Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2023 – 02:19 PM EST

PDB ID	:	3KS7
Title	:	Crystal structure of Putative Peptide:N-glycosidase F (PNGase F) (YP_210507.1) from Bacteroides fragilis NCTC 9343 at 2.30 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2009-11-20
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

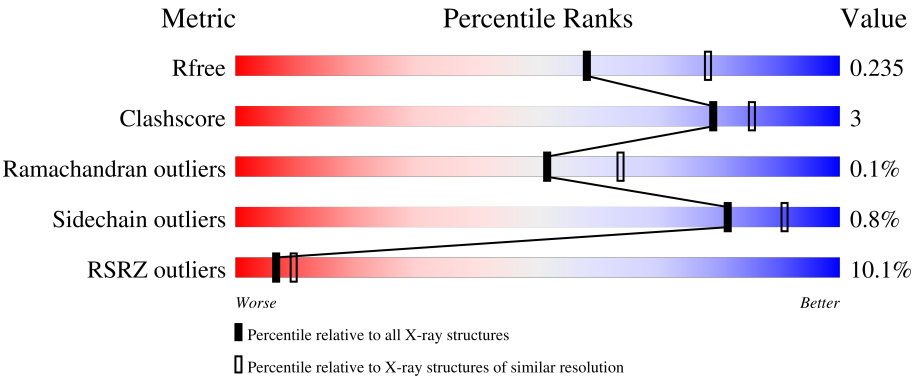
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	397	11% 90% 9%
1	B	397	8% 92% 6%
1	C	397	11% 93% 5%
1	D	397	9% 92% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12893 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 Putative Putative PNGase F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	Se	0	7	0
			3085	1973	520	582	4	6			
1	B	390	Total	C	N	O	S	Se	0	4	0
			3066	1956	519	581	4	6			
1	C	390	Total	C	N	O	S	Se	0	7	0
			3091	1977	522	582	4	6			
1	D	392	Total	C	N	O	S	Se	0	4	0
			3090	1975	522	583	4	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q5LH31
B	0	GLY	-	expression tag	UNP Q5LH31
C	0	GLY	-	expression tag	UNP Q5LH31
D	0	GLY	-	expression tag	UNP Q5LH31

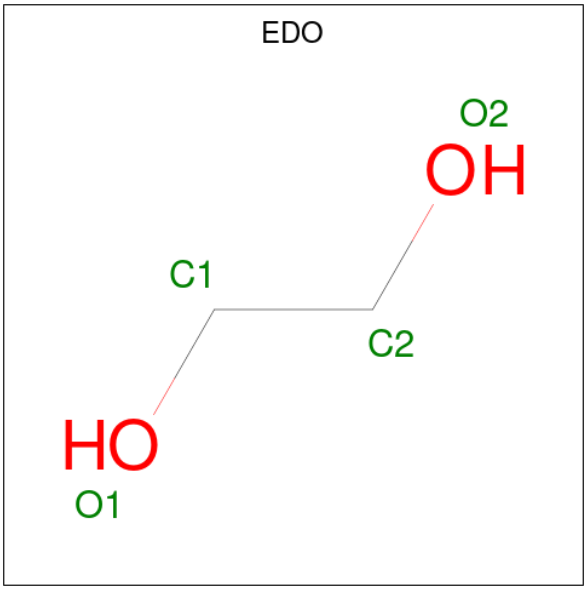
- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	I	0	0
			2	2		
2	B	2	Total	I	0	0
			2	2		
2	C	1	Total	I	0	0
			1	1		
2	D	2	Total	I	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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



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

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

- Molecule 5 is water.

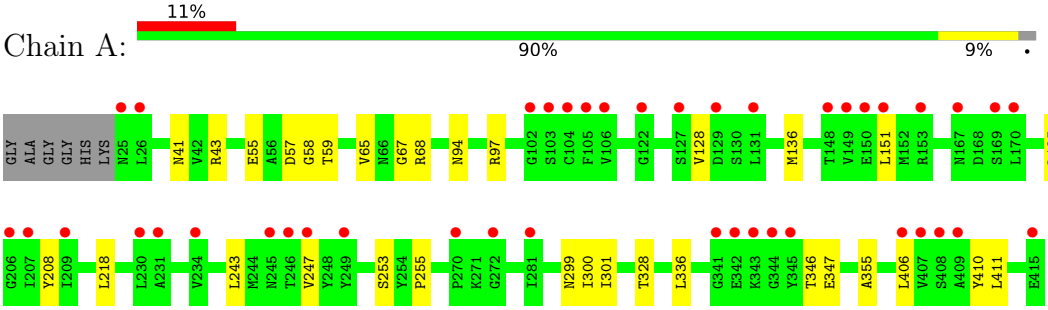
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	130	Total	O	0	1
			130	130		
5	C	106	Total	O	0	0
			106	106		
5	D	115	Total	O	0	1
			115	115		

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.

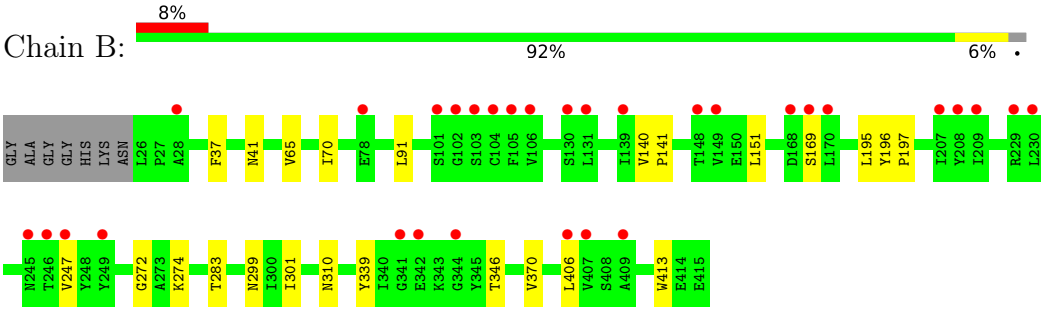
• Molecule 1: Putative Putative PNGase F

Chain A:



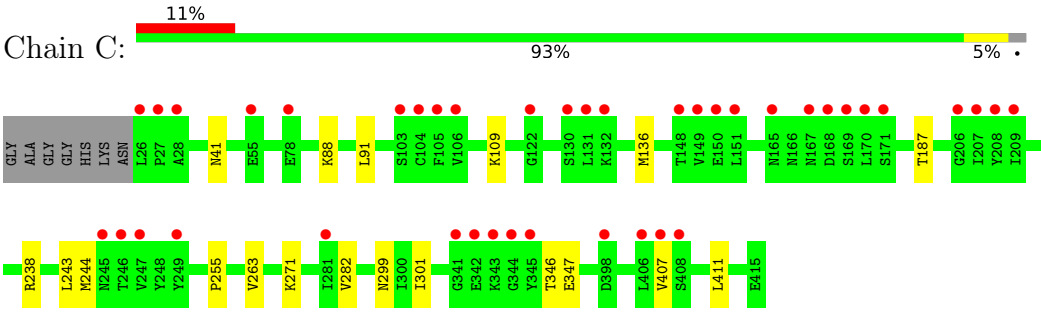
• Molecule 1: Putative Putative PNGase F

Chain B:



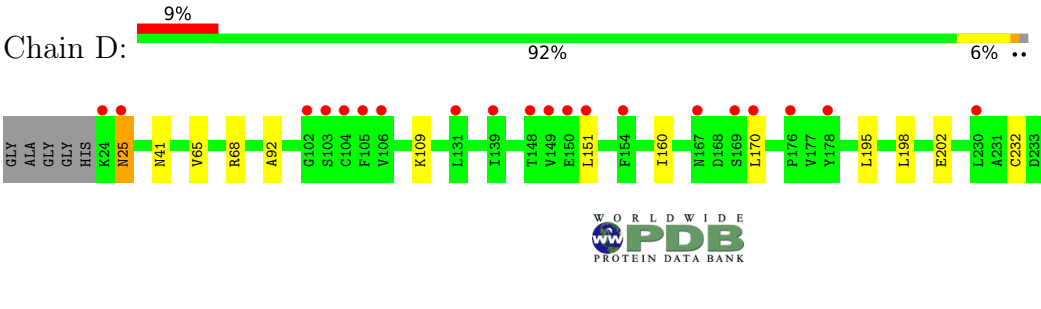
• Molecule 1: Putative Putative PNGase F

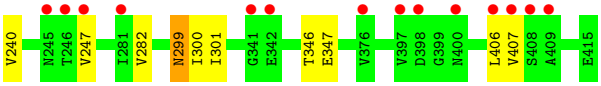
Chain C:



• Molecule 1: Putative Putative PNGase F

Chain D:




V240
N245
T246
V247
I281
V282
N299
I300
I301
G341
E342
T346
E347
V376
V397
D398
G399
N400
L406
V407
S408
A409
E415

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.06Å 119.22Å 154.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.30 29.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.88-2.30) 99.8 (29.88-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102, PHENIX	Depositor
R, R_{free}	0.201 , 0.237 0.200 , 0.235	Depositor DCC
R_{free} test set	4374 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12893	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% 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: EDO, IOD, CL

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	0.62	0/3179	0.53	0/4325
1	B	0.60	0/3151	0.53	0/4286
1	C	0.59	0/3185	0.53	0/4328
1	D	0.62	1/3175 (0.0%)	0.53	0/4317
All	All	0.61	1/12690 (0.0%)	0.53	0/17256

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	CYS	CB-SG	6.90	1.94	1.82

There are no bond angle outliers.

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	3085	0	2991	26	0
1	B	3066	0	2967	14	0
1	C	3091	0	3010	13	0
1	D	3090	0	3003	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	36	0	0
4	B	24	0	36	0	0
4	C	20	0	30	0	0
4	D	20	0	30	0	0
5	A	105	0	0	1	0
5	B	130	0	0	1	0
5	C	106	0	0	3	0
5	D	115	0	0	0	0
All	All	12893	0	12103	69	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 3.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:HG22	1:A:347:GLU:H	1.38	0.86
1:C:346:THR:HG22	1:C:347:GLU:H	1.49	0.78
1:C:136:MSE:HE1	1:C:255:PRO:HB3	1.77	0.66
1:A:301:ILE:N	1:A:301:ILE:HD12	2.12	0.65
1:C:238:ARG:HG2	5:C:432:HOH:O	1.98	0.63
1:D:109[A]:LYS:NZ	1:D:202:GLU:O	2.32	0.62
1:C:301:ILE:HD12	1:C:301:ILE:N	2.14	0.62
1:A:136:MSE:HA	1:A:136:MSE:HE2	1.80	0.62
1:A:65:VAL:HG11	1:A:68[A]:ARG:HH11	1.65	0.61
1:A:151:LEU:HD23	1:A:195:LEU:HD13	1.83	0.60
1:B:247:VAL:HA	1:B:406:LEU:HD22	1.85	0.58
1:B:301:ILE:HD12	1:B:301:ILE:N	2.17	0.58
1:C:243:LEU:HD11	1:C:411:LEU:HG	1.88	0.54
1:D:65:VAL:HG11	1:D:68[A]:ARG:HH11	1.73	0.54
1:D:346:THR:HG22	1:D:347:GLU:N	2.23	0.54
1:A:346:THR:HG22	1:A:347:GLU:N	2.18	0.53
1:B:151:LEU:HD23	1:B:195:LEU:HD13	1.92	0.51
1:A:300:ILE:HD12	1:A:300:ILE:N	2.26	0.50
1:A:57[B]:ASP:OD1	1:A:59:THR:OG1	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:HD12	1:D:170:LEU:O	2.12	0.49
1:A:243:LEU:HD11	1:A:411:LEU:HG	1.94	0.48
1:A:128:VAL:HG22	5:A:496:HOH:O	2.13	0.48
1:D:151:LEU:HD23	1:D:195:LEU:HD13	1.94	0.48
1:D:300:ILE:HD12	1:D:300:ILE:N	2.29	0.48
1:A:94:ASN:HB2	1:A:218[A]:LEU:HG	1.95	0.47
1:C:244:MSE:HE2	1:C:263:VAL:HG12	1.96	0.46
1:A:195:LEU:HD21	1:A:410:TYR:CZ	2.50	0.46
1:A:328:THR:HG21	1:A:355:ALA:HB1	1.97	0.46
1:D:282:VAL:HG23	1:D:407:VAL:HG22	1.98	0.46
1:C:109:LYS:N	5:C:478:HOH:O	2.47	0.46
1:D:299:ASN:HD22	1:D:299:ASN:N	2.13	0.46
1:D:346:THR:HG22	1:D:347:GLU:H	1.80	0.46
1:A:65:VAL:HG11	1:A:68[A]:ARG:NH1	2.29	0.46
1:C:136:MSE:HE1	1:C:255:PRO:CB	2.44	0.46
1:A:346:THR:CG2	1:A:347:GLU:H	2.18	0.45
1:B:339:TYR:CE1	1:B:346:THR:HG23	2.51	0.45
1:A:196:TYR:N	1:A:197:PRO:CD	2.79	0.45
1:D:247:VAL:HA	1:D:406:LEU:HD22	1.99	0.45
1:D:301:ILE:HD12	1:D:301:ILE:N	2.32	0.44
1:C:91:LEU:HD23	1:C:91:LEU:C	2.38	0.44
1:D:235:LEU:HD12	1:D:236:PRO:HD2	1.98	0.44
1:B:339:TYR:CZ	1:B:346:THR:HG23	2.53	0.43
1:A:97:ARG:HG2	3:A:12:CL:CL	2.55	0.43
1:B:37:PHE:CD1	1:B:70:ILE:HD12	2.52	0.43
1:D:25:ASN:ND2	1:D:25:ASN:O	2.52	0.43
1:B:140:VAL:HB	1:B:141:PRO:HD2	2.00	0.43
1:A:136:MSE:SE	1:A:255:PRO:HA	2.69	0.43
1:B:65:VAL:HG11	5:B:462[B]:HOH:O	2.18	0.43
1:A:195:LEU:HD21	1:A:410:TYR:CE1	2.54	0.42
1:B:140:VAL:HB	1:B:141:PRO:CD	2.49	0.42
1:B:239:HIS:CD2	1:B:413:TRP:CZ2	3.08	0.42
1:A:43:ARG:O	1:A:67:GLY:C	2.58	0.42
1:B:272:GLY:O	1:B:274:LYS:HG3	2.20	0.42
1:D:109[A]:LYS:HA	1:D:109[A]:LYS:HD3	1.72	0.42
1:B:91:LEU:C	1:B:91:LEU:HD23	2.40	0.41
1:D:198:LEU:HD11	1:D:240:VAL:HG11	2.01	0.41
1:B:196:TYR:N	1:B:197:PRO:CD	2.84	0.41
1:C:282:VAL:HG23	1:C:407:VAL:HG22	2.02	0.41
1:C:88:LYS:NZ	1:C:187:THR:HG21	2.34	0.41
1:A:68[A]:ARG:NH2	1:A:208:TYR:OH	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:THR:HG22	1:C:347:GLU:N	2.28	0.41
1:D:92:ALA:HA	1:D:160:ILE:HG23	2.02	0.41
1:A:57[A]:ASP:CG	1:A:58:GLY:H	2.24	0.41
1:B:283:THR:CG2	1:B:370:VAL:HG21	2.51	0.41
1:A:136:MSE:HE1	1:A:253:SER:OG	2.21	0.40
1:A:336:LEU:HD11	1:A:347:GLU:HG2	2.04	0.40
1:C:271[A]:LYS:HD3	5:C:439:HOH:O	2.20	0.40
1:A:247:VAL:HA	1:A:406:LEU:HD22	2.03	0.40
1:A:299:ASN:HB3	1:A:301:ILE:HD11	2.04	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	396/397 (100%)	378 (96%)	18 (4%)	0	100 100
1	B	392/397 (99%)	377 (96%)	14 (4%)	1 (0%)	41 50
1	C	395/397 (100%)	383 (97%)	12 (3%)	0	100 100
1	D	394/397 (99%)	375 (95%)	19 (5%)	0	100 100
All	All	1577/1588 (99%)	1513 (96%)	63 (4%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	SER

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	334/339 (98%)	332 (99%)	2 (1%)	86 94
1	B	333/339 (98%)	330 (99%)	3 (1%)	78 89
1	C	335/339 (99%)	333 (99%)	2 (1%)	86 94
1	D	335/339 (99%)	332 (99%)	3 (1%)	78 89
All	All	1337/1356 (99%)	1327 (99%)	10 (1%)	81 92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	55	GLU
1	B	41	ASN
1	B	299	ASN
1	B	310	ASN
1	C	41	ASN
1	C	299	ASN
1	D	25	ASN
1	D	41	ASN
1	D	299	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	41	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 17 are monoatomic - leaving 22 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	C	419	-	3,3,3	0.58	0	2,2,2	0.22	0
4	EDO	C	418	-	3,3,3	0.40	0	2,2,2	0.37	0
4	EDO	C	420	-	3,3,3	0.68	0	2,2,2	0.18	0
4	EDO	A	419	-	3,3,3	0.51	0	2,2,2	0.30	0
4	EDO	B	421	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	D	18	-	3,3,3	0.51	0	2,2,2	0.27	0
4	EDO	A	421	-	3,3,3	0.56	0	2,2,2	0.24	0
4	EDO	C	417	-	3,3,3	0.40	0	2,2,2	0.37	0
4	EDO	A	420	-	3,3,3	0.56	0	2,2,2	0.24	0
4	EDO	D	417	-	3,3,3	0.57	0	2,2,2	0.20	0
4	EDO	D	419	-	3,3,3	0.53	0	2,2,2	0.24	0
4	EDO	B	417	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	B	419	-	3,3,3	0.52	0	2,2,2	0.27	0
4	EDO	A	418	-	3,3,3	0.60	0	2,2,2	0.21	0
4	EDO	C	416	-	3,3,3	0.41	0	2,2,2	0.34	0
4	EDO	A	416	-	3,3,3	0.49	0	2,2,2	0.31	0
4	EDO	D	416	-	3,3,3	0.57	0	2,2,2	0.25	0
4	EDO	B	420	-	3,3,3	0.49	0	2,2,2	0.32	0
4	EDO	B	418	-	3,3,3	0.64	0	2,2,2	0.13	0
4	EDO	A	417	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	D	418	-	3,3,3	0.52	0	2,2,2	0.29	0
4	EDO	B	416	-	3,3,3	0.57	0	2,2,2	0.18	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	C	419	-	-	1/1/1/1	-
4	EDO	C	418	-	-	1/1/1/1	-
4	EDO	C	420	-	-	1/1/1/1	-
4	EDO	A	419	-	-	1/1/1/1	-
4	EDO	B	421	-	-	0/1/1/1	-
4	EDO	D	18	-	-	1/1/1/1	-
4	EDO	A	421	-	-	1/1/1/1	-
4	EDO	C	417	-	-	1/1/1/1	-
4	EDO	A	420	-	-	1/1/1/1	-
4	EDO	D	417	-	-	1/1/1/1	-
4	EDO	D	419	-	-	0/1/1/1	-
4	EDO	B	417	-	-	1/1/1/1	-
4	EDO	B	419	-	-	0/1/1/1	-
4	EDO	A	418	-	-	1/1/1/1	-
4	EDO	C	416	-	-	1/1/1/1	-
4	EDO	A	416	-	-	1/1/1/1	-
4	EDO	D	416	-	-	0/1/1/1	-
4	EDO	B	420	-	-	1/1/1/1	-
4	EDO	B	418	-	-	1/1/1/1	-
4	EDO	A	417	-	-	1/1/1/1	-
4	EDO	D	418	-	-	1/1/1/1	-
4	EDO	B	416	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	416	EDO	O1-C1-C2-O2
4	A	419	EDO	O1-C1-C2-O2
4	C	416	EDO	O1-C1-C2-O2
4	C	417	EDO	O1-C1-C2-O2
4	C	418	EDO	O1-C1-C2-O2
4	C	420	EDO	O1-C1-C2-O2
4	D	18	EDO	O1-C1-C2-O2
4	D	417	EDO	O1-C1-C2-O2
4	D	418	EDO	O1-C1-C2-O2
4	B	416	EDO	O1-C1-C2-O2
4	C	419	EDO	O1-C1-C2-O2
4	A	417	EDO	O1-C1-C2-O2
4	A	421	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	420	EDO	O1-C1-C2-O2
4	B	418	EDO	O1-C1-C2-O2
4	B	420	EDO	O1-C1-C2-O2
4	A	418	EDO	O1-C1-C2-O2
4	B	417	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	385/397 (96%)	0.35	42 (10%) 5 8	18, 25, 36, 46	0
1	B	384/397 (96%)	0.33	33 (8%) 10 14	18, 25, 35, 46	0
1	C	384/397 (96%)	0.41	45 (11%) 4 6	18, 25, 36, 46	0
1	D	386/397 (97%)	0.26	35 (9%) 9 12	18, 25, 35, 46	0
All	All	1539/1588 (96%)	0.34	155 (10%) 7 9	18, 25, 36, 46	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	LEU	8.0
1	C	167	ASN	6.4
1	B	231	ALA	6.2
1	B	131	LEU	5.8
1	C	131	LEU	5.7
1	B	232	CYS	5.4
1	A	131	LEU	5.2
1	B	247	VAL	4.9
1	C	168	ASP	4.7
1	C	169	SER	4.7
1	D	131	LEU	4.7
1	C	247	VAL	4.6
1	B	149	VAL	4.4
1	A	407	VAL	4.2
1	C	171	SER	4.2
1	A	247	VAL	4.1
1	D	247	VAL	4.1
1	C	343	LYS	4.1
1	A	167	ASN	4.0
1	C	105	PHE	4.0
1	A	103	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	105	PHE	3.9
1	D	167	ASN	3.9
1	C	406	LEU	3.9
1	A	169	SER	3.9
1	A	170	LEU	3.8
1	B	246	THR	3.7
1	C	408	SER	3.7
1	A	406	LEU	3.6
1	C	245	ASN	3.6
1	A	26	LEU	3.5
1	C	341	GLY	3.5
1	C	106	VAL	3.5
1	C	104	CYS	3.4
1	D	103	SER	3.4
1	A	105	PHE	3.4
1	D	104	CYS	3.4
1	C	407	VAL	3.3
1	D	149	VAL	3.3
1	C	344	GLY	3.3
1	A	341	GLY	3.3
1	C	229	ARG	3.3
1	D	106	VAL	3.3
1	B	106	VAL	3.2
1	C	149	VAL	3.2
1	C	103	SER	3.2
1	A	408	SER	3.2
1	C	398	ASP	3.2
1	D	407	VAL	3.2
1	C	148	THR	3.1
1	B	148	THR	3.0
1	B	130	SER	3.0
1	A	249	TYR	2.9
1	A	342	GLU	2.9
1	B	28	ALA	2.9
1	D	409	ALA	2.9
1	D	105	PHE	2.9
1	D	230	LEU	2.9
1	D	342	GLU	2.9
1	B	249	TYR	2.9
1	D	281	ILE	2.9
1	C	249	TYR	2.9
1	B	169	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	245	ASN	2.9
1	B	207	ILE	2.8
1	A	25	ASN	2.8
1	A	272	GLY	2.8
1	D	406	LEU	2.8
1	B	103	SER	2.8
1	B	406	LEU	2.8
1	D	408	SER	2.8
1	B	102	GLY	2.8
1	D	178	TYR	2.8
1	B	168	ASP	2.7
1	B	342	GLU	2.7
1	C	78	GLU	2.7
1	A	409	ALA	2.7
1	A	234	VAL	2.7
1	A	102	GLY	2.7
1	A	344	GLY	2.7
1	B	341	GLY	2.7
1	A	245	ASN	2.7
1	D	245	ASN	2.7
1	C	26	LEU	2.7
1	C	246	THR	2.7
1	C	231	ALA	2.6
1	C	130	SER	2.6
1	D	341	GLY	2.6
1	A	415	GLU	2.6
1	A	207	ILE	2.6
1	D	246	THR	2.6
1	B	407	VAL	2.6
1	C	345	TYR	2.6
1	D	25	ASN	2.6
1	A	281	ILE	2.6
1	A	127	SER	2.5
1	A	345	TYR	2.5
1	C	342	GLU	2.5
1	D	102	GLY	2.5
1	B	229	ARG	2.5
1	B	78	GLU	2.5
1	C	206	GLY	2.5
1	C	281	ILE	2.5
1	C	151	LEU	2.5
1	C	209	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	24	LYS	2.4
1	C	207	ILE	2.4
1	B	230	LEU	2.4
1	A	151	LEU	2.4
1	A	122	GLY	2.4
1	A	149	VAL	2.4
1	B	409	ALA	2.4
1	A	246	THR	2.4
1	D	151	LEU	2.3
1	A	106	VAL	2.3
1	A	153	ARG	2.3
1	C	27	PRO	2.3
1	D	170	LEU	2.3
1	C	28	ALA	2.3
1	A	230	LEU	2.3
1	D	148	THR	2.3
1	D	376	VAL	2.3
1	A	206	GLY	2.3
1	B	344	GLY	2.3
1	D	398	ASP	2.3
1	B	101	SER	2.3
1	A	270	PRO	2.2
1	A	209	ILE	2.2
1	D	234	VAL	2.2
1	D	169	SER	2.2
1	A	129	ASP	2.2
1	C	208	TYR	2.2
1	B	170	LEU	2.2
1	D	176	PRO	2.2
1	D	397	VAL	2.2
1	C	232	CYS	2.2
1	B	139	ILE	2.1
1	D	400	ASN	2.1
1	C	150	GLU	2.1
1	D	150	GLU	2.1
1	C	55	GLU	2.1
1	C	165	ASN	2.1
1	D	139	ILE	2.1
1	B	104	CYS	2.1
1	B	208	TYR	2.1
1	D	154	PHE	2.1
1	A	148	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	122	GLY	2.0
1	A	231	ALA	2.0
1	C	132	LYS	2.0
1	A	104	CYS	2.0
1	A	150	GLU	2.0
1	B	209	ILE	2.0
1	C	230	LEU	2.0
1	A	343	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
4	EDO	D	419	4/4	0.57	0.23	88,89,89,89	0
4	EDO	C	420	4/4	0.71	0.21	58,59,59,60	0
4	EDO	A	416	4/4	0.72	0.24	67,67,68,69	0
4	EDO	A	420	4/4	0.73	0.24	61,63,64,64	0
4	EDO	D	416	4/4	0.79	0.22	58,58,58,58	0
4	EDO	B	418	4/4	0.80	0.18	56,56,56,56	0
4	EDO	B	421	4/4	0.80	0.16	67,68,69,69	0
4	EDO	D	417	4/4	0.80	0.20	52,52,53,53	0
4	EDO	C	419	4/4	0.80	0.15	56,57,57,57	0
4	EDO	A	421	4/4	0.81	0.18	61,61,62,62	0
4	EDO	A	418	4/4	0.81	0.21	63,63,64,64	0
4	EDO	C	418	4/4	0.83	0.23	52,52,52,53	0
4	EDO	D	18	4/4	0.85	0.26	66,67,67,67	0
4	EDO	B	416	4/4	0.85	0.22	50,52,53,55	0
4	EDO	C	416	4/4	0.86	0.22	51,52,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	9	1/1	0.87	0.16	58,58,58,58	0
4	EDO	A	419	4/4	0.88	0.18	49,49,49,50	0
4	EDO	B	417	4/4	0.88	0.17	54,55,55,55	0
3	CL	C	15	1/1	0.90	0.22	49,49,49,49	0
4	EDO	A	417	4/4	0.90	0.12	54,55,55,55	0
4	EDO	B	420	4/4	0.91	0.15	58,59,59,60	0
4	EDO	D	418	4/4	0.92	0.11	65,66,66,66	0
4	EDO	C	417	4/4	0.93	0.19	62,62,62,63	0
4	EDO	B	419	4/4	0.95	0.11	61,63,64,64	0
3	CL	C	13	1/1	0.96	0.14	41,41,41,41	0
3	CL	B	14	1/1	0.96	0.09	48,48,48,48	0
3	CL	B	16	1/1	0.96	0.10	48,48,48,48	0
3	CL	B	8	1/1	0.97	0.13	36,36,36,36	0
3	CL	D	17	1/1	0.97	0.05	49,49,49,49	0
2	IOD	A	6	1/1	0.97	0.11	45,45,45,45	1
3	CL	A	11	1/1	0.98	0.24	40,40,40,40	0
2	IOD	B	5	1/1	0.98	0.24	45,45,45,45	1
2	IOD	D	7	1/1	0.98	0.21	44,44,44,44	1
2	IOD	A	4	1/1	0.98	0.11	36,36,36,36	1
3	CL	C	10	1/1	0.98	0.10	35,35,35,35	0
3	CL	A	12	1/1	0.99	0.08	42,42,42,42	0
2	IOD	D	3	1/1	0.99	0.14	33,33,33,33	1
2	IOD	C	2	1/1	0.99	0.13	35,35,35,35	1
2	IOD	B	1	1/1	1.00	0.10	36,36,36,36	1

6.5 Other polymers (i)

There are no such residues in this entry.