



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:23 am GMT

PDB ID : 3SL9
Title : X-ray structure of Beta catenin in complex with Bcl9
Authors : Gupta, D.; Bienz, M.
Deposited on : 2011-06-24
Resolution : 2.20 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:

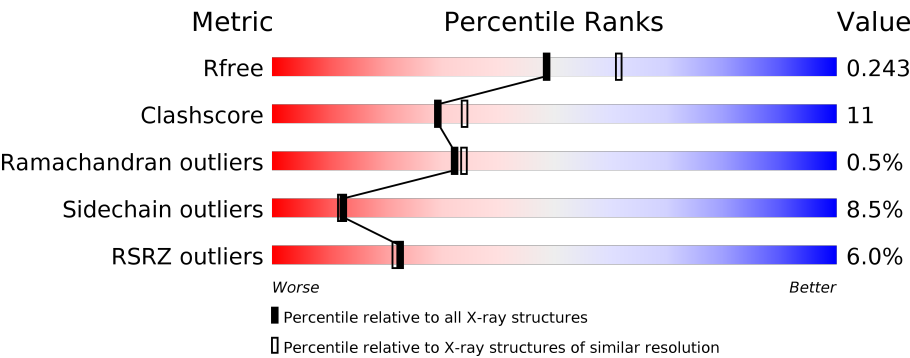
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

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 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 $\leq 5\%$. 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	167	<div><div>2%</div><div><div></div><div>86%</div><div>11%</div><div></div></div><div>..</div></div>
1	B	167	<div><div>2%</div><div><div></div><div>78%</div><div>17%</div><div></div></div><div>..</div></div>
1	E	167	<div><div>%</div><div><div></div><div>86%</div><div>11%</div><div></div></div><div>..</div></div>
1	G	167	<div><div>5%</div><div><div></div><div>77%</div><div>13%</div><div></div></div><div>.. 5%</div></div>
2	C	55	<div><div>9%</div><div><div></div><div>31%</div><div>13%</div><div>5%</div><div></div></div><div>51%</div></div>
2	D	55	<div><div>16%</div><div><div></div><div>29%</div><div>11%</div><div></div></div><div>58%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	55	
2	H	55	

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	5	-	-	X	-
3	EDO	C	3	-	-	-	X
3	EDO	E	9	-	-	-	X
4	PEG	B	306	-	-	-	X
4	PEG	E	5	-	-	-	X
5	IMD	A	308	-	-	-	X
5	IMD	B	307	-	-	-	X
6	GOL	B	309	-	-	-	X
6	GOL	F	4	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5813 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 Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1192	753	211	219	9			
1	B	165	Total	C	N	O	S	0	0	0
			1227	774	219	225	9			
1	E	165	Total	C	N	O	S	0	0	0
			1225	770	222	224	9			
1	G	158	Total	C	N	O	S	0	0	0
			1132	712	207	204	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	GLY	-	EXPRESSION TAG	UNP P35222
A	140	SER	-	EXPRESSION TAG	UNP P35222
B	139	GLY	-	EXPRESSION TAG	UNP P35222
B	140	SER	-	EXPRESSION TAG	UNP P35222
E	139	GLY	-	EXPRESSION TAG	UNP P35222
E	140	SER	-	EXPRESSION TAG	UNP P35222
G	139	GLY	-	EXPRESSION TAG	UNP P35222
G	140	SER	-	EXPRESSION TAG	UNP P35222

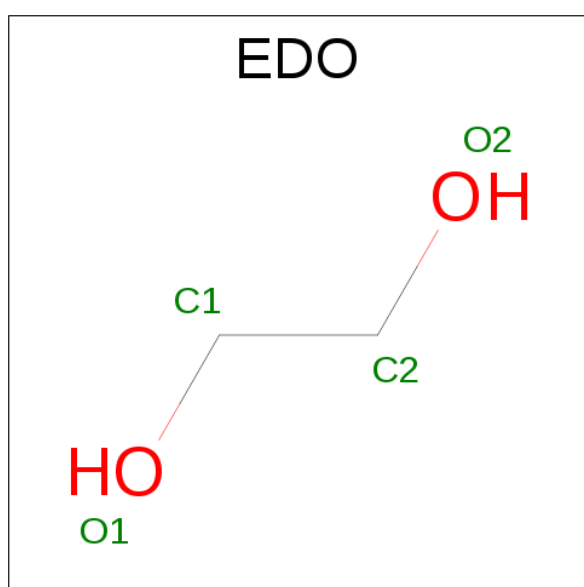
- Molecule 2 is a protein called B-cell CLL/lymphoma 9 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	S	0	0	0
			223	136	42	44	1			
2	D	23	Total	C	N	O	S	0	0	0
			178	109	37	31	1			
2	F	27	Total	C	N	O	S	0	0	0
			196	119	41	35	1			
2	H	20	Total	C	N	O		0	0	0
			144	83	30	31				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	342	MET	-	EXPRESSION TAG	UNP O00512
C	343	ALA	-	EXPRESSION TAG	UNP O00512
D	342	MET	-	EXPRESSION TAG	UNP O00512
D	343	ALA	-	EXPRESSION TAG	UNP O00512
F	342	MET	-	EXPRESSION TAG	UNP O00512
F	343	ALA	-	EXPRESSION TAG	UNP O00512
H	342	MET	-	EXPRESSION TAG	UNP O00512
H	343	ALA	-	EXPRESSION TAG	UNP O00512

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



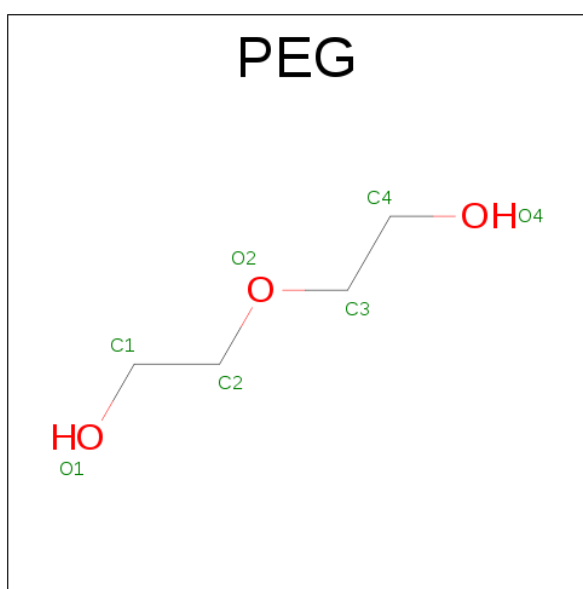
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

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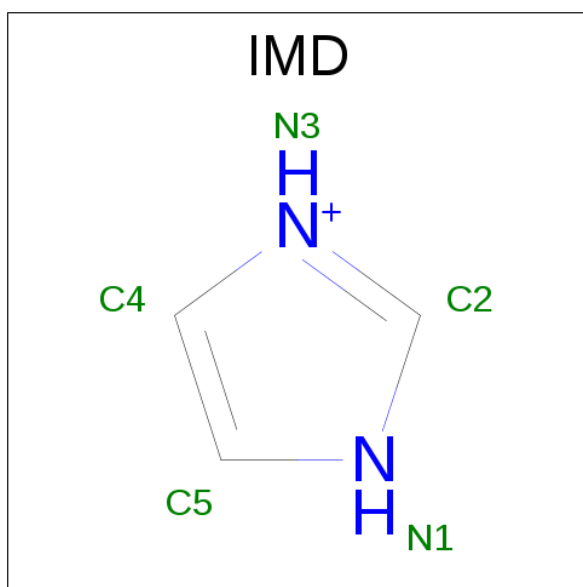
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		
5	A	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	E	1	Total	C	N	0	0
			5	3	2		
5	G	1	Total	C	N	0	0
			5	3	2		
5	G	1	Total	C	N	0	0
			5	3	2		
5	G	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		

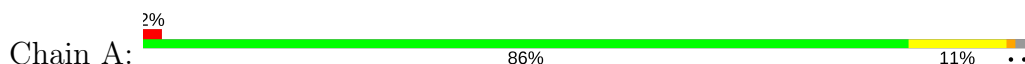
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	45	Total	O	0	0
			45	45		
7	C	7	Total	O	0	0
			7	7		
7	B	37	Total	O	0	0
			37	37		
7	E	38	Total	O	0	0
			38	38		
7	F	1	Total	O	0	0
			1	1		
7	G	22	Total	O	0	0
			22	22		
7	H	2	Total	O	0	0
			2	2		

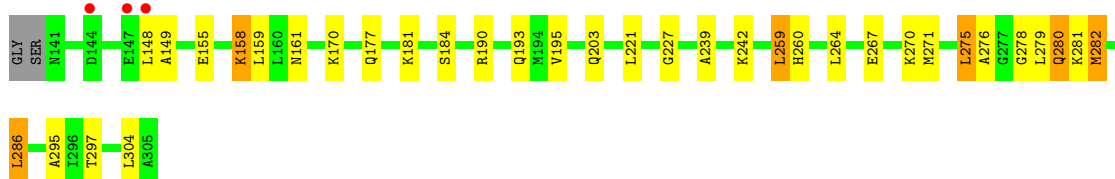
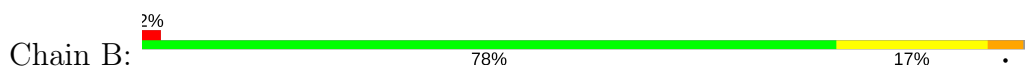
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

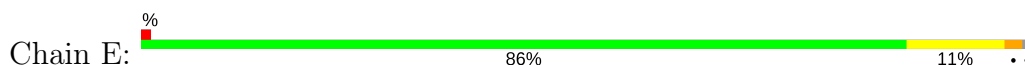
- Molecule 1: Catenin beta-1



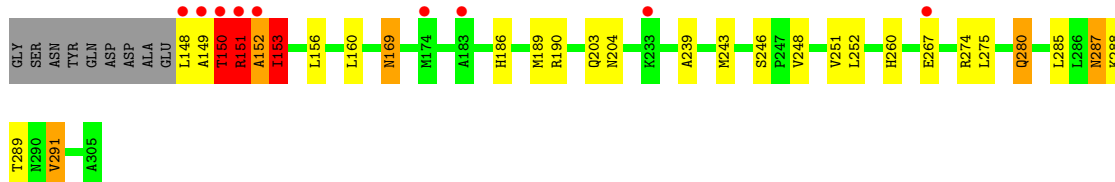
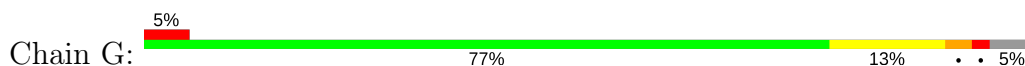
- Molecule 1: Catenin beta-1



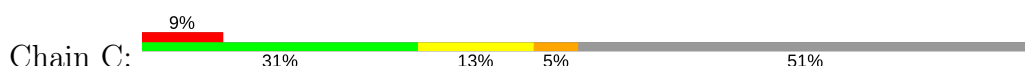
- Molecule 1: Catenin beta-1



- Molecule 1: Catenin beta-1



- Molecule 2: B-cell CLL/lymphoma 9 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.89Å 80.70Å 87.94Å 90.00° 102.00° 90.00°	Depositor
Resolution (Å)	29.43 – 2.20 29.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.43-2.20) 97.0 (29.43-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.249 0.191 , 0.243	Depositor DCC
R_{free} test set	2763 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5813	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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, 0.333 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: GOL, PEG, IMD, 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	1.13	0/1207	0.98	2/1639 (0.1%)
1	B	1.11	3/1242 (0.2%)	1.02	4/1684 (0.2%)
1	E	1.19	0/1239	1.00	2/1680 (0.1%)
1	G	0.92	0/1145	0.90	3/1552 (0.2%)
2	C	0.89	0/225	1.00	1/299 (0.3%)
2	D	0.69	0/179	0.93	0/237
2	F	0.78	0/197	0.96	1/263 (0.4%)
2	H	0.60	0/144	0.65	0/192
All	All	1.06	3/5578 (0.1%)	0.97	13/7546 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	ALA	CA-CB	8.17	1.69	1.52
1	B	195	VAL	CB-CG1	6.05	1.65	1.52
1	B	281	LYS	CD-CE	5.47	1.65	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	MET	CG-SD-CE	-10.88	82.78	100.20
1	G	291	VAL	CG1-CB-CG2	7.75	123.30	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	291	VAL	CB-CA-C	-7.21	97.71	111.40
2	F	375	PRO	N-CA-CB	7.10	111.82	103.30
1	A	200	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	E	304	LEU	CB-CG-CD1	-6.19	100.48	111.00
1	E	185	ARG	NE-CZ-NH1	-6.01	117.30	120.30
2	C	356	LEU	CA-CB-CG	5.85	128.75	115.30
1	B	190	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	252	LEU	CA-CB-CG	5.32	127.53	115.30
1	G	291	VAL	CA-CB-CG2	5.23	118.75	110.90
1	B	286	LEU	CB-CG-CD2	5.04	119.57	111.00
1	B	259	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	153	ILE	Peptide

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	1192	0	1210	21	0
1	B	1227	0	1265	22	0
1	E	1225	0	1262	16	0
1	G	1132	0	1150	47	0
2	C	223	0	216	9	0
2	D	178	0	170	8	0
2	F	196	0	171	3	0
2	H	144	0	115	3	0
3	A	12	0	18	7	0
3	B	12	0	18	0	0
3	C	4	0	6	0	0
3	E	16	0	24	3	0
4	A	7	0	10	2	0
4	B	14	0	20	1	0
4	C	7	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	7	0	10	0	0
5	A	10	0	10	0	0
5	B	5	0	5	3	0
5	E	5	0	5	0	0
5	G	15	0	15	2	0
6	B	12	0	16	0	0
6	E	6	0	8	0	0
6	F	6	0	8	0	0
6	G	6	0	8	1	0
7	A	45	0	0	0	0
7	B	37	0	0	0	0
7	C	7	0	0	3	0
7	E	38	0	0	2	0
7	F	1	0	0	0	0
7	G	22	0	0	0	0
7	H	2	0	0	0	0
All	All	5813	0	5750	123	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 11.

All (123) 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:G:148:LEU:CB	1:G:150:THR:HG22	1.67	1.25
1:G:150:THR:O	1:G:152:ALA:N	1.78	1.15
1:G:148:LEU:CB	1:G:150:THR:CG2	2.30	1.09
1:A:159:LEU:HD13	2:C:366:LEU:HD13	1.29	1.05
1:G:148:LEU:C	1:G:150:THR:CG2	2.30	0.98
1:G:151:ARG:C	1:G:151:ARG:HE	1.73	0.91
1:G:169:ASN:HD22	1:G:169:ASN:C	1.77	0.87
1:G:148:LEU:C	1:G:150:THR:HG22	1.97	0.83
1:A:274:ARG:HD3	3:A:5:EDO:C2	2.08	0.83
1:A:274:ARG:HD3	3:A:5:EDO:O2	1.79	0.82
1:G:248:VAL:HB	1:G:251:VAL:CG1	2.11	0.81
1:E:161:ASN:ND2	1:E:200:ARG:NH1	2.27	0.81
1:G:148:LEU:CA	1:G:150:THR:CG2	2.59	0.80
1:G:148:LEU:C	1:G:150:THR:HG23	2.02	0.79
1:G:248:VAL:HB	1:G:251:VAL:HG12	1.64	0.79
1:A:159:LEU:HD13	2:C:366:LEU:CD1	2.09	0.79
1:E:161:ASN:ND2	1:E:200:ARG:HH12	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:LEU:O	1:G:150:THR:HG23	1.87	0.75
1:G:148:LEU:CB	1:G:150:THR:HG21	2.17	0.73
1:G:148:LEU:CA	1:G:150:THR:HG22	2.17	0.73
1:G:248:VAL:O	1:G:251:VAL:HG12	1.90	0.72
1:B:158:LYS:HE3	1:B:158:LYS:HA	1.70	0.71
1:G:186:HIS:O	1:G:190:ARG:HD2	1.90	0.71
1:G:150:THR:O	1:G:151:ARG:C	2.28	0.70
1:E:161:ASN:HD21	1:E:200:ARG:NH1	1.90	0.69
1:G:169:ASN:C	1:G:169:ASN:ND2	2.45	0.67
1:B:203:GLN:HE21	1:B:239:ALA:HA	1.60	0.66
2:D:364:GLN:OE1	2:D:367:ARG:HD3	1.97	0.65
2:D:367:ARG:HG2	2:D:367:ARG:HH11	1.61	0.64
1:G:151:ARG:O	1:G:153:ILE:N	2.30	0.64
2:D:367:ARG:NH1	2:D:367:ARG:HG2	2.13	0.63
2:D:364:GLN:HG3	1:G:204:ASN:OD1	1.98	0.63
1:G:248:VAL:O	1:G:251:VAL:CG1	2.47	0.63
1:B:278:GLY:O	1:B:282:MET:HB2	1.99	0.62
1:B:280:GLN:NE2	1:B:280:GLN:H	1.97	0.62
1:A:170:LYS:HD2	2:C:363:LEU:HD22	1.82	0.62
1:E:161:ASN:HD21	1:E:200:ARG:HH12	1.45	0.62
1:B:242:LYS:HE2	4:B:306:PEG:H31	1.82	0.62
1:A:159:LEU:CD1	2:C:366:LEU:HD13	2.20	0.61
2:C:357:GLU:OE1	7:C:45:HOH:O	2.15	0.61
1:G:151:ARG:C	1:G:153:ILE:H	2.03	0.61
1:G:150:THR:O	1:G:152:ALA:CA	2.49	0.61
1:B:203:GLN:NE2	1:B:239:ALA:HB2	2.17	0.60
2:F:363:LEU:O	2:F:367:ARG:HG3	2.01	0.60
2:C:364:GLN:HG3	7:C:50:HOH:O	2.01	0.59
1:G:246:SER:OG	1:G:251:VAL:HG11	2.03	0.59
1:B:203:GLN:NE2	5:B:307:IMD:HN3	2.01	0.58
1:B:203:GLN:HE21	1:B:239:ALA:CA	2.14	0.58
2:D:352:SER:HA	2:D:355:GLN:HB2	1.86	0.58
1:E:232:PHE:HE2	3:E:11:EDO:H22	1.69	0.57
1:B:158:LYS:CE	1:B:158:LYS:HA	2.29	0.57
1:G:150:THR:OG1	1:G:151:ARG:N	2.37	0.57
2:C:354:GLU:OE1	1:E:242:LYS:NZ	2.35	0.57
1:G:248:VAL:HB	1:G:251:VAL:HG11	1.84	0.55
1:B:279:LEU:HD23	1:B:279:LEU:C	2.26	0.55
1:E:290:ASN:C	1:E:290:ASN:HD22	2.10	0.54
1:G:151:ARG:O	1:G:151:ARG:NE	2.41	0.54
1:G:280:GLN:H	1:G:280:GLN:HE21	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:ALA:O	1:G:243:MET:HG2	2.08	0.53
4:A:306:PEG:H22	4:A:306:PEG:O4	2.08	0.52
1:A:142:TYR:CD2	1:A:143:GLN:N	2.78	0.52
1:A:221:LEU:O	1:A:227:GLY:HA3	2.09	0.52
1:G:203:GLN:HA	1:G:243:MET:HE1	1.91	0.52
2:D:364:GLN:CG	1:G:204:ASN:OD1	2.58	0.51
1:A:274:ARG:HG2	3:A:5:EDO:H21	1.92	0.51
1:B:149:ALA:HB2	1:B:184:SER:HB3	1.91	0.51
1:B:158:LYS:CE	1:B:161:ASN:HD22	2.23	0.50
1:G:149:ALA:N	1:G:150:THR:HG22	2.25	0.50
1:B:282:MET:HE3	1:B:297:THR:HG23	1.93	0.50
1:E:178:LEU:HD21	2:F:373:LEU:HD23	1.93	0.50
1:A:274:ARG:CD	3:A:5:EDO:C2	2.87	0.50
1:B:155:GLU:O	1:B:159:LEU:HG	2.12	0.49
1:E:271:MET:CE	1:E:274:ARG:NH1	2.76	0.49
3:E:8:EDO:H22	7:E:93:HOH:O	2.13	0.49
1:G:151:ARG:HH21	1:G:152:ALA:HA	1.77	0.48
1:A:274:ARG:CD	3:A:5:EDO:H21	2.43	0.48
1:A:253:PHE:HA	1:A:293:PHE:HE2	1.78	0.48
1:A:170:LYS:HD2	2:C:363:LEU:CD2	2.43	0.48
1:G:203:GLN:HA	1:G:243:MET:CE	2.43	0.48
4:A:306:PEG:C2	4:A:306:PEG:O4	2.61	0.48
6:G:1:GOL:O1	6:G:1:GOL:O3	2.25	0.48
1:A:274:ARG:HD3	3:A:5:EDO:H21	1.91	0.48
1:A:238:PRO:HG3	5:B:307:IMD:H5	1.95	0.47
1:E:221:LEU:O	1:E:227:GLY:HA3	2.14	0.47
1:G:148:LEU:CA	1:G:150:THR:HG21	2.40	0.47
1:A:274:ARG:CG	3:A:5:EDO:H21	2.44	0.47
1:B:159:LEU:HD13	2:D:366:LEU:HD22	1.97	0.47
1:G:280:GLN:NE2	1:G:280:GLN:H	2.12	0.46
1:A:275:LEU:HA	1:B:276:ALA:O	2.15	0.46
1:A:271:MET:O	1:A:275:LEU:HD13	2.16	0.46
4:C:2:PEG:O4	7:C:51:HOH:O	2.20	0.46
1:E:290:ASN:HD22	1:E:292:LYS:H	1.63	0.46
1:G:287:ASN:H	1:G:287:ASN:HD22	1.63	0.46
1:E:290:ASN:HD21	1:E:292:LYS:HG2	1.80	0.46
3:E:8:EDO:C2	7:E:93:HOH:O	2.63	0.45
1:G:260:HIS:HE1	5:G:5:IMD:H2	1.81	0.45
2:H:352:SER:HB3	2:H:355:GLN:CD	2.36	0.45
1:E:203:GLN:HE21	1:E:242:LYS:HD2	1.82	0.45
1:B:221:LEU:O	1:B:227:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:MET:HE1	1:E:274:ARG:NH1	2.33	0.44
2:D:364:GLN:CD	1:G:204:ASN:OD1	2.56	0.44
1:G:287:ASN:HD21	1:G:288:LYS:NZ	2.15	0.44
1:G:160:LEU:HD12	1:G:160:LEU:HA	1.63	0.44
1:A:217:THR:O	1:A:221:LEU:HG	2.17	0.44
1:B:260:HIS:CE1	1:B:264:LEU:HD11	2.53	0.44
1:A:142:TYR:HD2	1:A:143:GLN:N	2.15	0.43
1:B:203:GLN:NE2	5:B:307:IMD:N3	2.66	0.43
1:B:271:MET:HG2	1:B:275:LEU:HD22	2.00	0.43
2:C:349:ASP:HB2	2:C:351:LEU:HD13	2.01	0.43
2:H:369:ILE:HG22	2:H:370:GLN:N	2.34	0.43
2:F:364:GLN:OE1	2:F:367:ARG:NH1	2.52	0.42
1:E:271:MET:HE2	1:E:274:ARG:NH1	2.35	0.42
1:G:151:ARG:HE	1:G:151:ARG:CA	2.29	0.42
1:G:151:ARG:C	1:G:153:ILE:N	2.70	0.41
1:G:246:SER:OG	1:G:251:VAL:CG1	2.67	0.41
1:G:260:HIS:CE1	5:G:5:IMD:H2	2.55	0.41
1:G:156:LEU:HA	1:G:156:LEU:HD23	1.80	0.41
1:B:282:MET:CE	1:B:297:THR:HG23	2.50	0.41
1:A:253:PHE:HA	1:A:293:PHE:CE2	2.55	0.41
1:E:252:LEU:O	1:E:252:LEU:HD22	2.21	0.41
2:H:352:SER:HB3	2:H:355:GLN:HB2	2.02	0.41
1:B:270:LYS:HE3	1:B:304:LEU:O	2.21	0.40
1:G:186:HIS:O	1:G:189:MET:HG2	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	A	162/167 (97%)	161 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/167 (98%)	163 (100%)	0	0	100	100
1	E	163/167 (98%)	163 (100%)	0	0	100	100
1	G	156/167 (93%)	152 (97%)	0	4 (3%)	6	3
2	C	25/55 (46%)	25 (100%)	0	0	100	100
2	D	21/55 (38%)	21 (100%)	0	0	100	100
2	F	25/55 (46%)	24 (96%)	1 (4%)	0	100	100
2	H	18/55 (33%)	14 (78%)	4 (22%)	0	100	100
All	All	733/888 (82%)	723 (99%)	6 (1%)	4 (0%)	32	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	150	THR
1	G	151	ARG
1	G	152	ALA
1	G	153	ILE

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	124/139 (89%)	118 (95%)	6 (5%)	30	36
1	B	131/139 (94%)	120 (92%)	11 (8%)	13	12
1	E	130/139 (94%)	121 (93%)	9 (7%)	18	19
1	G	116/139 (84%)	104 (90%)	12 (10%)	8	7
2	C	25/47 (53%)	20 (80%)	5 (20%)	1	1
2	D	18/47 (38%)	15 (83%)	3 (17%)	2	2
2	F	17/47 (36%)	14 (82%)	3 (18%)	2	1
2	H	13/47 (28%)	13 (100%)	0	100	100
All	All	574/744 (77%)	525 (92%)	49 (8%)	12	12

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	GLU
1	A	193	GLN
1	A	252	LEU
1	A	280	GLN
1	A	288	LYS
1	A	292	LYS
2	C	356	LEU
2	C	364	GLN
2	C	366	LEU
2	C	373	LEU
2	C	374	PHE
1	B	148	LEU
1	B	158	LYS
1	B	170	LYS
1	B	177	GLN
1	B	181	LYS
1	B	193	GLN
1	B	259	LEU
1	B	267	GLU
1	B	275	LEU
1	B	280	GLN
1	B	286	LEU
2	D	356	LEU
2	D	366	LEU
2	D	373	LEU
1	E	148	LEU
1	E	154	PRO
1	E	177	GLN
1	E	193	GLN
1	E	196	SER
1	E	200	ARG
1	E	252	LEU
1	E	275	LEU
1	E	290	ASN
2	F	352	SER
2	F	364	GLN
2	F	366	LEU
1	G	150	THR
1	G	151	ARG
1	G	169	ASN
1	G	252	LEU
1	G	267	GLU

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Mol	Chain	Res	Type
1	G	274	ARG
1	G	275	LEU
1	G	280	GLN
1	G	285	LEU
1	G	287	ASN
1	G	289	THR
1	G	291	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	193	GLN
2	C	353	GLN
2	C	364	GLN
1	B	193	GLN
1	B	203	GLN
1	B	280	GLN
1	E	161	ASN
1	E	193	GLN
1	E	203	GLN
1	E	290	ASN
1	G	169	ASN
1	G	280	GLN
1	G	287	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 ⓘ

28 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	A	1	-	3,3,3	0.52	0	2,2,2	0.38	0
3	EDO	A	2	-	3,3,3	0.61	0	2,2,2	0.47	0
4	PEG	A	306	-	6,6,6	0.66	0	5,5,5	0.61	0
5	IMD	A	307	-	3,5,5	0.55	0	4,5,5	0.62	0
5	IMD	A	308	-	3,5,5	0.54	0	4,5,5	0.61	0
3	EDO	A	5	-	3,3,3	0.27	0	2,2,2	0.32	0
4	PEG	B	3	-	6,6,6	0.36	0	5,5,5	0.79	0
4	PEG	B	306	-	6,6,6	0.74	0	5,5,5	1.04	0
5	IMD	B	307	-	3,5,5	0.62	0	4,5,5	0.58	0
6	GOL	B	308	-	5,5,5	0.52	0	5,5,5	0.83	0
6	GOL	B	309	-	5,5,5	0.32	0	5,5,5	0.56	0
3	EDO	B	4	-	3,3,3	0.46	0	2,2,2	0.49	0
3	EDO	B	6	-	3,3,3	0.58	0	2,2,2	0.28	0
3	EDO	B	7	-	3,3,3	0.94	0	2,2,2	0.10	0
4	PEG	C	2	-	6,6,6	0.50	0	5,5,5	0.47	0
3	EDO	C	3	-	3,3,3	1.12	0	2,2,2	0.74	0
3	EDO	E	10	-	3,3,3	0.48	0	2,2,2	0.56	0
3	EDO	E	11	-	3,3,3	0.56	0	2,2,2	0.44	0
6	GOL	E	2	-	5,5,5	0.41	0	5,5,5	0.24	0
5	IMD	E	4	-	3,5,5	0.54	0	4,5,5	0.60	0
4	PEG	E	5	-	6,6,6	0.64	0	5,5,5	0.82	0
3	EDO	E	8	-	3,3,3	0.27	0	2,2,2	0.60	0
3	EDO	E	9	-	3,3,3	0.48	0	2,2,2	0.42	0
6	GOL	F	4	-	5,5,5	0.31	0	5,5,5	0.88	0
6	GOL	G	1	-	5,5,5	0.35	0	5,5,5	0.60	0
5	IMD	G	5	-	3,5,5	0.53	0	4,5,5	0.40	0
5	IMD	G	6	-	3,5,5	0.55	0	4,5,5	0.46	0
5	IMD	G	7	-	3,5,5	0.43	0	4,5,5	0.95	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	A	1	-	-	0/1/1/1	0/0/0/0
3	EDO	A	2	-	-	0/1/1/1	0/0/0/0
4	PEG	A	306	-	-	0/4/4/4	0/0/0/0
5	IMD	A	307	-	-	0/0/0/0	0/1/1/1
5	IMD	A	308	-	-	0/0/0/0	0/1/1/1
3	EDO	A	5	-	-	0/1/1/1	0/0/0/0
4	PEG	B	3	-	-	0/4/4/4	0/0/0/0
4	PEG	B	306	-	-	0/4/4/4	0/0/0/0
5	IMD	B	307	-	-	0/0/0/0	0/1/1/1
6	GOL	B	308	-	-	0/4/4/4	0/0/0/0
6	GOL	B	309	-	-	0/4/4/4	0/0/0/0
3	EDO	B	4	-	-	0/1/1/1	0/0/0/0
3	EDO	B	6	-	-	0/1/1/1	0/0/0/0
3	EDO	B	7	-	-	0/1/1/1	0/0/0/0
4	PEG	C	2	-	-	0/4/4/4	0/0/0/0
3	EDO	C	3	-	-	0/1/1/1	0/0/0/0
3	EDO	E	10	-	-	0/1/1/1	0/0/0/0
3	EDO	E	11	-	-	0/1/1/1	0/0/0/0
6	GOL	E	2	-	-	0/4/4/4	0/0/0/0
5	IMD	E	4	-	-	0/0/0/0	0/1/1/1
4	PEG	E	5	-	-	0/4/4/4	0/0/0/0
3	EDO	E	8	-	-	0/1/1/1	0/0/0/0
3	EDO	E	9	-	-	0/1/1/1	0/0/0/0
6	GOL	F	4	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1	-	-	0/4/4/4	0/0/0/0
5	IMD	G	5	-	-	0/0/0/0	0/1/1/1
5	IMD	G	6	-	-	0/0/0/0	0/1/1/1
5	IMD	G	7	-	-	0/0/0/0	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	PEG	2	0
3	A	5	EDO	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	306	PEG	1	0
5	B	307	IMD	3	0
4	C	2	PEG	1	0
3	E	11	EDO	1	0
3	E	8	EDO	2	0
6	G	1	GOL	1	0
5	G	5	IMD	2	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	164/167 (98%)	-0.09	4 (2%) 59 57	15, 30, 60, 99	0
1	B	165/167 (98%)	-0.11	3 (1%) 69 66	16, 31, 56, 75	0
1	E	165/167 (98%)	-0.13	1 (0%) 89 88	15, 26, 47, 57	0
1	G	158/167 (94%)	0.24	9 (5%) 24 24	20, 46, 88, 119	0
2	C	27/55 (49%)	0.58	5 (18%) 1 1	22, 43, 65, 85	0
2	D	23/55 (41%)	1.73	9 (39%) 0 0	48, 60, 80, 88	0
2	F	27/55 (49%)	0.93	6 (22%) 1 1	29, 50, 91, 96	0
2	H	20/55 (36%)	1.54	8 (40%) 0 0	58, 68, 86, 87	0
All	All	749/888 (84%)	0.13	45 (6%) 23 22	15, 35, 77, 119	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	353	GLN	7.0
1	G	149	ALA	5.6
2	F	351	LEU	5.2
2	C	374	PHE	5.1
1	A	142	TYR	5.0
1	G	150	THR	4.9
2	D	354	GLU	4.5
1	E	141	ASN	4.4
2	D	356	LEU	4.3
1	G	148	LEU	4.2
2	F	350	GLY	4.1
2	D	355	GLN	4.0
1	A	144	ASP	4.0
2	D	358	HIS	3.4
2	H	369	ILE	3.3
1	B	148	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	152	ALA	3.2
1	B	147	GLU	2.8
1	B	144	ASP	2.8
1	G	151	ARG	2.8
2	F	349	ASP	2.7
2	F	355	GLN	2.7
2	D	352	SER	2.7
2	H	353	GLN	2.7
2	D	357	GLU	2.7
1	G	183	ALA	2.6
1	G	267	GLU	2.5
2	H	368	ASP	2.5
2	H	371	ARG	2.4
2	H	358	HIS	2.4
2	C	371	ARG	2.4
1	A	147	GLU	2.4
2	C	372	MET	2.3
2	C	349	ASP	2.3
2	D	359	ARG	2.3
2	D	361	ARG	2.2
2	H	355	GLN	2.2
2	F	358	HIS	2.1
2	C	348	PRO	2.1
2	F	375	PRO	2.1
2	H	363	LEU	2.0
1	G	233	LYS	2.0
2	H	359	ARG	2.0
1	A	143	GLN	2.0
1	G	174	MET	2.0

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

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

6.3 Carbohydrates ⓘ

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
4	PEG	E	5	7/7	0.78	0.35	13.86	64,66,69,71	0
5	IMD	B	307	5/5	0.90	0.25	11.24	68,69,70,72	0
6	GOL	B	309	6/6	0.79	0.20	6.63	53,66,68,70	0
5	IMD	A	308	5/5	0.86	0.18	4.79	82,84,84,85	0
3	EDO	C	3	4/4	0.82	0.24	4.06	31,38,49,54	0
3	EDO	E	9	4/4	0.84	0.23	3.45	69,71,72,72	0
6	GOL	F	4	6/6	0.75	0.23	3.37	62,70,71,76	0
4	PEG	B	306	7/7	0.75	0.23	2.60	56,68,72,73	0
4	PEG	B	3	7/7	0.90	0.15	1.95	57,62,71,73	0
4	PEG	A	306	7/7	0.83	0.15	1.55	41,63,64,70	0
3	EDO	E	8	4/4	0.94	0.16	1.19	34,39,44,53	0
3	EDO	B	4	4/4	0.81	0.13	0.76	64,71,72,74	0
3	EDO	E	11	4/4	0.89	0.15	0.37	52,55,56,64	0
4	PEG	C	2	7/7	0.90	0.15	0.29	54,60,65,65	0
3	EDO	A	2	4/4	0.87	0.17	0.24	45,57,58,65	0
5	IMD	A	307	5/5	0.87	0.16	0.23	73,75,76,78	0
3	EDO	A	5	4/4	0.90	0.12	-1.37	20,20,20,20	0
5	IMD	G	7	5/5	0.81	0.26	-	71,73,80,81	0
6	GOL	B	308	6/6	0.87	0.13	-	65,69,75,81	0
5	IMD	G	6	5/5	0.86	0.15	-	92,92,93,93	0
5	IMD	E	4	5/5	0.79	0.31	-	85,86,88,88	0
3	EDO	B	6	4/4	0.85	0.21	-	63,66,69,71	0
3	EDO	B	7	4/4	0.92	0.47	-	90,92,94,99	0
6	GOL	G	1	6/6	0.91	0.17	-	62,66,69,72	0
3	EDO	A	1	4/4	0.89	0.13	-	59,62,65,67	0
3	EDO	E	10	4/4	0.93	0.19	-	56,57,61,62	0
6	GOL	E	2	6/6	0.69	0.28	-	71,73,79,80	0
5	IMD	G	5	5/5	0.87	0.19	-	71,72,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.