Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 08:27 AM EDT

PDB ID	:	6TGF
Title	:	Pantoea stewartii WceF is a glycan biofilm modifying enzyme with a bacteriophage tailspike-like parallel beta-helix fold
Authors	:	Irmscher, T.; Roske, Y.; Gayk, I.; Heinemann, U.; Barbirz, S.
Deposited on	:	2019-11-15
Resolution	:	2.55 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 (i)) were used in the production of this report:

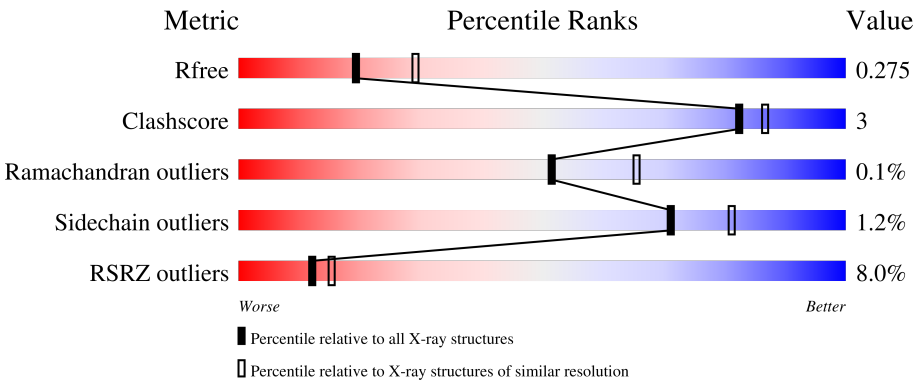
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	D	736	4% 86% 7% 7%
1	E	736	13% 85% 6% • 9%
1	F	736	5% 86% 6% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	D	805	-	-	-	X
3	EDO	D	814	-	-	-	X
3	EDO	F	805	-	-	-	X

2 Entry composition (i)

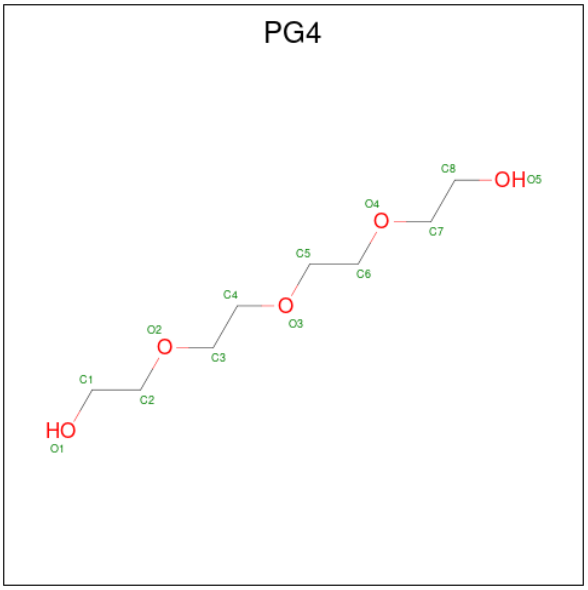
There are 4 unique types of molecules in this entry. The entry contains 16651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Exopolysaccharide biosynthesis protein.

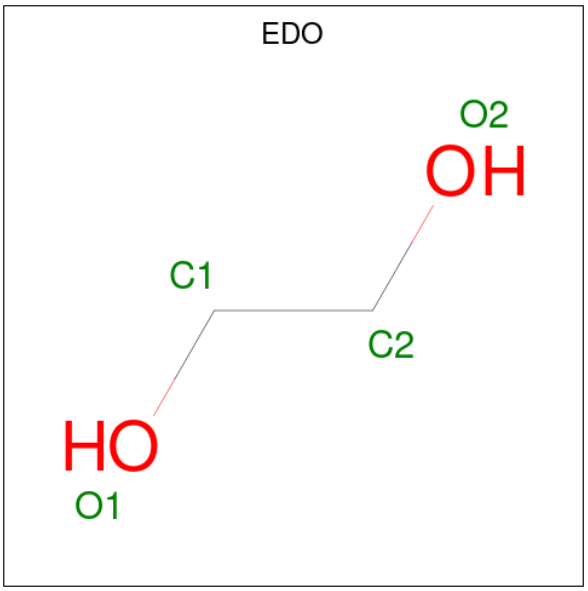
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	682	5295	3329	939	1008	19	0	2	0
1	D	687	5318	3345	941	1013	19	0	0	0
1	E	673	5226	3286	926	995	19	0	1	0

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	F	1	13	8	5	0	0
2	D	1	13	8	5	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

- Molecule 4 is water.

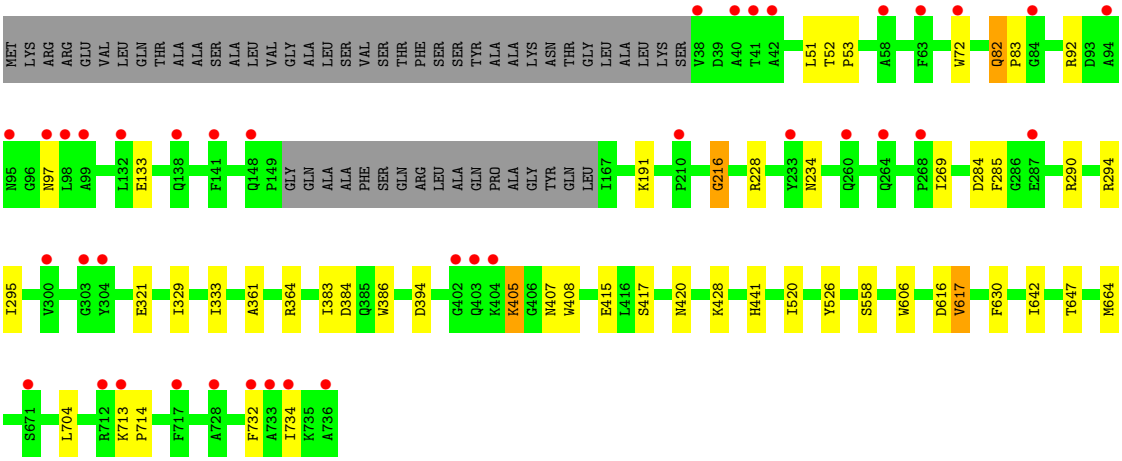
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	F	216	216	216	0	0
			Total	O		
4	D	214	214	214	0	0
			Total	O		
4	E	188	188	188	0	0

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.

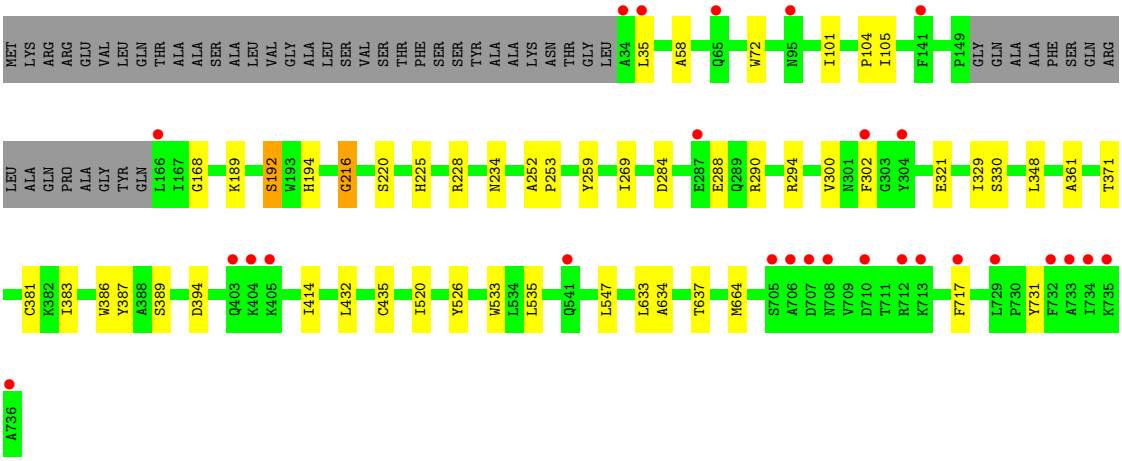
• Molecule 1: Exopolysaccharide biosynthesis protein

Chain F:



• Molecule 1: Exopolysaccharide biosynthesis protein

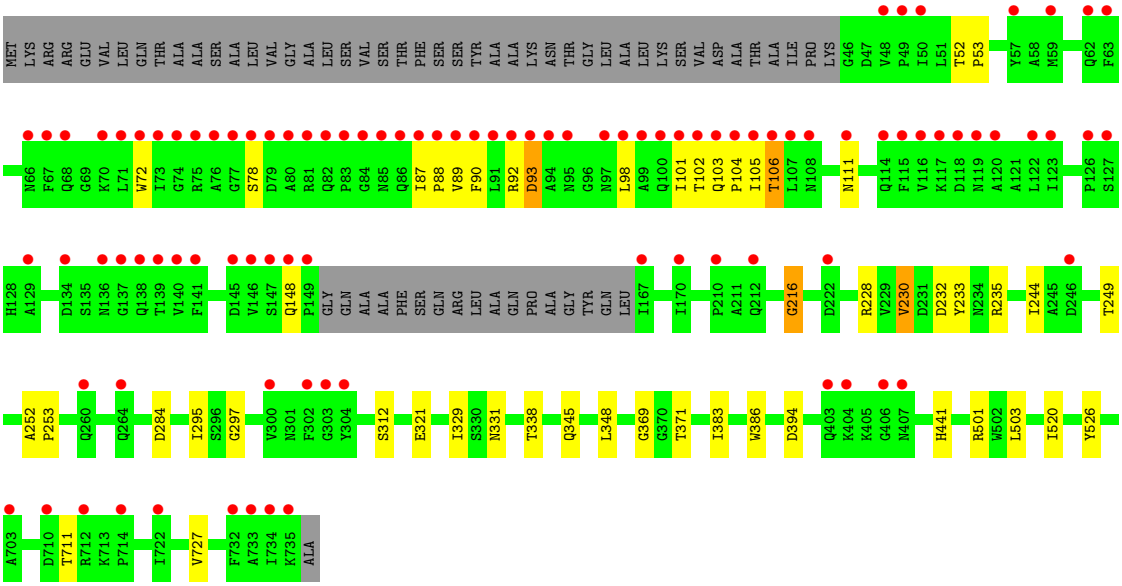
Chain D:



• Molecule 1: Exopolysaccharide biosynthesis protein

Chain E:

13%
85%
6%
9%


MET LYS ARG ARG GLU VAL LEU GLN THR ALA ALA SER ALA LEU VAL GLY ALA LEU SER VAL SER THR PHE SER SER TYR ALA ALA LYS ASN THR GLY LEU ALA LEU LYS SER VAL ASP ALA THR ALA ILE PRO LYS G46 D47 V48 P49 I50 L51 T52 P53 Y57 A58 M59 Q62 F63
N66 F67 Q68 G69 K70 L71 W72 I73 G74 R75 A76 G77 S78 D79 A80 R81 Q82 P83 G84 N85 Q86 I87 P88 V89 F90 L91 R92 D93 A94 N95 G96 N97 L98 A99 Q100 I101 T102 Q103 P104 I105 T106 L107 N108 N111 Q114 F115 V116 K117 D118 N119 A120 A121 L122 I123 P126 S127
H128 A129 D134 S135 N136 G137 Q138 T139 V140 F141 D145 V146 S147 Q148 P149 GLY GLN ALA ALA PHE SER GLN ARG LEU ALA GLN PRO ALA GLY TYR GLN LEU I167 I170 P210 A211 Q212 G216 D222 R228 V229 V230 D231 D232 Y233 N234 R235 I244 A245 D246 T249
A252 P253 Q260 Q264 D284 I295 S296 G297 V300 N301 F302 G303 Y304 S312 E321 I329 S330 N331 T338 Q345 L348 G369 G370 T371 I383 W386 D394 Q403 K404 K405 G406 N407 H441 R501 W502 L503 I520 Y526
A703 D710 T711 R712 K713 P714 I722 V727 F732 A733 I734 K735 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.18Å 97.20Å 128.95Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	48.60 – 2.55 48.60 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.60-2.55) 96.5 (48.60-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.227 , 0.273 0.228 , 0.275	Depositor DCC
R_{free} test set	2101 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16651	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 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	D	0.64	0/5449	0.71	0/7403
1	E	0.65	0/5359	0.71	0/7281
1	F	0.64	0/5432	0.71	0/7380
All	All	0.64	0/16240	0.71	0/22064

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 (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	D	5318	0	5118	31	0
1	E	5226	0	5015	25	0
1	F	5295	0	5092	30	0
2	D	13	0	18	0	0
2	F	13	0	18	1	0
3	D	64	0	96	2	0
3	E	32	0	48	0	0
3	F	72	0	105	1	0
4	D	214	0	0	0	0
4	E	188	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	216	0	0	0	0
All	All	16651	0	15510	80	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 (80) 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:E:338:THR:HG21	1:E:369:GLY:HA3	1.69	0.75
1:F:558:SER:H	1:F:647:THR:HG22	1.52	0.74
1:D:58:ALA:O	1:D:168:GLY:HA3	1.94	0.66
1:E:338:THR:HG21	1:E:369:GLY:CA	2.28	0.63
1:E:216:GLY:O	1:E:228:ARG:NH1	2.34	0.59
1:F:732:PHE:CD1	1:D:717:PHE:HE2	2.21	0.58
1:F:269:ILE:O	1:F:294:ARG:NH1	2.37	0.58
1:D:192:SER:OG	1:D:194:HIS:O	2.22	0.57
1:F:617:VAL:HG23	1:F:630:PHE:O	2.05	0.56
1:F:216:GLY:O	1:F:228:ARG:NH1	2.38	0.55
1:D:535:LEU:HD21	1:D:664:MET:HG3	1.89	0.54
1:D:731:TYR:HB2	1:E:727:VAL:CG1	2.37	0.54
1:D:387:TYR:HB3	3:D:815:EDO:H22	1.90	0.54
1:D:234:ASN:HA	1:D:269:ILE:HD12	1.90	0.53
1:E:329:ILE:HD11	1:E:348:LEU:HD13	1.89	0.53
1:D:533:TRP:HB3	1:D:664:MET:HG2	1.90	0.53
1:E:230:VAL:HG21	1:E:233:TYR:CE1	2.45	0.51
1:F:606:TRP:CD1	1:F:617:VAL:CG1	2.94	0.51
1:D:101:ILE:HD13	1:D:105:ILE:HG12	1.93	0.51
1:D:381:CYS:HB3	1:D:414:ILE:HD13	1.93	0.50
1:D:72:TRP:CE2	1:D:104:PRO:HB3	2.46	0.50
1:D:389:SER:HB2	3:D:815:EDO:H21	1.92	0.50
1:F:92:ARG:HA	1:F:97:ASN:O	2.12	0.50
1:D:383:ILE:HG22	1:D:386:TRP:CD1	2.46	0.49
1:D:329:ILE:HD11	1:D:348:LEU:HD13	1.95	0.49
1:E:383:ILE:HG22	1:E:386:TRP:CD1	2.48	0.49
1:E:101:ILE:HD12	1:E:105:ILE:HD12	1.95	0.48
1:D:216:GLY:O	1:D:228:ARG:NH1	2.47	0.48
1:F:520:ILE:O	1:D:526:TYR:HA	2.14	0.47
1:E:501:ARG:HD2	1:E:503:LEU:O	2.13	0.47
1:F:526:TYR:HA	1:E:520:ILE:O	2.15	0.46
1:D:633:LEU:HG	1:D:637:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:VAL:HB	1:D:302:PHE:CE2	2.49	0.46
1:D:520:ILE:O	1:E:526:TYR:HA	2.16	0.46
1:F:642:ILE:HG13	1:F:664:MET:HE1	1.98	0.46
1:E:244:ILE:HD12	1:E:249:THR:HG21	1.98	0.46
1:D:259:TYR:OH	1:D:290:ARG:HD2	2.16	0.45
1:F:405:LYS:C	1:F:407:ASN:H	2.19	0.45
1:F:333:ILE:HG12	1:F:364:ARG:HB2	2.00	0.44
1:F:295:ILE:O	1:F:329:ILE:HA	2.18	0.44
1:F:394:ASP:HA	1:F:428:LYS:O	2.18	0.44
1:D:220:SER:HA	1:D:225:HIS:HA	1.99	0.44
1:D:633:LEU:HG	1:D:637:THR:CG2	2.48	0.44
1:D:330:SER:HA	1:D:361:ALA:O	2.17	0.44
1:F:234:ASN:HA	1:F:269:ILE:HD12	2.00	0.43
1:F:714:PRO:N	1:F:732:PHE:CE2	2.87	0.43
1:E:252:ALA:N	1:E:253:PRO:CD	2.81	0.43
1:D:634:ALA:O	1:D:637:THR:HG22	2.19	0.43
1:D:371:THR:HA	1:D:394:ASP:O	2.18	0.43
1:F:415:GLU:OE2	1:E:441:HIS:NE2	2.45	0.43
1:F:713:LYS:C	1:F:732:PHE:CE2	2.93	0.43
1:F:72:TRP:HZ3	1:F:133:GLU:HG2	1.83	0.43
1:E:232:ASP:HB3	1:E:235:ARG:HG3	2.00	0.42
1:E:72:TRP:CE2	1:E:104:PRO:HB3	2.55	0.42
1:F:52:THR:HB	1:F:53:PRO:HD2	2.01	0.42
1:F:82:GLN:HG3	1:F:83:PRO:HD2	2.01	0.42
1:E:93:ASP:N	1:E:93:ASP:OD1	2.52	0.42
1:D:269:ILE:O	1:D:294:ARG:NH1	2.52	0.42
1:E:87:ILE:HB	1:E:88:PRO:HD2	2.02	0.41
1:E:103:GLN:HA	1:E:104:PRO:C	2.40	0.41
1:F:361:ALA:HA	1:F:384:ASP:O	2.20	0.41
1:F:417:SER:HA	1:F:441:HIS:O	2.20	0.41
1:E:297:GLY:HA3	1:E:331:ASN:O	2.21	0.41
1:F:383:ILE:HG22	1:F:386:TRP:CD1	2.56	0.41
1:D:547:LEU:O	1:D:664:MET:HE1	2.21	0.41
1:F:704:LEU:HD21	1:F:734:ILE:CD1	2.51	0.41
1:D:252:ALA:HB3	1:D:253:PRO:HD3	2.03	0.41
1:F:405:LYS:O	1:F:408:TRP:CD1	2.74	0.41
1:F:420:ASN:HD21	3:F:809:EDO:H11	1.86	0.41
1:D:284:ASP:HA	1:D:321:GLU:HB2	2.02	0.41
1:E:52:THR:HB	1:E:53:PRO:HD2	2.03	0.41
1:E:284:ASP:HA	1:E:321:GLU:HB2	2.03	0.41
1:F:51:LEU:HD13	2:F:801:PG4:H41	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:THR:HA	1:E:394:ASP:O	2.21	0.40
1:F:285:PHE:O	1:F:290:ARG:NH1	2.51	0.40
1:D:432:LEU:HB3	1:D:435:CYS:SG	2.61	0.40
1:E:106:THR:O	1:E:111:ASN:ND2	2.52	0.40
1:D:414:ILE:HG13	1:D:435:CYS:SG	2.61	0.40
1:F:284:ASP:HA	1:F:321:GLU:HB2	2.04	0.40
1:E:312:SER:HB3	1:E:345:GLN:OE1	2.21	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	D	683/736 (93%)	648 (95%)	34 (5%)	1 (0%)	51	65
1	E	670/736 (91%)	629 (94%)	40 (6%)	1 (0%)	51	65
1	F	680/736 (92%)	647 (95%)	32 (5%)	1 (0%)	51	65
All	All	2033/2208 (92%)	1924 (95%)	106 (5%)	3 (0%)	51	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	216	GLY
1	E	216	GLY
1	F	216	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	565/600 (94%)	561 (99%)	4 (1%)	84	90
1	E	556/600 (93%)	544 (98%)	12 (2%)	52	66
1	F	563/600 (94%)	558 (99%)	5 (1%)	78	86
All	All	1684/1800 (94%)	1663 (99%)	21 (1%)	71	81

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	82	GLN
1	F	191	LYS
1	F	405	LYS
1	F	616	ASP
1	F	617	VAL
1	D	35	LEU
1	D	189	LYS
1	D	192	SER
1	D	288	GLU
1	E	78	SER
1	E	89	VAL
1	E	90	PHE
1	E	92	ARG
1	E	93	ASP
1	E	98	LEU
1	E	102	THR
1	E	106	THR
1	E	148	GLN
1	E	230	VAL
1	E	295	ILE
1	E	711	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	450	ASN
1	F	628	GLN
1	D	264	GLN
1	D	301	ASN
1	D	422	GLN

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Mol	Chain	Res	Type
1	E	264	GLN
1	E	337	ASN
1	E	367	ASN
1	E	450	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)

44 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	$\#\|Z\| > 2$
3	EDO	D	815	-	3,3,3	0.05	0	2,2,2	0.13	0
2	PG4	F	801	-	12,12,12	0.18	0	11,11,11	0.12	0
3	EDO	E	805	-	3,3,3	0.07	0	2,2,2	0.12	0
3	EDO	F	809	-	3,3,3	0.05	0	2,2,2	0.12	0
3	EDO	F	810	-	3,3,3	0.06	0	2,2,2	0.16	0
3	EDO	D	805	-	3,3,3	0.08	0	2,2,2	0.21	0
3	EDO	F	816	-	3,3,3	0.07	0	2,2,2	0.20	0
2	PG4	D	801	-	12,12,12	0.18	0	11,11,11	0.11	0
3	EDO	F	805	-	3,3,3	0.06	0	2,2,2	0.15	0
3	EDO	F	817	-	3,3,3	0.07	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	F	803	3	3,3,3	0.17	0	2,2,2	0.10	0
3	EDO	F	802	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	F	819	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	E	807	-	3,3,3	0.06	0	2,2,2	0.14	0
3	EDO	E	803	-	3,3,3	0.09	0	2,2,2	0.23	0
3	EDO	E	806	-	3,3,3	0.08	0	2,2,2	0.17	0
3	EDO	D	806	-	3,3,3	0.07	0	2,2,2	0.16	0
3	EDO	D	817	-	3,3,3	0.07	0	2,2,2	0.13	0
3	EDO	E	801	-	3,3,3	0.06	0	2,2,2	0.16	0
3	EDO	D	807	-	3,3,3	0.06	0	2,2,2	0.15	0
3	EDO	D	808	-	3,3,3	0.08	0	2,2,2	0.23	0
3	EDO	F	814	-	3,3,3	0.06	0	2,2,2	0.14	0
3	EDO	D	809	-	3,3,3	0.08	0	2,2,2	0.23	0
3	EDO	F	813	-	3,3,3	0.08	0	2,2,2	0.19	0
3	EDO	F	804	3	3,3,3	0.15	0	2,2,2	0.07	0
3	EDO	D	813	-	3,3,3	0.07	0	2,2,2	0.16	0
3	EDO	E	802	-	3,3,3	0.06	0	2,2,2	0.15	0
3	EDO	D	816	-	3,3,3	0.07	0	2,2,2	0.13	0
3	EDO	E	808	-	3,3,3	0.05	0	2,2,2	0.09	0
3	EDO	F	806	-	3,3,3	0.07	0	2,2,2	0.12	0
3	EDO	E	804	-	3,3,3	0.05	0	2,2,2	0.14	0
3	EDO	D	814	-	3,3,3	0.06	0	2,2,2	0.13	0
3	EDO	D	802	-	3,3,3	0.06	0	2,2,2	0.17	0
3	EDO	F	818	-	3,3,3	0.07	0	2,2,2	0.11	0
3	EDO	F	808	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	F	811	-	3,3,3	0.06	0	2,2,2	0.18	0
3	EDO	F	812	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	D	804	-	3,3,3	0.09	0	2,2,2	0.23	0
3	EDO	D	810	-	3,3,3	0.06	0	2,2,2	0.17	0
3	EDO	D	803	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	F	807	-	3,3,3	0.07	0	2,2,2	0.16	0
3	EDO	D	811	-	3,3,3	0.07	0	2,2,2	0.14	0
3	EDO	D	812	-	3,3,3	0.05	0	2,2,2	0.09	0
3	EDO	F	815	-	3,3,3	0.07	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
3	EDO	D	815	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	F	801	-	-	7/10/10/10	-
3	EDO	E	805	-	-	0/1/1/1	-
3	EDO	F	809	-	-	0/1/1/1	-
3	EDO	F	810	-	-	0/1/1/1	-
3	EDO	D	805	-	-	1/1/1/1	-
3	EDO	F	816	-	-	1/1/1/1	-
2	PG4	D	801	-	-	6/10/10/10	-
3	EDO	F	805	-	-	0/1/1/1	-
3	EDO	F	817	-	-	0/1/1/1	-
3	EDO	F	803	3	-	1/1/1/1	-
3	EDO	F	802	-	-	0/1/1/1	-
3	EDO	F	819	-	-	0/1/1/1	-
3	EDO	E	807	-	-	0/1/1/1	-
3	EDO	E	803	-	-	1/1/1/1	-
3	EDO	E	806	-	-	1/1/1/1	-
3	EDO	D	806	-	-	1/1/1/1	-
3	EDO	D	817	-	-	0/1/1/1	-
3	EDO	E	801	-	-	0/1/1/1	-
3	EDO	D	807	-	-	0/1/1/1	-
3	EDO	D	808	-	-	1/1/1/1	-
3	EDO	F	814	-	-	0/1/1/1	-
3	EDO	D	809	-	-	1/1/1/1	-
3	EDO	F	813	-	-	1/1/1/1	-
3	EDO	F	804	3	-	0/1/1/1	-
3	EDO	D	813	-	-	0/1/1/1	-
3	EDO	E	802	-	-	0/1/1/1	-
3	EDO	D	816	-	-	0/1/1/1	-
3	EDO	E	808	-	-	1/1/1/1	-
3	EDO	F	806	-	-	0/1/1/1	-
3	EDO	E	804	-	-	0/1/1/1	-
3	EDO	D	814	-	-	0/1/1/1	-
3	EDO	D	802	-	-	1/1/1/1	-
3	EDO	F	818	-	-	1/1/1/1	-
3	EDO	F	808	-	-	0/1/1/1	-
3	EDO	F	811	-	-	1/1/1/1	-
3	EDO	F	812	-	-	0/1/1/1	-
3	EDO	D	804	-	-	1/1/1/1	-
3	EDO	D	810	-	-	1/1/1/1	-
3	EDO	D	803	-	-	0/1/1/1	-
3	EDO	F	807	-	-	1/1/1/1	-
3	EDO	D	811	-	-	0/1/1/1	-
3	EDO	D	812	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	F	815	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	PG4	O3-C5-C6-O4
2	F	801	PG4	O2-C3-C4-O3
2	F	801	PG4	O3-C5-C6-O4
2	D	801	PG4	O2-C3-C4-O3
2	F	801	PG4	O1-C1-C2-O2
3	D	804	EDO	O1-C1-C2-O2
3	D	805	EDO	O1-C1-C2-O2
3	D	808	EDO	O1-C1-C2-O2
3	E	803	EDO	O1-C1-C2-O2
3	D	809	EDO	O1-C1-C2-O2
2	F	801	PG4	C4-C3-O2-C2
2	D	801	PG4	C3-C4-O3-C5
2	F	801	PG4	C8-C7-O4-C6
2	D	801	PG4	C8-C7-O4-C6
3	F	803	EDO	O1-C1-C2-O2
2	F	801	PG4	C5-C6-O4-C7
2	D	801	PG4	O4-C7-C8-O5
2	F	801	PG4	C3-C4-O3-C5
3	F	813	EDO	O1-C1-C2-O2
3	F	816	EDO	O1-C1-C2-O2
2	D	801	PG4	C4-C3-O2-C2
3	F	811	EDO	O1-C1-C2-O2
3	F	818	EDO	O1-C1-C2-O2
3	D	802	EDO	O1-C1-C2-O2
3	F	815	EDO	O1-C1-C2-O2
3	D	810	EDO	O1-C1-C2-O2
3	E	808	EDO	O1-C1-C2-O2
3	F	807	EDO	O1-C1-C2-O2
3	D	806	EDO	O1-C1-C2-O2
3	E	806	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	815	EDO	2	0
2	F	801	PG4	1	0
3	F	809	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 (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(Å^2)	Q<0.9
1	D	687/736 (93%)	0.38	27 (3%) 39 45	23, 41, 71, 92	0
1	E	673/736 (91%)	0.85	98 (14%) 2 3	20, 49, 120, 143	0
1	F	682/736 (92%)	0.45	38 (5%) 24 29	22, 42, 73, 95	0
All	All	2042/2208 (92%)	0.56	163 (7%) 12 15	20, 43, 92, 143	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	98	LEU	11.4
1	E	77	GLY	10.5
1	E	99	ALA	7.1
1	E	97	ASN	7.0
1	E	74	GLY	6.0
1	E	48	VAL	5.9
1	E	90	PHE	5.7
1	E	115	PHE	5.3
1	E	94	ALA	5.2
1	E	101	ILE	5.2
1	D	35	LEU	5.1
1	E	403	GLN	5.0
1	E	137	GLY	5.0
1	E	92	ARG	4.8
1	E	89	VAL	4.6
1	F	732	PHE	4.4
1	E	59	MET	4.4
1	E	87	ILE	4.4
1	E	105	ILE	4.3
1	E	81	ARG	4.3
1	E	91	LEU	4.2
1	D	141	PHE	4.2
1	F	41	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	139	THR	4.1
1	D	34	ALA	4.1
1	F	97	ASN	4.1
1	D	707	ASP	4.0
1	E	167	ILE	4.0
1	D	403	GLN	4.0
1	E	149	PRO	3.8
1	E	103	GLN	3.8
1	E	100	GLN	3.8
1	D	287	GLU	3.8
1	E	68	GLN	3.6
1	E	83	PRO	3.5
1	E	82	GLN	3.5
1	E	85	ASN	3.5
1	E	95	ASN	3.5
1	E	127	SER	3.5
1	E	67	PHE	3.4
1	E	222	ASP	3.4
1	E	118	ASP	3.4
1	E	732	PHE	3.3
1	F	95	ASN	3.2
1	E	136	ASN	3.2
1	E	88	PRO	3.2
1	F	40	ALA	3.1
1	F	233	TYR	3.1
1	E	119	ASN	3.1
1	E	714	PRO	3.1
1	F	42	ALA	3.1
1	E	73	ILE	3.1
1	F	148	GLN	3.1
1	E	116	VAL	3.1
1	F	404	LYS	3.0
1	E	304	TYR	3.0
1	E	122	LEU	3.0
1	E	63	PHE	3.0
1	D	706	ALA	3.0
1	E	120	ALA	3.0
1	E	50	ILE	3.0
1	E	102	THR	3.0
1	E	106	THR	3.0
1	E	703	ALA	2.9
1	E	406	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	76	ALA	2.9
1	E	404	LYS	2.9
1	E	84	GLY	2.9
1	E	210	PRO	2.9
1	E	108	ASN	2.8
1	F	733	ALA	2.8
1	E	104	PRO	2.8
1	F	734	ILE	2.7
1	E	71	LEU	2.7
1	F	99	ALA	2.7
1	E	72	TRP	2.7
1	D	736	ALA	2.7
1	E	80	ALA	2.7
1	D	733	ALA	2.6
1	F	98	LEU	2.6
1	E	141	PHE	2.6
1	D	717	PHE	2.6
1	E	145	ASP	2.6
1	F	141	PHE	2.6
1	F	58	ALA	2.6
1	E	129	ALA	2.6
1	D	735	LYS	2.6
1	E	66	ASN	2.6
1	E	75	ARG	2.6
1	F	300	VAL	2.5
1	E	111	ASN	2.5
1	D	404	LYS	2.5
1	E	260[A]	GLN	2.5
1	E	93	ASP	2.5
1	D	713	LYS	2.5
1	F	671	SER	2.5
1	F	736	ALA	2.5
1	E	117	LYS	2.5
1	E	107	LEU	2.5
1	E	114	GLN	2.5
1	E	710	ASP	2.5
1	E	57	TYR	2.4
1	E	303	GLY	2.4
1	F	138	GLN	2.4
1	D	405	LYS	2.4
1	D	734	ILE	2.4
1	E	734	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	717	PHE	2.4
1	F	84	GLY	2.4
1	D	705	SER	2.4
1	E	147	SER	2.4
1	D	304	TYR	2.4
1	D	712	ARG	2.4
1	E	78	SER	2.4
1	D	95	ASN	2.3
1	F	268	PRO	2.3
1	E	148	GLN	2.3
1	F	132	LEU	2.3
1	D	541	GLN	2.3
1	D	710	ASP	2.3
1	E	62	GLN	2.3
1	E	123	ILE	2.3
1	F	712	ARG	2.3
1	E	712	ARG	2.3
1	D	732	PHE	2.3
1	E	70	LYS	2.2
1	E	126	PRO	2.2
1	F	713	LYS	2.2
1	E	735	LYS	2.2
1	E	86	GLN	2.2
1	E	733	ALA	2.2
1	D	166	LEU	2.2
1	F	210	PRO	2.2
1	F	403	GLN	2.2
1	E	140	VAL	2.2
1	F	63	PHE	2.2
1	E	212	GLN	2.2
1	E	170	ILE	2.2
1	D	65	GLN	2.2
1	E	138	GLN	2.2
1	E	49	PRO	2.2
1	E	264	GLN	2.2
1	E	300	VAL	2.2
1	F	260	GLN	2.1
1	E	407	ASN	2.1
1	E	722	ILE	2.1
1	F	38	VAL	2.1
1	F	94	ALA	2.1
1	F	287	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	302	PHE	2.1
1	F	728	ALA	2.1
1	D	708	ASN	2.1
1	F	264	GLN	2.1
1	E	134	ASP	2.1
1	F	303	GLY	2.1
1	F	72	TRP	2.1
1	E	79	ASP	2.0
1	E	146	VAL	2.0
1	D	729	LEU	2.0
1	E	246	ASP	2.0
1	F	304	TYR	2.0
1	D	302	PHE	2.0
1	F	402	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 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
3	EDO	D	807	4/4	0.61	0.37	82,83,83,83	0
3	EDO	D	814	4/4	0.62	0.53	88,89,89,89	0
3	EDO	F	808	4/4	0.66	0.34	83,84,84,84	0
3	EDO	F	818	4/4	0.66	0.39	73,73,73,73	0
3	EDO	D	813	4/4	0.68	0.33	72,72,73,73	0
3	EDO	E	801	4/4	0.68	0.27	81,81,81,81	0
3	EDO	D	805	4/4	0.71	0.41	84,84,84,84	0
3	EDO	F	804	4/4	0.74	0.30	107,108,108,108	0
3	EDO	D	808	4/4	0.75	0.23	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	F	805	4/4	0.75	0.48	88,88,88,88	0
3	EDO	F	819	4/4	0.76	0.34	71,71,72,72	0
3	EDO	F	807	4/4	0.76	0.38	79,79,80,80	0
3	EDO	D	811	4/4	0.76	0.19	82,82,83,83	0
3	EDO	F	806	4/4	0.78	0.31	83,83,83,83	0
3	EDO	D	806	4/4	0.78	0.33	73,73,73,74	0
3	EDO	F	812	4/4	0.79	0.30	78,78,78,78	0
3	EDO	F	815	4/4	0.79	0.23	71,71,72,72	0
3	EDO	E	803	4/4	0.80	0.16	67,68,68,68	0
3	EDO	E	805	4/4	0.80	0.31	67,68,68,68	0
3	EDO	F	816	4/4	0.81	0.37	86,86,86,87	0
3	EDO	F	803	4/4	0.81	0.30	105,105,105,106	0
3	EDO	D	817	4/4	0.81	0.19	79,79,79,80	0
3	EDO	F	811	4/4	0.82	0.45	64,65,65,65	0
3	EDO	F	802	4/4	0.82	0.57	68,68,68,68	0
3	EDO	F	813	4/4	0.82	0.35	78,79,79,79	0
3	EDO	D	815	4/4	0.84	0.32	66,66,66,66	0
3	EDO	E	808	4/4	0.84	0.50	67,67,67,67	0
3	EDO	D	816	4/4	0.85	0.32	78,79,79,79	0
3	EDO	F	810	4/4	0.85	1.18	100,100,100,101	0
3	EDO	D	809	4/4	0.85	0.36	82,83,83,83	0
3	EDO	F	817	4/4	0.86	0.28	76,76,76,76	0
3	EDO	F	814	4/4	0.87	0.22	84,84,84,84	0
3	EDO	E	806	4/4	0.88	0.28	85,86,86,86	0
3	EDO	E	807	4/4	0.88	0.16	76,76,77,77	0
3	EDO	D	802	4/4	0.88	0.23	57,58,58,58	0
3	EDO	D	810	4/4	0.89	0.15	71,72,72,72	0
3	EDO	E	804	4/4	0.89	0.33	75,75,75,75	0
3	EDO	F	809	4/4	0.90	0.47	72,72,73,73	0
2	PG4	F	801	13/13	0.91	0.40	88,89,90,90	0
3	EDO	D	812	4/4	0.91	0.21	80,80,80,81	0
3	EDO	D	803	4/4	0.93	0.48	71,71,71,71	0
3	EDO	D	804	4/4	0.93	0.25	69,70,70,70	0
2	PG4	D	801	13/13	0.94	0.33	77,78,80,81	0
3	EDO	E	802	4/4	0.94	0.41	92,93,93,93	0

6.5 Other polymers (i)

There are no such residues in this entry.