506	4/4	0.81	0.17	39,40,49,59	0
5	NH4	C	510	1/1	0.81	0.38	31,31,31,31	0
4	EDO	C	503	4/4	0.82	0.17	48,55,56,57	0
3	GOL	D	504	6/6	0.83	0.38	52,57,60,62	0
3	GOL	A	502	6/6	0.85	0.16	40,56,59,69	0
7	PEG	D	505	7/7	0.86	0.39	33,40,49,51	0
3	GOL	C	501	6/6	0.86	0.31	37,45,48,50	0
3	GOL	C	502	6/6	0.88	0.39	37,40,55,61	0
4	EDO	A	509	4/4	0.88	0.34	38,39,40,51	0
4	EDO	A	510	4/4	0.88	0.18	40,41,46,48	0
3	GOL	A	503	6/6	0.89	0.45	44,55,58,63	0
3	GOL	D	501	6/6	0.89	0.22	43,56,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	EDO	C	505	4/4	0.89	0.28	46,47,52,58	0
5	NH4	C	511	1/1	0.89	0.47	34,34,34,34	0
7	PEG	C	506	7/7	0.89	0.20	35,47,53,54	0
4	EDO	A	508	4/4	0.90	0.12	34,48,51,62	0
4	EDO	B	503	4/4	0.90	0.20	32,40,43,57	0
5	NH4	A	513	1/1	0.91	0.24	39,39,39,39	0
5	NH4	D	507	1/1	0.91	0.13	32,32,32,32	0
5	NH4	C	512	1/1	0.92	0.22	15,15,15,15	0
4	EDO	A	504	4/4	0.92	0.15	31,33,44,53	0
5	NH4	B	505	1/1	0.92	0.09	23,23,23,23	0
4	EDO	B	502	4/4	0.92	0.33	32,34,36,49	0
3	GOL	B	501	6/6	0.92	0.11	35,43,53,57	0
4	EDO	C	504	4/4	0.93	0.31	38,38,40,41	0
4	EDO	A	505	4/4	0.94	0.29	28,38,39,47	0
4	EDO	A	512	4/4	0.94	0.21	28,38,41,48	0
5	NH4	A	515	1/1	0.94	0.17	31,31,31,31	0
4	EDO	A	511	4/4	0.95	0.20	29,29,43,43	0
2	PO4	A	501	5/5	0.95	0.15	57,57,61,67	0
4	EDO	A	507	4/4	0.96	0.16	28,28,29,33	0
5	NH4	B	506	1/1	0.96	0.15	32,32,32,32	0
4	EDO	D	502	4/4	0.96	0.12	22,22,24,29	0
5	NH4	D	506	1/1	0.97	0.06	32,32,32,32	0
5	NH4	C	509	1/1	0.97	0.14	22,22,22,22	0
4	EDO	B	507	4/4	0.97	0.12	29,31,35,47	0
5	NH4	A	514	1/1	0.98	0.14	15,15,15,15	0
5	NH4	C	508	1/1	0.99	0.18	16,16,16,16	0
5	NH4	A	516	1/1	0.99	0.16	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.