



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 PM GMT

PDB ID : 4TUH
Title : Bcl-xL in complex with inhibitor (Compound 10)
Authors : Czabotar, P.E.; Lessense, G.; Smith, B.J.; Colman, P.M.
Deposited on : 2014-06-24
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

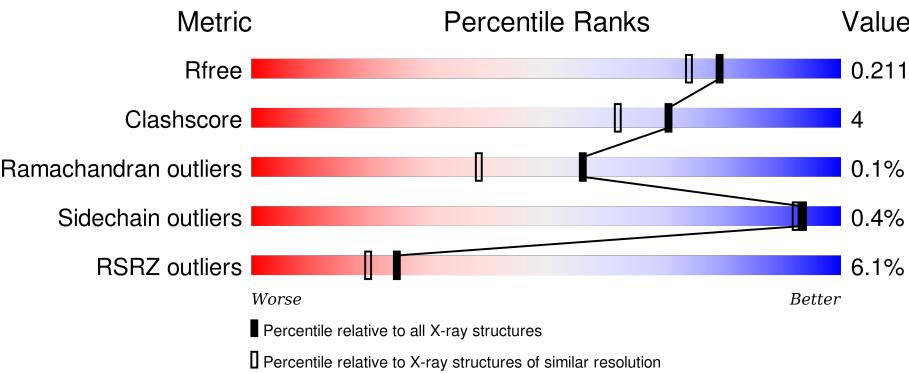
1 Overall quality at a glance i

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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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. 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	158	<div><div></div><div>89%9%</div></div>
1	B	158	<div><div>3%</div><div>82%9%8%</div></div>
1	C	158	<div><div>8%</div><div>81%9%10%</div></div>
1	D	158	<div><div>5%</div><div>84%6%11%</div></div>
1	E	158	<div><div>%</div><div>83%6%11%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	158	
1	G	158	
1	H	158	

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	A	302	-	-	-	X
3	EDO	A	304	-	-	-	X
3	EDO	A	306	-	-	-	X
3	EDO	C	302	-	-	-	X
3	EDO	F	302	-	-	-	X
3	EDO	G	302	-	-	-	X
4	ACT	B	302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10587 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 Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	2	0
			1174	750	199	220	5			
1	B	145	Total	C	N	O	S	0	3	0
			1179	752	198	224	5			
1	C	142	Total	C	N	O	S	0	1	0
			1155	736	195	219	5			
1	D	141	Total	C	N	O	S	0	1	0
			1149	733	194	217	5			
1	E	140	Total	C	N	O	S	0	1	0
			1138	728	191	214	5			
1	F	146	Total	C	N	O	S	0	2	0
			1190	758	203	224	5			
1	G	141	Total	C	N	O	S	0	0	0
			1141	729	192	215	5			
1	H	143	Total	C	N	O	S	0	0	0
			1153	735	195	218	5			

There are 40 discrepancies between the modelled and reference sequences:

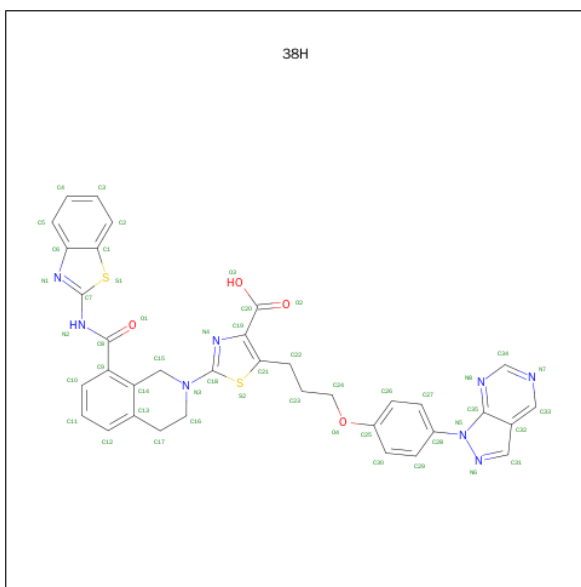
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q07817
A	-3	PRO	-	expression tag	UNP Q07817
A	-2	LEU	-	expression tag	UNP Q07817
A	-1	GLY	-	expression tag	UNP Q07817
A	0	SER	-	expression tag	UNP Q07817
B	-4	GLY	-	expression tag	UNP Q07817
B	-3	PRO	-	expression tag	UNP Q07817
B	-2	LEU	-	expression tag	UNP Q07817
B	-1	GLY	-	expression tag	UNP Q07817
B	0	SER	-	expression tag	UNP Q07817
C	-4	GLY	-	expression tag	UNP Q07817
C	-3	PRO	-	expression tag	UNP Q07817
C	-2	LEU	-	expression tag	UNP Q07817

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q07817
C	0	SER	-	expression tag	UNP Q07817
D	-4	GLY	-	expression tag	UNP Q07817
D	-3	PRO	-	expression tag	UNP Q07817
D	-2	LEU	-	expression tag	UNP Q07817
D	-1	GLY	-	expression tag	UNP Q07817
D	0	SER	-	expression tag	UNP Q07817
E	-4	GLY	-	expression tag	UNP Q07817
E	-3	PRO	-	expression tag	UNP Q07817
E	-2	LEU	-	expression tag	UNP Q07817
E	-1	GLY	-	expression tag	UNP Q07817
E	0	SER	-	expression tag	UNP Q07817
F	-4	GLY	-	expression tag	UNP Q07817
F	-3	PRO	-	expression tag	UNP Q07817
F	-2	LEU	-	expression tag	UNP Q07817
F	-1	GLY	-	expression tag	UNP Q07817
F	0	SER	-	expression tag	UNP Q07817
G	-4	GLY	-	expression tag	UNP Q07817
G	-3	PRO	-	expression tag	UNP Q07817
G	-2	LEU	-	expression tag	UNP Q07817
G	-1	GLY	-	expression tag	UNP Q07817
G	0	SER	-	expression tag	UNP Q07817
H	-4	GLY	-	expression tag	UNP Q07817
H	-3	PRO	-	expression tag	UNP Q07817
H	-2	LEU	-	expression tag	UNP Q07817
H	-1	GLY	-	expression tag	UNP Q07817
H	0	SER	-	expression tag	UNP Q07817

- Molecule 2 is 2-[8-(1,3-benzothiazol-2-ylcarbamoyl)-3,4-dihydroisoquinolin-2(1H)-yl]-5-{3-[4-(1H-pyrazolo[3,4-d]pyrimidin-1-yl)phenoxy]propyl}-1,3-thiazole-4-carboxylic acid (three-letter code: 38H) (formula: C₃₅H₂₈N₈O₄S₂).



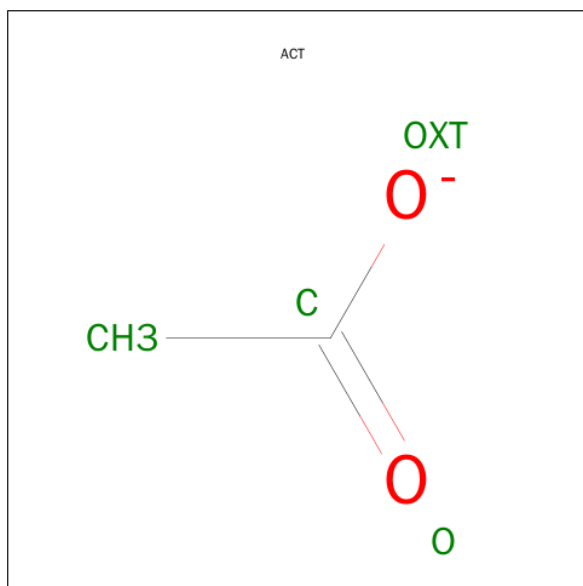
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			49	35	8	4	2		
2	B	1	Total	C	N	O	S	0	0
			49	35	8	4	2		
2	C	1	Total	C	N	O	S	0	0
			49	35	8	4	2		
2	D	1	Total	C	N	O	S	0	0
			49	35	8	4	2		
2	E	1	Total	C	N	O	S	0	0
			49	35	8	4	2		
2	F	1	Total	C	N	O	S	0	0
			49	35	8	4	2		
2	G	1	Total	C	N	O	S	0	0
			49	35	8	4	2		
2	H	1	Total	C	N	O	S	0	0
			49	35	8	4	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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


- Molecule 5 is water.

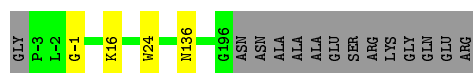
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total	O	0	0
			140	140		
5	B	110	Total	O	0	0
			110	110		
5	C	75	Total	O	0	0
			75	75		
5	D	100	Total	O	0	0
			100	100		
5	E	138	Total	O	0	0
			138	138		
5	F	130	Total	O	0	0
			130	130		
5	G	48	Total	O	0	0
			48	48		
5	H	115	Total	O	0	0
			115	115		

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 errors 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.

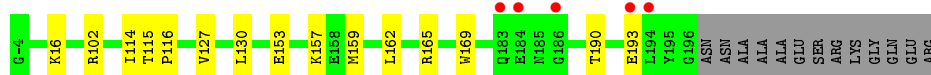
- Molecule 1: Bcl-2-like protein 1

Chain A: 




- Molecule 1: Bcl-2-like protein 1

Chain B: 




- Molecule 1: Bcl-2-like protein 1

Chain C: 




- Molecule 1: Bcl-2-like protein 1

Chain D: 




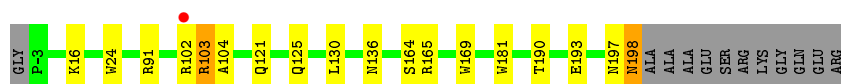
- Molecule 1: Bcl-2-like protein 1

Chain E: 

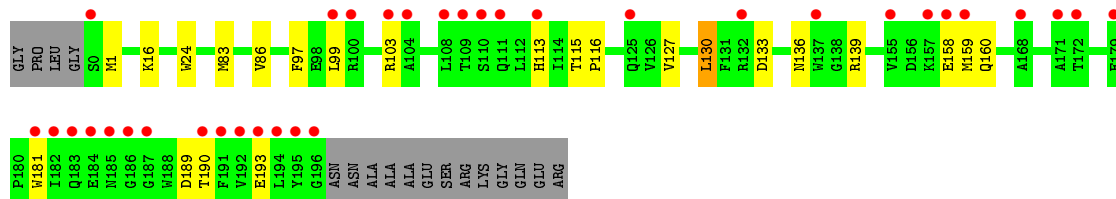
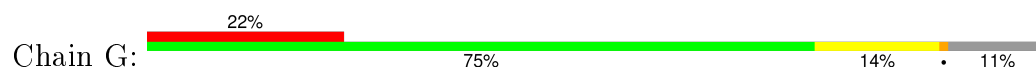


- Molecule 1: Bcl-2-like protein 1

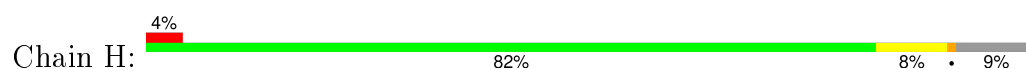
Chain F: 



- Molecule 1: Bcl-2-like protein 1



- Molecule 1: Bcl-2-like protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.83Å 109.66Å 102.10Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	31.37 – 1.80 31.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (31.37-1.80) 98.1 (31.36-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.172 , 0.209 0.177 , 0.211	Depositor DCC
R_{free} test set	5993 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 119248 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10587	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 38H, EDO, ACT

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	0.47	0/1206	0.55	0/1631
1	B	0.41	0/1211	0.57	0/1639
1	C	0.34	0/1183	0.50	0/1601
1	D	0.39	0/1177	0.57	0/1593
1	E	0.42	0/1169	0.55	0/1582
1	F	0.39	0/1222	0.55	0/1653
1	G	0.35	0/1169	0.53	1/1582 (0.1%)
1	H	0.44	0/1181	0.55	1/1598 (0.1%)
All	All	0.40	0/9518	0.55	2/12879 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	130	LEU	CA-CB-CG	5.42	127.76	115.30
1	H	1	MET	CG-SD-CE	-5.32	91.69	100.20

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	A	1174	0	1126	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1179	0	1125	11	0
1	C	1155	0	1098	10	0
1	D	1149	0	1093	5	0
1	E	1138	0	1088	8	0
1	F	1190	0	1138	13	0
1	G	1141	0	1088	19	0
1	H	1153	0	1097	14	0
2	A	49	0	27	1	0
2	B	49	0	27	1	0
2	C	49	0	27	1	0
2	D	49	0	27	1	0
2	E	49	0	27	1	0
2	F	49	0	27	4	0
2	G	49	0	27	4	0
2	H	49	0	27	1	0
3	A	28	0	42	5	0
3	C	12	0	18	3	0
3	F	4	0	6	0	0
3	G	4	0	6	0	0
3	H	8	0	12	0	0
4	B	4	0	3	0	0
5	A	140	0	0	1	0
5	B	110	0	0	1	0
5	C	75	0	0	0	0
5	D	100	0	0	1	0
5	E	138	0	0	2	0
5	F	130	0	0	0	0
5	G	48	0	0	0	0
5	H	115	0	0	1	0
All	All	10587	0	9156	83	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 4.

All (83) 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:190:THR:HA	1:F:193:GLU:HG2	1.72	0.70
1:E:121:GLN:O	1:E:125:GLN:HG3	1.91	0.70
1:G:130:LEU:HD13	2:G:301:38H:H11	1.80	0.63
1:G:97:PHE:HD2	2:G:301:38H:H21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:CYS:SG	1:E:163:VAL:HG13	2.41	0.60
1:F:197:ASN:O	1:F:198:ASN:HB2	2.03	0.59
1:C:2:SER:HB3	3:C:303:EDO:H22	1.87	0.57
1:A:136:ASN:HB2	3:A:306:EDO:H11	1.87	0.57
1:A:-1:GLY:HA3	1:E:24:TRP:CE2	2.40	0.56
1:G:130:LEU:CD1	2:G:301:38H:H11	2.36	0.55
1:A:24:TRP:CZ2	3:A:308:EDO:H11	2.42	0.55
1:G:1:MET:SD	1:H:83:MET:HE1	2.48	0.54
1:B:115:THR:HB	1:B:116:PRO:HD2	1.90	0.54
2:H:301:38H:S1	2:H:301:38H:O1	2.66	0.53
2:E:301:38H:S1	2:E:301:38H:O1	2.67	0.52
1:E:163:VAL:HG12	1:F:24:TRP:CZ3	2.45	0.52
1:B:165:ARG:HG2	1:B:169:TRP:CE2	2.45	0.52
1:D:175:ASN:ND2	5:D:479:HOH:O	2.41	0.52
1:C:100:ARG:HA	1:C:103:ARG:HH12	1.75	0.51
1:G:160:GLN:H	1:G:160:GLN:CD	2.12	0.51
1:D:96:GLU:OE2	1:D:100:ARG:NE	2.41	0.51
2:B:301:38H:S1	2:B:301:38H:O1	2.69	0.51
1:F:102:ARG:HE	2:F:301:38H:C4	2.23	0.51
1:E:1:MET:N	5:E:502:HOH:O	2.30	0.51
2:A:301:38H:S1	2:A:301:38H:O1	2.67	0.51
3:A:304:EDO:H22	1:H:136:ASN:HD22	1.76	0.50
1:D:3:GLN:O	1:H:6:ARG:NH2	2.41	0.49
1:C:2:SER:HB2	1:H:164:SER:HB2	1.95	0.49
1:G:86:VAL:HG12	1:H:8:LEU:HD21	1.95	0.49
2:D:301:38H:O1	2:D:301:38H:S1	2.71	0.48
1:H:-1:GLY:N	5:H:468:HOH:O	2.30	0.48
2:F:301:38H:S1	2:F:301:38H:O1	2.71	0.48
1:B:153:GLU:OE2	1:B:157:LYS:NZ	2.45	0.48
1:B:102:ARG:NH2	5:B:428:HOH:O	2.41	0.47
1:E:103:ARG:HG2	1:E:103:ARG:HH11	1.78	0.47
1:G:16:LYS:HD3	1:G:16:LYS:HA	1.72	0.47
1:D:16:LYS:HD3	1:D:16:LYS:HA	1.73	0.47
1:B:16:LYS:HA	1:B:16:LYS:HD3	1.77	0.47
1:B:114:ILE:HG12	1:B:162:LEU:HD13	1.96	0.47
1:B:116:PRO:HA	1:B:162:LEU:HD21	1.97	0.47
1:C:114:ILE:HG22	1:C:162:LEU:HD13	1.96	0.47
1:B:127:VAL:O	1:B:130:LEU:HB3	2.14	0.46
3:C:303:EDO:H11	1:H:164:SER:HB3	1.97	0.46
1:F:16:LYS:HD3	1:F:16:LYS:HA	1.79	0.46
1:H:83:MET:SD	1:H:87:LYS:HE3	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:303:EDO:H21	1:G:24:TRP:CZ2	2.51	0.46
1:F:103:ARG:HG3	1:F:104:ALA:N	2.29	0.46
1:G:99:LEU:O	1:G:103:ARG:NH2	2.49	0.45
1:G:1:MET:HE1	1:H:83:MET:HB2	1.99	0.45
1:G:158:GLU:CD	1:G:160:GLN:HE22	2.19	0.45
1:A:16:LYS:HA	1:A:16:LYS:HD3	1.75	0.45
1:D:116:PRO:HD3	1:D:159:MET:SD	2.57	0.45
1:A:24:TRP:CE2	3:A:308:EDO:H11	2.51	0.45
1:C:16:LYS:HA	1:C:16:LYS:HD3	1.77	0.44
1:H:1:MET:HB3	1:H:1:MET:HE3	1.60	0.44
1:E:153:GLU:HG3	5:E:526:HOH:O	2.18	0.44
2:G:301:38H:H10	2:G:301:38H:O1	2.16	0.44
1:H:157:LYS:HB2	1:H:159:MET:HE2	1.98	0.43
5:A:510:HOH:O	1:F:164:SER:HB2	2.17	0.43
1:C:129:GLU:HA	1:C:132:ARG:HG2	2.00	0.43
1:G:133:ASP:HB2	1:G:139:ARG:HH12	1.84	0.43
1:F:130:LEU:HD13	2:F:301:38H:H11	2.01	0.43
1:G:116:PRO:HD3	1:G:159:MET:SD	2.59	0.42
1:B:165:ARG:HG2	1:B:169:TRP:CZ2	2.53	0.42
1:F:165:ARG:HG2	1:F:169:TRP:CE2	2.54	0.42
1:H:116:PRO:HD3	1:H:159:MET:SD	2.60	0.42
1:B:116:PRO:HD3	1:B:159:MET:SD	2.59	0.42
1:F:121:GLN:O	1:F:125:GLN:HG2	2.20	0.42
1:G:127:VAL:O	1:G:130:LEU:HB3	2.20	0.42
1:G:115:THR:HB	1:G:116:PRO:HD2	2.01	0.41
1:F:136:ASN:HA	1:F:181:TRP:CZ2	2.55	0.41
1:G:189:ASP:O	1:G:193:GLU:HG2	2.20	0.41
1:F:130:LEU:CD1	2:F:301:38H:H11	2.50	0.41
1:B:190:THR:HA	1:B:193:GLU:HG2	2.01	0.41
1:G:83:MET:HE1	1:H:4:SER:HB3	2.01	0.41
1:C:93:ALA:HA	2:C:301:38H:N6	2.35	0.41
1:A:136:ASN:HB2	3:A:306:EDO:C1	2.49	0.41
1:C:127:VAL:O	1:C:130:LEU:HB2	2.21	0.40
1:C:137:TRP:CZ3	1:C:191:PHE:HB2	2.57	0.40
1:E:15:TYR:CG	1:F:91[B]:ARG:HD2	2.56	0.40
1:G:190:THR:HA	1:G:193:GLU:CG	2.51	0.40
1:C:164:SER:HB2	1:H:2:SER:HB2	2.02	0.40
1:G:136:ASN:HA	1:G:181:TRP:CZ2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	144/158 (91%)	142 (99%)	2 (1%)	0	100	100
1	B	146/158 (92%)	144 (99%)	2 (1%)	0	100	100
1	C	141/158 (89%)	140 (99%)	1 (1%)	0	100	100
1	D	140/158 (89%)	138 (99%)	2 (1%)	0	100	100
1	E	139/158 (88%)	138 (99%)	1 (1%)	0	100	100
1	F	146/158 (92%)	144 (99%)	2 (1%)	0	100	100
1	G	139/158 (88%)	137 (99%)	1 (1%)	1 (1%)	26	11
1	H	141/158 (89%)	139 (99%)	2 (1%)	0	100	100
All	All	1136/1264 (90%)	1122 (99%)	13 (1%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	113	HIS

5.3.2 Protein sidechains

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	124/131 (95%)	124 (100%)	0	100	100
1	B	125/131 (95%)	125 (100%)	0	100	100
1	C	122/131 (93%)	122 (100%)	0	100	100
1	D	121/131 (92%)	119 (98%)	2 (2%)	68	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	120/131 (92%)	120 (100%)	0	100	100
1	F	126/131 (96%)	124 (98%)	2 (2%)	70	59
1	G	120/131 (92%)	120 (100%)	0	100	100
1	H	121/131 (92%)	121 (100%)	0	100	100
All	All	979/1048 (93%)	975 (100%)	4 (0%)	93	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1	MET
1	D	102	ARG
1	F	103	ARG
1	F	198	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	125	GLN
1	F	198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

23 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	38H	A	301	-	44,56,56	1.07	1 (2%)	47,80,80	1.84	11 (23%)
3	EDO	A	302	-	3,3,3	0.47	0	2,2,2	0.50	0
3	EDO	A	303	-	3,3,3	0.47	0	2,2,2	0.50	0
3	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	A	305	-	3,3,3	0.40	0	2,2,2	0.46	0
3	EDO	A	306	-	3,3,3	0.46	0	2,2,2	0.54	0
3	EDO	A	307	-	3,3,3	0.43	0	2,2,2	0.68	0
3	EDO	A	308	-	3,3,3	0.47	0	2,2,2	0.53	0
2	38H	B	301	-	44,56,56	1.14	2 (4%)	47,80,80	1.86	11 (23%)
4	ACT	B	302	-	1,3,3	1.17	0	0,3,3	0.00	-
2	38H	C	301	-	44,56,56	1.09	2 (4%)	47,80,80	1.87	11 (23%)
3	EDO	C	302	-	3,3,3	0.45	0	2,2,2	0.68	0
3	EDO	C	303	-	3,3,3	0.45	0	2,2,2	0.45	0
3	EDO	C	304	-	3,3,3	0.43	0	2,2,2	0.47	0
2	38H	D	301	-	44,56,56	1.08	2 (4%)	47,80,80	1.94	11 (23%)
2	38H	E	301	-	44,56,56	1.05	2 (4%)	47,80,80	2.08	12 (25%)
2	38H	F	301	-	44,56,56	1.07	1 (2%)	47,80,80	1.91	12 (25%)
3	EDO	F	302	-	3,3,3	0.49	0	2,2,2	0.34	0
2	38H	G	301	-	44,56,56	1.08	2 (4%)	47,80,80	2.02	11 (23%)
3	EDO	G	302	-	3,3,3	0.47	0	2,2,2	0.40	0
2	38H	H	301	-	44,56,56	1.04	1 (2%)	47,80,80	1.99	12 (25%)
3	EDO	H	302	-	3,3,3	0.43	0	2,2,2	0.65	0
3	EDO	H	303	-	3,3,3	0.45	0	2,2,2	0.41	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	38H	A	301	-	-	0/18/36/36	0/8/8/8
3	EDO	A	302	-	-	0/1/1/1	0/0/0/0
3	EDO	A	303	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	304	-	-	0/1/1/1	0/0/0/0
3	EDO	A	305	-	-	0/1/1/1	0/0/0/0
3	EDO	A	306	-	-	0/1/1/1	0/0/0/0
3	EDO	A	307	-	-	0/1/1/1	0/0/0/0
3	EDO	A	308	-	-	0/1/1/1	0/0/0/0
2	38H	B	301	-	-	0/18/36/36	0/8/8/8
4	ACT	B	302	-	-	0/0/0/0	0/0/0/0
2	38H	C	301	-	-	0/18/36/36	0/8/8/8
3	EDO	C	302	-	-	0/1/1/1	0/0/0/0
3	EDO	C	303	-	-	0/1/1/1	0/0/0/0
3	EDO	C	304	-	-	0/1/1/1	0/0/0/0
2	38H	D	301	-	-	0/18/36/36	0/8/8/8
2	38H	E	301	-	-	0/18/36/36	0/8/8/8
2	38H	F	301	-	-	0/18/36/36	0/8/8/8
3	EDO	F	302	-	-	0/1/1/1	0/0/0/0
2	38H	G	301	-	-	0/18/36/36	0/8/8/8
3	EDO	G	302	-	-	0/1/1/1	0/0/0/0
2	38H	H	301	-	-	0/18/36/36	0/8/8/8
3	EDO	H	302	-	-	0/1/1/1	0/0/0/0
3	EDO	H	303	-	-	0/1/1/1	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	38H	C28-N5	-4.94	1.34	1.44
2	F	301	38H	C28-N5	-4.88	1.34	1.44
2	E	301	38H	C28-N5	-4.72	1.34	1.44
2	A	301	38H	C28-N5	-4.65	1.34	1.44
2	C	301	38H	C28-N5	-4.63	1.34	1.44
2	D	301	38H	C28-N5	-4.63	1.34	1.44
2	G	301	38H	C28-N5	-4.59	1.34	1.44
2	H	301	38H	C28-N5	-4.55	1.35	1.44
2	E	301	38H	C18-N3	2.24	1.35	1.32
2	B	301	38H	C18-N3	2.66	1.36	1.32
2	C	301	38H	C18-N3	2.67	1.36	1.32
2	D	301	38H	C18-N3	2.90	1.36	1.32
2	G	301	38H	C18-N3	2.95	1.36	1.32

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	38H	C28-N5-C35	-7.43	122.17	130.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	38H	C28-N5-C35	-5.97	123.74	130.11
2	E	301	38H	C28-N5-C35	-5.96	123.75	130.11
2	A	301	38H	C28-N5-C35	-5.51	124.22	130.11
2	H	301	38H	C28-N5-C35	-5.51	124.23	130.11
2	F	301	38H	C28-N5-C35	-5.11	124.66	130.11
2	C	301	38H	C28-N5-C35	-4.42	125.39	130.11
2	D	301	38H	C28-N5-C35	-4.16	125.67	130.11
2	C	301	38H	O1-C8-N2	-4.05	114.79	123.68
2	G	301	38H	O1-C8-N2	-3.57	115.84	123.68
2	D	301	38H	O1-C8-N2	-3.54	115.91	123.68
2	A	301	38H	O1-C8-N2	-3.50	115.98	123.68
2	B	301	38H	O1-C8-N2	-3.38	116.25	123.68
2	E	301	38H	O1-C8-N2	-3.19	116.66	123.68
2	F	301	38H	O1-C8-N2	-2.81	117.51	123.68
2	H	301	38H	O1-C8-N2	-2.74	117.67	123.68
2	G	301	38H	C15-C14-C13	-2.58	118.69	121.03
2	C	301	38H	C32-C31-N6	-2.58	104.96	111.38
2	F	301	38H	C32-C31-N6	-2.50	105.16	111.38
2	E	301	38H	C32-C31-N6	-2.46	105.25	111.38
2	A	301	38H	C32-C31-N6	-2.43	105.34	111.38
2	H	301	38H	C32-C31-N6	-2.34	105.56	111.38
2	D	301	38H	C32-C31-N6	-2.34	105.56	111.38
2	B	301	38H	C32-C31-N6	-2.31	105.65	111.38
2	G	301	38H	C32-C31-N6	-2.21	105.89	111.38
2	H	301	38H	C30-C29-C28	2.01	121.27	119.23
2	F	301	38H	C16-C17-C13	2.12	114.40	111.20
2	H	301	38H	C16-C17-C13	2.14	114.42	111.20
2	H	301	38H	C9-C8-N2	2.19	120.57	116.13
2	C	301	38H	C9-C8-N2	2.22	120.63	116.13
2	A	301	38H	C24-O4-C25	2.31	123.59	117.91
2	E	301	38H	C24-O4-C25	2.31	123.61	117.91
2	E	301	38H	C9-C8-N2	2.34	120.88	116.13
2	A	301	38H	C14-C15-N3	2.37	116.31	111.71
2	F	301	38H	C9-C8-N2	2.37	120.94	116.13
2	B	301	38H	C14-C15-N3	2.40	116.37	111.71
2	E	301	38H	C16-C17-C13	2.41	114.83	111.20
2	G	301	38H	C14-C15-N3	2.42	116.41	111.71
2	F	301	38H	C24-O4-C25	2.45	123.95	117.91
2	A	301	38H	C9-C8-N2	2.48	121.16	116.13
2	D	301	38H	C1-C6-N1	2.57	114.11	108.16
2	C	301	38H	C14-C15-N3	2.58	116.72	111.71
2	H	301	38H	C14-C15-N3	2.62	116.81	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	38H	C15-N3-C16	2.66	120.69	114.21
2	A	301	38H	C15-N3-C16	2.70	120.77	114.21
2	B	301	38H	C1-C6-N1	2.72	114.46	108.16
2	C	301	38H	C15-N3-C16	2.74	120.87	114.21
2	B	301	38H	C9-C8-N2	2.75	121.70	116.13
2	A	301	38H	C1-C6-N1	2.75	114.53	108.16
2	G	301	38H	C1-C6-N1	2.80	114.66	108.16
2	D	301	38H	C14-C15-N3	2.81	117.16	111.71
2	D	301	38H	C9-C8-N2	2.84	121.90	116.13
2	H	301	38H	C1-C6-N1	2.85	114.76	108.16
2	C	301	38H	C1-C6-N1	2.85	114.76	108.16
2	E	301	38H	C14-C15-N3	2.86	117.27	111.71
2	E	301	38H	C1-C6-N1	2.88	114.84	108.16
2	F	301	38H	C14-C15-N3	2.89	117.33	111.71
2	F	301	38H	C1-C6-N1	2.90	114.88	108.16
2	D	301	38H	C15-N3-C16	2.92	121.32	114.21
2	D	301	38H	C24-O4-C25	3.05	125.43	117.91
2	B	301	38H	C15-N3-C16	3.12	121.81	114.21
2	F	301	38H	C15-N3-C16	3.32	122.28	114.21
2	B	301	38H	C31-N6-N5	3.33	108.45	104.02
2	C	301	38H	C24-O4-C25	3.33	126.12	117.91
2	G	301	38H	C31-N6-N5	3.37	108.50	104.02
2	E	301	38H	C15-N3-C16	3.41	122.52	114.21
2	C	301	38H	C17-C16-N3	3.47	113.65	109.75
2	B	301	38H	C24-O4-C25	3.47	126.46	117.91
2	E	301	38H	C31-N6-N5	3.53	108.72	104.02
2	H	301	38H	C15-N3-C16	3.57	122.91	114.21
2	B	301	38H	C17-C16-N3	3.63	113.83	109.75
2	A	301	38H	C31-N6-N5	3.67	108.91	104.02
2	H	301	38H	C31-N6-N5	3.67	108.91	104.02
2	G	301	38H	C17-C16-N3	3.72	113.93	109.75
2	A	301	38H	C17-C16-N3	3.98	114.22	109.75
2	D	301	38H	C31-N6-N5	3.98	109.32	104.02
2	C	301	38H	C31-N6-N5	4.13	109.53	104.02
2	F	301	38H	C31-N6-N5	4.15	109.55	104.02
2	G	301	38H	C31-C32-C35	4.37	109.23	105.20
2	H	301	38H	C31-C32-C35	4.42	109.28	105.20
2	G	301	38H	C24-O4-C25	4.55	129.10	117.91
2	D	301	38H	C31-C32-C35	4.67	109.52	105.20
2	B	301	38H	C31-C32-C35	4.69	109.53	105.20
2	F	301	38H	C31-C32-C35	4.72	109.56	105.20
2	F	301	38H	C17-C16-N3	4.84	115.19	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	38H	C31-C32-C35	4.94	109.77	105.20
2	E	301	38H	C31-C32-C35	4.98	109.80	105.20
2	C	301	38H	C31-C32-C35	5.04	109.86	105.20
2	D	301	38H	C17-C16-N3	5.49	115.92	109.75
2	H	301	38H	C17-C16-N3	6.60	117.17	109.75
2	E	301	38H	C17-C16-N3	6.84	117.44	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	38H	1	0
3	A	304	EDO	1	0
3	A	306	EDO	2	0
3	A	308	EDO	2	0
2	B	301	38H	1	0
2	C	301	38H	1	0
3	C	303	EDO	3	0
2	D	301	38H	1	0
2	E	301	38H	1	0
2	F	301	38H	4	0
2	G	301	38H	4	0
2	H	301	38H	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, 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	A	144/158 (91%)	-0.17	0 100 100	16, 28, 47, 79	0
1	B	145/158 (91%)	0.05	5 (3%) 49 43	18, 35, 60, 82	0
1	C	142/158 (89%)	0.40	12 (8%) 13 10	20, 46, 76, 99	0
1	D	141/158 (89%)	0.21	8 (5%) 27 22	21, 35, 59, 88	0
1	E	140/158 (88%)	-0.03	2 (1%) 78 74	18, 31, 52, 65	0
1	F	146/158 (92%)	-0.15	1 (0%) 89 87	20, 33, 58, 95	0
1	G	141/158 (89%)	1.24	35 (24%) 1 0	23, 64, 96, 109	0
1	H	143/158 (90%)	-0.01	7 (4%) 33 27	17, 31, 63, 117	0
All	All	1142/1264 (90%)	0.19	70 (6%) 25 20	16, 36, 75, 117	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	187	GLY	5.1
1	G	196	GLY	5.1
1	G	190	THR	4.8
1	G	186	GLY	4.7
1	G	194	LEU	4.3
1	H	0	SER	4.3
1	G	104	ALA	4.2
1	G	183	GLN	4.2
1	D	1	MET	4.2
1	G	155	VAL	4.0
1	D	26	GLN	4.0
1	G	195	TYR	3.9
1	G	111	GLN	3.8
1	G	182	ILE	3.7
1	C	160	GLN	3.7
1	G	99	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	193	GLU	3.7
1	G	158	GLU	3.4
1	D	22	TYR	3.3
1	G	185	ASN	3.2
1	H	9	VAL	3.2
1	B	193	GLU	3.2
1	G	132	ARG	3.2
1	G	157	LYS	3.1
1	C	161	VAL	3.1
1	C	159	MET	3.1
1	G	171	ALA	3.1
1	G	103	ARG	3.1
1	C	103	ARG	3.0
1	G	192	VAL	3.0
1	E	26	GLN	3.0
1	G	191	PHE	3.0
1	G	110	SER	3.0
1	F	102	ARG	2.9
1	G	113	HIS	2.9
1	G	108	LEU	2.9
1	G	168	ALA	2.8
1	G	159	MET	2.8
1	G	125	GLN	2.8
1	D	8	LEU	2.7
1	B	186	GLY	2.7
1	C	132	ARG	2.6
1	D	197	ASN	2.5
1	C	158	GLU	2.5
1	G	184	GLU	2.5
1	B	194	LEU	2.5
1	C	110	SER	2.4
1	D	9	VAL	2.4
1	G	137	TRP	2.4
1	H	197	ASN	2.4
1	G	100	ARG	2.4
1	C	0	SER	2.3
1	G	109	THR	2.3
1	G	179	GLU	2.3
1	D	186	GLY	2.3
1	G	172	THR	2.3
1	G	181	TRP	2.2
1	E	193	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	171	ALA	2.2
1	H	1	MET	2.2
1	B	183	GLN	2.2
1	H	22	TYR	2.1
1	C	1	MET	2.1
1	H	160	GLN	2.1
1	D	193	GLU	2.1
1	C	184	GLU	2.1
1	G	0	SER	2.1
1	B	184	GLU	2.0
1	C	153	GLU	2.0
1	H	-1	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	G	302	4/4	0.82	0.25	8.85	54,61,71,79	0
3	EDO	A	306	4/4	0.89	0.14	8.01	30,38,40,44	0
3	EDO	A	304	4/4	0.70	0.25	6.73	58,58,60,64	0
4	ACT	B	302	4/4	0.87	0.27	4.83	41,54,56,56	0
3	EDO	A	302	4/4	0.91	0.19	3.99	36,39,48,49	0
3	EDO	C	302	4/4	0.92	0.14	3.70	49,53,54,55	0
3	EDO	F	302	4/4	0.94	0.12	2.24	26,37,43,66	0
3	EDO	A	307	4/4	0.91	0.15	1.71	37,38,42,50	0
3	EDO	C	304	4/4	0.89	0.23	0.81	39,49,64,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	38H	A	301	49/49	0.96	0.10	0.47	15,22,31,40	0
2	38H	E	301	49/49	0.96	0.11	-0.03	16,26,58,60	0
2	38H	B	301	49/49	0.95	0.10	-0.04	17,30,63,69	0
2	38H	G	301	49/49	0.89	0.17	-0.18	38,54,89,92	0
3	EDO	C	303	4/4	0.89	0.14	-0.20	69,70,70,75	0
2	38H	H	301	49/49	0.97	0.09	-0.43	15,24,31,34	0
2	38H	F	301	49/49	0.97	0.08	-0.55	21,28,46,52	0
2	38H	C	301	49/49	0.95	0.09	-0.57	29,39,52,58	0
2	38H	D	301	49/49	0.96	0.09	-0.80	24,33,51,58	0
3	EDO	H	302	4/4	0.81	0.17	-	45,52,60,69	0
3	EDO	H	303	4/4	0.92	0.20	-	44,50,60,71	0
3	EDO	A	303	4/4	0.76	0.23	-	57,64,67,68	0
3	EDO	A	308	4/4	0.85	0.16	-	40,47,49,53	0
3	EDO	A	305	4/4	0.97	0.12	-	26,30,39,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.