Full wwPDB X-ray Structure Validation Report (i)

May 12, 2025 – 12:50 PM EDT

PDB ID	:	9OJL / pdb_00009ojl
Title	:	Crystal Structure of GH18 Chitinase Domain from Vibrio splendidus
Authors	:	Horton, J.G.; Jackson, C.J.; Frkic, R.L.
Deposited on	:	2025-05-08
Resolution	:	1.80 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 (i) 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 (1)) were used in the production of this report:

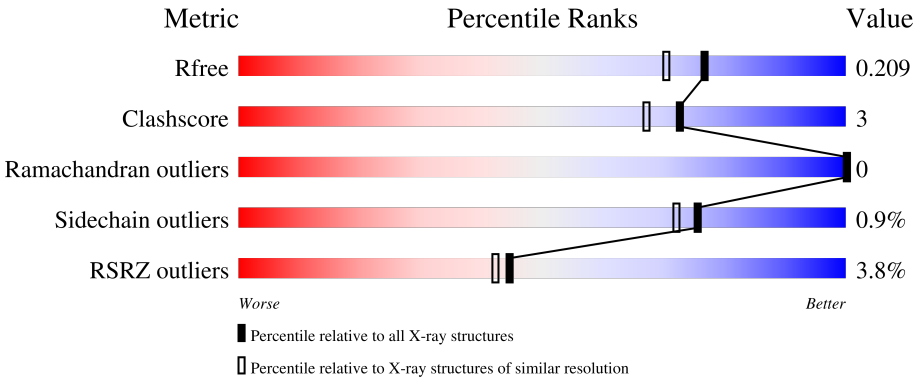
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 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	336	90% · 6%
1	B	336	90% · 5%
1	C	336	2% 92% · ·
1	D	336	89% · · 6%
1	E	336	11% 86% 9% 5%

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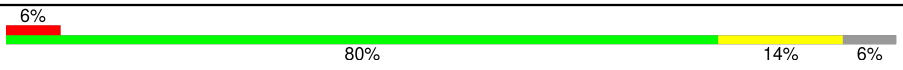
Mol	Chain	Length	Quality of chain
1	F	336	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17698 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 Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	4	0
			2531	1611	413	499	8			
1	B	318	Total	C	N	O	S	0	5	0
			2538	1615	414	501	8			
1	C	323	Total	C	N	O	S	0	3	0
			2567	1636	420	503	8			
1	D	317	Total	C	N	O	S	0	5	0
			2536	1614	413	501	8			
1	E	318	Total	C	N	O	S	0	0	0
			2502	1596	409	489	8			
1	F	316	Total	C	N	O	S	0	1	0
			2502	1596	409	489	8			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP A0A837NXJ2
A	2	PRO	-	expression tag	UNP A0A837NXJ2
A	3	THR	-	expression tag	UNP A0A837NXJ2
A	4	ALA	-	expression tag	UNP A0A837NXJ2
A	5	PRO	-	expression tag	UNP A0A837NXJ2
A	329	LEU	-	expression tag	UNP A0A837NXJ2
A	330	GLU	-	expression tag	UNP A0A837NXJ2
A	331	HIS	-	expression tag	UNP A0A837NXJ2
A	332	HIS	-	expression tag	UNP A0A837NXJ2
A	333	HIS	-	expression tag	UNP A0A837NXJ2
A	334	HIS	-	expression tag	UNP A0A837NXJ2
A	335	HIS	-	expression tag	UNP A0A837NXJ2
A	336	HIS	-	expression tag	UNP A0A837NXJ2
B	1	ALA	-	expression tag	UNP A0A837NXJ2
B	2	PRO	-	expression tag	UNP A0A837NXJ2
B	3	THR	-	expression tag	UNP A0A837NXJ2
B	4	ALA	-	expression tag	UNP A0A837NXJ2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	PRO	-	expression tag	UNP A0A837NXJ2
B	329	LEU	-	expression tag	UNP A0A837NXJ2
B	330	GLU	-	expression tag	UNP A0A837NXJ2
B	331	HIS	-	expression tag	UNP A0A837NXJ2
B	332	HIS	-	expression tag	UNP A0A837NXJ2
B	333	HIS	-	expression tag	UNP A0A837NXJ2
B	334	HIS	-	expression tag	UNP A0A837NXJ2
B	335	HIS	-	expression tag	UNP A0A837NXJ2
B	336	HIS	-	expression tag	UNP A0A837NXJ2
C	1	ALA	-	expression tag	UNP A0A837NXJ2
C	2	PRO	-	expression tag	UNP A0A837NXJ2
C	3	THR	-	expression tag	UNP A0A837NXJ2
C	4	ALA	-	expression tag	UNP A0A837NXJ2
C	5	PRO	-	expression tag	UNP A0A837NXJ2
C	329	LEU	-	expression tag	UNP A0A837NXJ2
C	330	GLU	-	expression tag	UNP A0A837NXJ2
C	331	HIS	-	expression tag	UNP A0A837NXJ2
C	332	HIS	-	expression tag	UNP A0A837NXJ2
C	333	HIS	-	expression tag	UNP A0A837NXJ2
C	334	HIS	-	expression tag	UNP A0A837NXJ2
C	335	HIS	-	expression tag	UNP A0A837NXJ2
C	336	HIS	-	expression tag	UNP A0A837NXJ2
D	1	ALA	-	expression tag	UNP A0A837NXJ2
D	2	PRO	-	expression tag	UNP A0A837NXJ2
D	3	THR	-	expression tag	UNP A0A837NXJ2
D	4	ALA	-	expression tag	UNP A0A837NXJ2
D	5	PRO	-	expression tag	UNP A0A837NXJ2
D	329	LEU	-	expression tag	UNP A0A837NXJ2
D	330	GLU	-	expression tag	UNP A0A837NXJ2
D	331	HIS	-	expression tag	UNP A0A837NXJ2
D	332	HIS	-	expression tag	UNP A0A837NXJ2
D	333	HIS	-	expression tag	UNP A0A837NXJ2
D	334	HIS	-	expression tag	UNP A0A837NXJ2
D	335	HIS	-	expression tag	UNP A0A837NXJ2
D	336	HIS	-	expression tag	UNP A0A837NXJ2
E	1	ALA	-	expression tag	UNP A0A837NXJ2
E	2	PRO	-	expression tag	UNP A0A837NXJ2
E	3	THR	-	expression tag	UNP A0A837NXJ2
E	4	ALA	-	expression tag	UNP A0A837NXJ2
E	5	PRO	-	expression tag	UNP A0A837NXJ2
E	329	LEU	-	expression tag	UNP A0A837NXJ2
E	330	GLU	-	expression tag	UNP A0A837NXJ2

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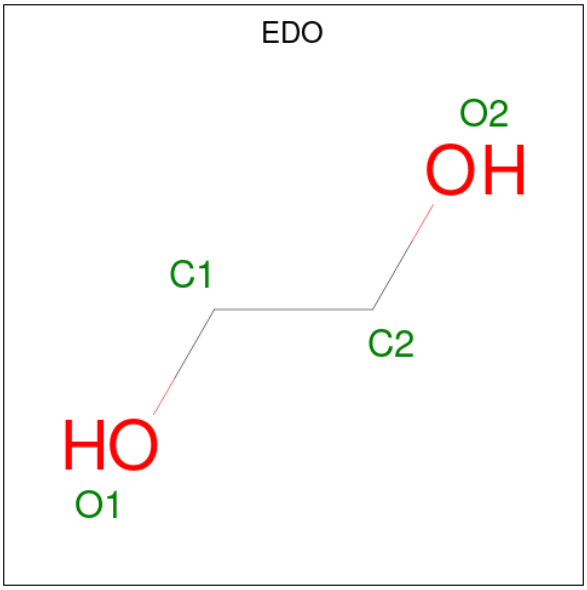
Chain	Residue	Modelled	Actual	Comment	Reference
E	331	HIS	-	expression tag	UNP A0A837NXJ2
E	332	HIS	-	expression tag	UNP A0A837NXJ2
E	333	HIS	-	expression tag	UNP A0A837NXJ2
E	334	HIS	-	expression tag	UNP A0A837NXJ2
E	335	HIS	-	expression tag	UNP A0A837NXJ2
E	336	HIS	-	expression tag	UNP A0A837NXJ2
F	1	ALA	-	expression tag	UNP A0A837NXJ2
F	2	PRO	-	expression tag	UNP A0A837NXJ2
F	3	THR	-	expression tag	UNP A0A837NXJ2
F	4	ALA	-	expression tag	UNP A0A837NXJ2
F	5	PRO	-	expression tag	UNP A0A837NXJ2
F	329	LEU	-	expression tag	UNP A0A837NXJ2
F	330	GLU	-	expression tag	UNP A0A837NXJ2
F	331	HIS	-	expression tag	UNP A0A837NXJ2
F	332	HIS	-	expression tag	UNP A0A837NXJ2
F	333	HIS	-	expression tag	UNP A0A837NXJ2
F	334	HIS	-	expression tag	UNP A0A837NXJ2
F	335	HIS	-	expression tag	UNP A0A837NXJ2
F	336	HIS	-	expression tag	UNP A0A837NXJ2

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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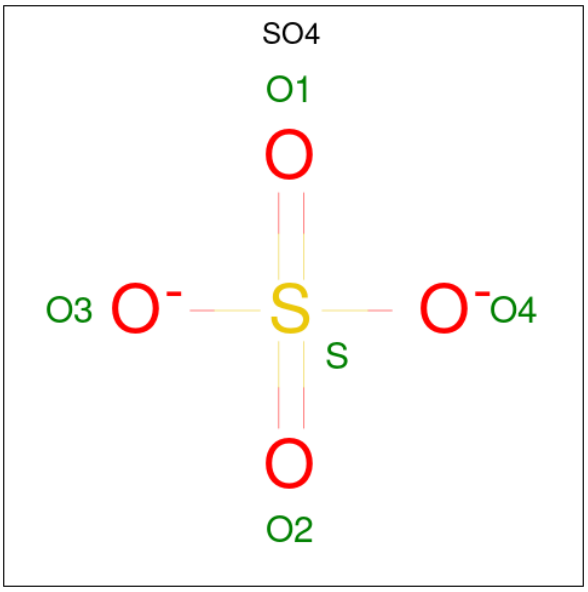
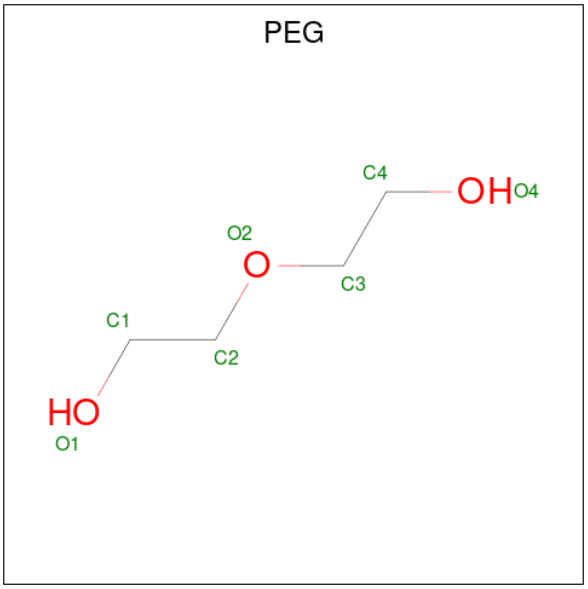
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: 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	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0

- Molecule 5 is water.

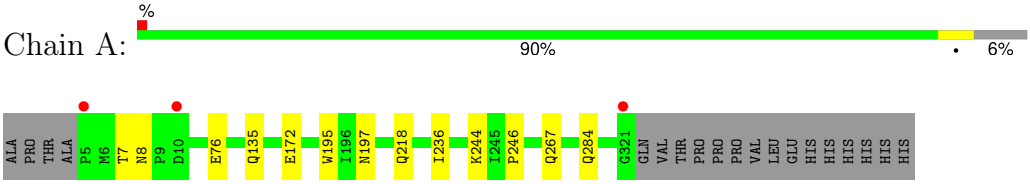
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	519	Total O 519 519	0	0
5	B	498	Total O 498 498	0	0
5	C	531	Total O 531 531	0	0
5	D	468	Total O 468 468	0	0
5	E	231	Total O 231 231	0	0
5	F	153	Total O 153 153	0	0

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.

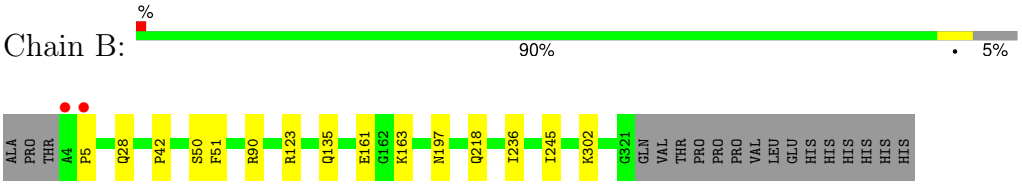
- Molecule 1: Chitinase

Chain A:



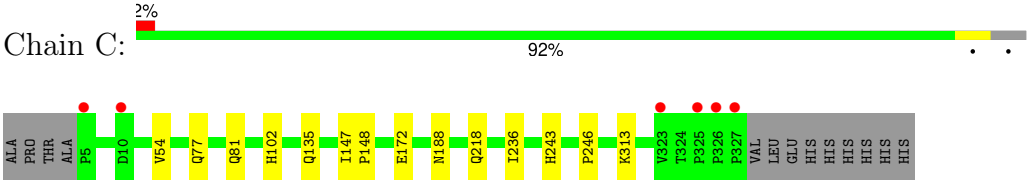
- Molecule 1: Chitinase

Chain B:



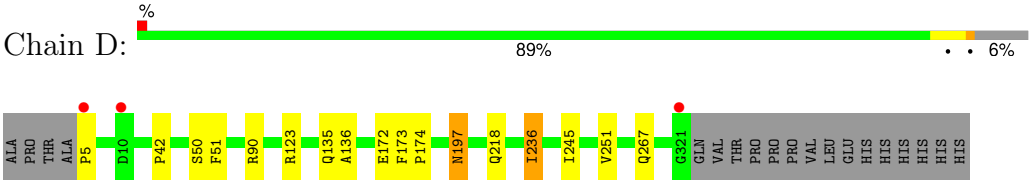
- Molecule 1: Chitinase

Chain C:



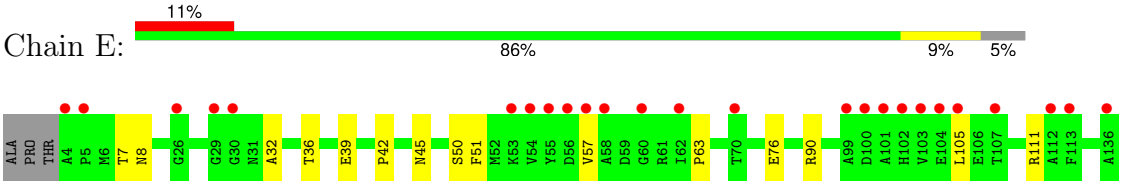
- Molecule 1: Chitinase

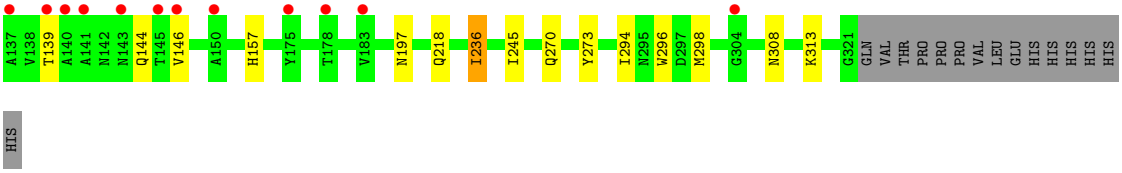
Chain D:



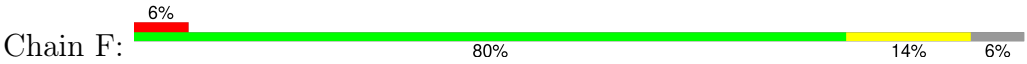
- Molecule 1: Chitinase

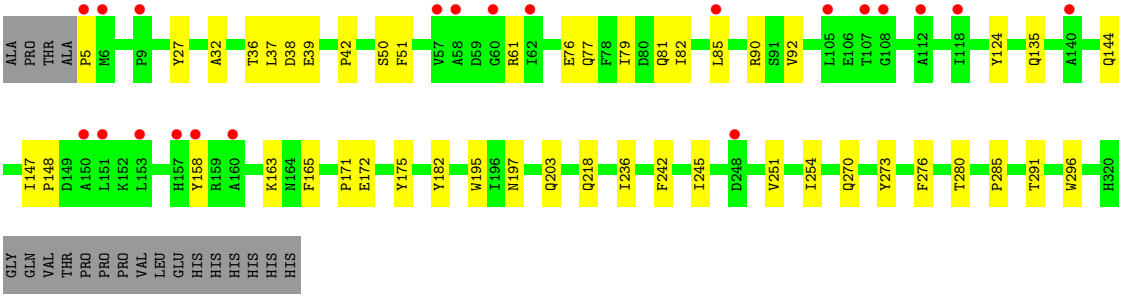
Chain E:





• Molecule 1: Chitinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.92Å 154.03Å 156.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 1.80 49.44 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.44-1.80) 100.0 (49.44-1.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.169 , 0.210 0.167 , 0.209	Depositor DCC
R_{free} test set	12204 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17698	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: PEG, SO4, EDO

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	0/2598	0.69	0/3539
1	B	0.61	0/2608	0.71	0/3554
1	C	0.62	0/2637	0.70	0/3596
1	D	0.56	0/2606	0.65	0/3550
1	E	0.44	0/2569	0.59	0/3501
1	F	0.39	0/2569	0.52	0/3500
All	All	0.55	0/15587	0.65	0/21240

There are no bond length outliers.

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	2531	0	2365	9	0
1	B	2538	0	2372	8	0
1	C	2567	0	2409	10	0
1	D	2536	0	2369	12	0
1	E	2502	0	2351	16	0
1	F	2502	0	2351	36	0
2	A	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	18	1	0
2	C	20	0	30	0	0
2	D	16	0	24	0	0
2	E	4	0	6	1	0
2	F	12	0	18	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	A	7	0	10	2	0
4	B	7	0	10	0	0
4	C	7	0	10	1	0
5	A	519	0	0	4	0
5	B	498	0	0	3	0
5	C	531	0	0	4	0
5	D	468	0	0	4	0
5	E	231	0	0	0	0
5	F	153	0	0	0	0
All	All	17698	0	14361	91	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 (91) 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:F:280:THR:HG22	1:F:285:PRO:HB3	1.49	0.94
1:F:5:PRO:HG2	1:F:158:TYR:CG	2.21	0.75
1:D:123:ARG:HD2	5:D:811:HOH:O	1.95	0.66
1:F:5:PRO:HG3	1:F:165:PHE:HD1	1.59	0.65
1:F:79:ILE:HG12	1:F:124:TYR:HA	1.81	0.63
1:C:135[A]:GLN:HG3	5:C:719:HOH:O	1.98	0.62
1:F:135:GLN:HG2	1:F:175:TYR:CE1	2.35	0.61
1:E:157:HIS:ND1	2:E:402:EDO:H21	2.17	0.59
1:F:61:ARG:HH12	2:F:403:EDO:H22	1.68	0.57
1:F:77:GLN:O	1:F:81:GLN:HG2	2.04	0.57
1:F:37:LEU:HB2	1:F:81:GLN:HB3	1.88	0.56
1:F:280:THR:HG22	1:F:285:PRO:CB	2.31	0.56
1:C:188:ASN:HB2	5:C:861:HOH:O	2.08	0.53
1:F:5:PRO:HB2	1:F:163:LYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:HG3	5:A:903:HOH:O	2.09	0.52
2:B:402:EDO:H11	5:B:685:HOH:O	2.09	0.52
1:E:139:THR:HA	1:E:144:GLN:HE21	1.75	0.52
1:E:294:ILE:O	1:E:298:MET:HG3	2.10	0.51
1:B:236:ILE:HA	1:B:245:ILE:O	2.11	0.51
1:F:195:TRP:HE1	1:F:197:ASN:ND2	2.08	0.50
1:C:135[B]:GLN:HG2	5:C:513:HOH:O	2.10	0.50
1:F:197:ASN:HA	1:F:251:VAL:O	2.12	0.50
1:D:135[B]:GLN:HG3	1:D:136:ALA:N	2.26	0.49
1:A:246:PRO:HB3	4:A:404:PEG:H11	1.94	0.49
1:E:63:PRO:HD3	1:E:105:LEU:HD21	1.94	0.49
1:A:135[A]:GLN:HG3	5:A:816:HOH:O	2.13	0.48
1:E:36:THR:OG1	1:E:39:GLU:HG3	2.14	0.48
1:D:267:GLN:HG3	5:D:860:HOH:O	2.14	0.47
1:A:195:TRP:HE1	1:A:197:ASN:HD22	1.63	0.47
1:B:135[A]:GLN:HG3	5:B:769:HOH:O	2.15	0.47
1:F:197:ASN:HB3	1:F:251:VAL:HB	1.96	0.47
1:E:7:THR:C	1:E:8:ASN:HD22	2.22	0.47
1:F:42:PRO:HA	1:F:90:ARG:CZ	2.44	0.47
1:E:105:LEU:HB3	1:E:146:VAL:HG11	1.96	0.46
1:D:135[A]:GLN:HG3	5:D:837:HOH:O	2.14	0.46
1:F:195:TRP:HE1	1:F:197:ASN:HD22	1.63	0.46
1:D:236:ILE:HA	1:D:245:ILE:O	2.15	0.46
1:D:42:PRO:HA	1:D:90:ARG:CZ	2.46	0.46
1:D:172[B]:GLU:H	1:D:172[B]:GLU:CD	2.23	0.46
1:D:173:PHE:CD2	1:D:174:PRO:HD3	2.51	0.46
1:B:123:ARG:CZ	1:E:76:GLU:HB3	2.46	0.45
1:F:171:PRO:HB3	1:F:182:TYR:CD2	2.52	0.45
2:A:401:EDO:H11	5:A:939:HOH:O	2.17	0.45
1:F:36:THR:OG1	1:F:39:GLU:HG3	2.17	0.45
1:B:161:GLU:OE1	1:B:163:LYS:HE2	2.17	0.45
1:F:50:SER:HA	1:F:51:PHE:HA	1.69	0.44
1:F:276:PHE:O	1:F:280:THR:HG23	2.17	0.44
1:F:32:ALA:HB2	1:F:296:TRP:CE2	2.52	0.44
1:F:82:ILE:HG12	1:F:92:VAL:HG11	1.99	0.44
1:C:135[A]:GLN:HG2	1:C:172:GLU:OE1	2.18	0.44
1:E:236:ILE:HA	1:E:245:ILE:O	2.17	0.44
1:E:270:GLN:HA	1:E:273:TYR:CD2	2.52	0.44
1:E:308:ASN:O	1:E:313:LYS:NZ	2.50	0.43
1:E:50:SER:HA	1:E:51:PHE:HA	1.68	0.43
1:F:242:PHE:CZ	2:F:402:EDO:H21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ARG:O	1:E:111:ARG:HD3	2.19	0.43
1:C:313:LYS:HD2	1:F:27:TYR:CZ	2.54	0.43
1:C:54:VAL:HB	1:C:102:HIS:HB2	2.01	0.43
1:D:5:PRO:HD3	5:D:785:HOH:O	2.19	0.43
1:A:76[B]:GLU:HG3	5:A:546:HOH:O	2.18	0.43
1:F:144:GLN:O	1:F:148:PRO:HG2	2.19	0.42
1:A:236:ILE:HD12	1:A:284:GLN:HB3	2.01	0.42
1:C:147:ILE:HB	1:C:148:PRO:HD3	2.01	0.42
1:F:172:GLU:HG2	1:F:203:GLN:OE1	2.19	0.42
1:F:5:PRO:HB3	1:F:165:PHE:HA	2.00	0.42
1:F:76:GLU:H	1:F:76:GLU:CD	2.26	0.42
1:F:254:ILE:O	1:F:291:THR:HA	2.19	0.42
1:A:244:LYS:NZ	4:A:404:PEG:H22	2.34	0.42
1:B:50:SER:HA	1:B:51:PHE:HA	1.88	0.42
1:E:45:ASN:HA	1:E:90:ARG:HG2	2.01	0.42
1:F:5:PRO:HB3	1:F:165:PHE:CA	2.50	0.42
1:E:32:ALA:HB2	1:E:296:TRP:CD2	2.53	0.42
1:D:135[A]:GLN:HG2	1:D:172[A]:GLU:CD	2.45	0.41
1:E:42:PRO:HA	1:E:90:ARG:CZ	2.50	0.41
1:B:5:PRO:HD2	5:B:606:HOH:O	2.19	0.41
1:F:32:ALA:HB2	1:F:296:TRP:CD2	2.55	0.41
1:C:246:PRO:HB3	4:C:402:PEG:H42	2.01	0.41
1:D:197:ASN:HA	1:D:251:VAL:O	2.21	0.41
1:F:5:PRO:HG2	1:F:158:TYR:CD1	2.53	0.41
1:B:28:GLN:O	1:B:302:LYS:HE3	2.20	0.41
1:A:135[A]:GLN:HG2	1:A:172:GLU:OE1	2.21	0.41
1:B:42:PRO:HA	1:B:90:ARG:CZ	2.51	0.41
1:C:77:GLN:O	1:C:81:GLN:HG3	2.21	0.41
1:C:243:HIS:HD2	5:C:670:HOH:O	2.03	0.41
1:D:50:SER:HA	1:D:51:PHE:HA	1.77	0.41
1:A:7:THR:C	1:A:8:ASN:HD22	2.29	0.40
1:F:147:ILE:HB	1:F:148:PRO:HD3	2.02	0.40
1:F:270:GLN:HA	1:F:273:TYR:CD2	2.56	0.40
1:F:38:ASP:CG	1:F:81:GLN:HE22	2.30	0.40
1:F:236:ILE:HA	1:F:245:ILE:O	2.21	0.40
1:F:135:GLN:HG3	1:F:172:GLU:CD	2.46	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	319/336 (95%)	312 (98%)	7 (2%)	0	100	100
1	B	321/336 (96%)	311 (97%)	10 (3%)	0	100	100
1	C	324/336 (96%)	316 (98%)	8 (2%)	0	100	100
1	D	320/336 (95%)	312 (98%)	8 (2%)	0	100	100
1	E	316/336 (94%)	309 (98%)	7 (2%)	0	100	100
1	F	315/336 (94%)	304 (96%)	11 (4%)	0	100	100
All	All	1915/2016 (95%)	1864 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/280 (95%)	266 (100%)	1 (0%)	89	88
1	B	268/280 (96%)	266 (99%)	2 (1%)	81	79
1	C	272/280 (97%)	270 (99%)	2 (1%)	81	79
1	D	268/280 (96%)	265 (99%)	3 (1%)	70	65
1	E	263/280 (94%)	259 (98%)	4 (2%)	60	53
1	F	264/280 (94%)	262 (99%)	2 (1%)	79	76
All	All	1602/1680 (95%)	1588 (99%)	14 (1%)	75	72

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
1	B	197	ASN
1	B	218	GLN
1	C	218	GLN
1	C	236	ILE
1	D	197	ASN
1	D	218	GLN
1	D	236	ILE
1	E	57	VAL
1	E	197	ASN
1	E	218	GLN
1	E	236	ILE
1	F	85	LEU
1	F	218	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	197	ASN
1	A	267	GLN
1	A	310	GLN
1	B	203	GLN
1	B	237	ASN
1	B	282	GLN
1	B	284	GLN
1	C	197	ASN
1	C	237	ASN
1	C	270	GLN
1	C	282	GLN
1	C	284	GLN
1	C	306	GLN
1	D	237	ASN
1	D	282	GLN
1	D	284	GLN
1	D	310	GLN
1	E	144	GLN
1	E	243	HIS
1	F	28	GLN
1	F	144	GLN
1	F	197	ASN

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Mol	Chain	Res	Type
1	F	237	ASN
1	F	267	GLN
1	F	282	GLN
1	F	284	GLN
1	F	310	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	C	407	-	3,3,3	0.28	0	2,2,2	0.37	0
3	SO4	D	402	-	4,4,4	0.66	0	6,6,6	0.26	0
3	SO4	C	401	-	4,4,4	0.73	0	6,6,6	0.46	0
2	EDO	C	404	-	3,3,3	0.26	0	2,2,2	0.40	0
2	EDO	F	401	-	3,3,3	0.27	0	2,2,2	0.39	0
2	EDO	B	404	-	3,3,3	0.32	0	2,2,2	0.19	0
2	EDO	D	404	-	3,3,3	0.25	0	2,2,2	0.62	0
4	PEG	C	402	-	6,6,6	0.49	0	5,5,5	1.95	2 (40%)
2	EDO	C	405	-	3,3,3	0.29	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	D	405	-	3,3,3	0.27	0	2,2,2	0.47	0
4	PEG	B	403	-	6,6,6	0.45	0	5,5,5	1.55	1 (20%)
3	SO4	A	402	-	4,4,4	0.75	0	6,6,6	0.29	0
2	EDO	E	402	-	3,3,3	0.21	0	2,2,2	0.48	0
3	SO4	B	401	-	4,4,4	0.74	0	6,6,6	0.25	0
2	EDO	A	405	-	3,3,3	0.32	0	2,2,2	0.19	0
2	EDO	C	406	-	3,3,3	0.16	0	2,2,2	0.89	0
2	EDO	C	403	-	3,3,3	0.24	0	2,2,2	0.72	0
2	EDO	F	402	-	3,3,3	0.24	0	2,2,2	0.31	0
2	EDO	B	405	-	3,3,3	0.32	0	2,2,2	0.25	0
2	EDO	A	403	-	3,3,3	0.30	0	2,2,2	0.20	0
3	SO4	E	401	-	4,4,4	0.72	0	6,6,6	0.24	0
2	EDO	D	403	-	3,3,3	0.28	0	2,2,2	0.14	0
2	EDO	B	402	-	3,3,3	0.14	0	2,2,2	0.67	0
4	PEG	A	404	-	6,6,6	0.42	0	5,5,5	1.80	2 (40%)
2	EDO	D	401	-	3,3,3	0.40	0	2,2,2	1.73	0
2	EDO	A	401	-	3,3,3	0.26	0	2,2,2	0.96	0
2	EDO	F	403	-	3,3,3	0.27	0	2,2,2	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	407	-	-	0/1/1/1	-
2	EDO	C	404	-	-	1/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-
2	EDO	B	404	-	-	1/1/1/1	-
2	EDO	D	404	-	-	0/1/1/1	-
4	PEG	C	402	-	-	1/4/4/4	-
2	EDO	C	405	-	-	0/1/1/1	-
2	EDO	D	405	-	-	1/1/1/1	-
4	PEG	B	403	-	-	3/4/4/4	-
2	EDO	E	402	-	-	1/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
2	EDO	C	406	-	-	0/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	F	402	-	-	0/1/1/1	-
2	EDO	B	405	-	-	1/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	D	403	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	402	-	-	0/1/1/1	-
4	PEG	A	404	-	-	3/4/4/4	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	F	403	-	-	1/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	402	PEG	O2-C2-C1	-3.24	95.86	110.11
4	A	404	PEG	O4-C4-C3	-2.93	94.59	111.82
4	C	402	PEG	O1-C1-C2	-2.88	94.90	111.82
4	A	404	PEG	O2-C3-C4	-2.72	98.14	110.11
4	B	403	PEG	O1-C1-C2	-2.56	96.77	111.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	PEG	O1-C1-C2-O2
2	B	405	EDO	O1-C1-C2-O2
4	A	404	PEG	C4-C3-O2-C2
4	A	404	PEG	O2-C3-C4-O4
4	B	403	PEG	C4-C3-O2-C2
2	D	405	EDO	O1-C1-C2-O2
2	E	402	EDO	O1-C1-C2-O2
4	C	402	PEG	C4-C3-O2-C2
4	B	403	PEG	O2-C3-C4-O4
2	A	401	EDO	O1-C1-C2-O2
4	B	403	PEG	C1-C2-O2-C3
2	C	404	EDO	O1-C1-C2-O2
2	C	403	EDO	O1-C1-C2-O2
2	F	403	EDO	O1-C1-C2-O2
2	B	404	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	PEG	1	0
2	E	402	EDO	1	0
2	F	402	EDO	1	0
2	B	402	EDO	1	0
4	A	404	PEG	2	0
2	A	401	EDO	1	0
2	F	403	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	317/336 (94%)	-0.84	3 (0%) 81 80	11, 18, 32, 71	4 (1%)
1	B	318/336 (94%)	-0.84	2 (0%) 85 85	10, 18, 32, 65	5 (1%)
1	C	323/336 (96%)	-0.84	6 (1%) 66 64	10, 17, 35, 81	3 (0%)
1	D	317/336 (94%)	-0.66	3 (0%) 81 80	12, 22, 41, 85	5 (1%)
1	E	318/336 (94%)	0.68	37 (11%) 11 9	23, 38, 69, 90	0
1	F	316/336 (94%)	0.68	21 (6%) 26 22	21, 46, 73, 94	1 (0%)
All	All	1909/2016 (94%)	-0.30	72 (3%) 44 42	10, 23, 62, 94	18 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	PRO	5.1
1	C	5	PRO	5.0
1	E	4	ALA	4.8
1	E	146	VAL	4.4
1	B	4	ALA	4.3
1	A	321	GLY	4.0
1	E	54	VAL	3.9
1	E	60	GLY	3.9
1	A	5	PRO	3.9
1	E	105	LEU	3.7
1	E	141	ALA	3.6
1	E	57	VAL	3.6
1	E	5	PRO	3.5
1	E	29	GLY	3.4
1	E	137	ALA	3.4
1	F	57	VAL	3.3
1	C	327	PRO	3.3
1	E	30	GLY	3.2
1	E	103	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	326	PRO	3.1
1	E	99	ALA	3.1
1	E	101	ALA	3.1
1	F	118	ILE	3.0
1	E	26	GLY	2.9
1	E	70	THR	2.9
1	E	100	ASP	2.8
1	F	5	PRO	2.8
1	F	9	PRO	2.8
1	E	136	ALA	2.8
1	E	183	VAL	2.8
1	E	145	THR	2.8
1	E	58	ALA	2.8
1	F	85	LEU	2.7
1	E	102	HIS	2.7
1	F	153	LEU	2.7
1	E	150	ALA	2.6
1	A	10	ASP	2.6
1	F	107	THR	2.5
1	F	160	ALA	2.5
1	E	140	ALA	2.5
1	C	325	PRO	2.5
1	D	10	ASP	2.5
1	F	58	ALA	2.5
1	F	150	ALA	2.5
1	F	140	ALA	2.4
1	B	5	PRO	2.4
1	E	107	THR	2.4
1	E	139	THR	2.4
1	F	158	TYR	2.4
1	E	178	THR	2.3
1	E	53	LYS	2.3
1	C	10	ASP	2.3
1	F	62	ILE	2.2
1	E	304	GLY	2.2
1	F	248	ASP	2.2
1	F	6	MET	2.2
1	E	113	PHE	2.2
1	F	60	GLY	2.2
1	F	151	LEU	2.2
1	E	55	TYR	2.2
1	E	104	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	108	GLY	2.1
1	E	62	ILE	2.1
1	D	321	GLY	2.1
1	F	112	ALA	2.1
1	F	157	HIS	2.1
1	E	112	ALA	2.1
1	F	105	LEU	2.1
1	E	56	ASP	2.0
1	C	323	VAL	2.0
1	E	143	ASN	2.0
1	E	175	TYR	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
2	EDO	F	403	4/4	0.70	0.16	70,71,73,75	0
2	EDO	E	402	4/4	0.79	0.17	38,48,56,66	0
2	EDO	F	401	4/4	0.82	0.16	42,49,52,55	0
2	EDO	C	404	4/4	0.83	0.15	45,55,60,61	0
2	EDO	B	405	4/4	0.89	0.14	34,40,48,53	0
2	EDO	A	401	4/4	0.89	0.13	23,32,36,43	0
2	EDO	D	401	4/4	0.89	0.17	25,25,34,49	0
3	SO4	E	401	5/5	0.89	0.09	39,61,79,80	0
4	PEG	A	404	7/7	0.89	0.14	23,29,42,49	0
4	PEG	C	402	7/7	0.89	0.14	22,29,38,50	0
2	EDO	B	402	4/4	0.90	0.10	24,31,33,44	0
4	PEG	B	403	7/7	0.90	0.13	25,30,43,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	C	403	4/4	0.90	0.12	34,40,52,55	0
2	EDO	F	402	4/4	0.91	0.16	38,39,44,50	0
2	EDO	D	404	4/4	0.91	0.14	28,29,34,44	0
2	EDO	D	405	4/4	0.93	0.10	29,33,37,45	0
2	EDO	C	406	4/4	0.94	0.09	25,28,40,42	0
2	EDO	B	404	4/4	0.95	0.14	26,27,35,44	0
2	EDO	A	405	4/4	0.95	0.08	27,29,33,44	0
2	EDO	C	407	4/4	0.96	0.10	25,28,31,44	0
2	EDO	C	405	4/4	0.97	0.06	19,20,20,22	0
3	SO4	B	401	5/5	0.97	0.12	29,34,37,42	0
3	SO4	D	402	5/5	0.98	0.04	35,36,44,51	0
2	EDO	D	403	4/4	0.98	0.04	17,20,21,27	0
3	SO4	A	402	5/5	0.98	0.09	32,35,41,46	0
2	EDO	A	403	4/4	0.98	0.06	21,22,31,46	0
3	SO4	C	401	5/5	0.98	0.09	29,32,39,41	0

6.5 Other polymers (i)

There are no such residues in this entry.