



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:55 AM UTC

PDB ID : 6EMX / pdb_00006emx
Title : X-ray structure of the N15'C mutant of GLIC in complex with bromoform
Authors : Fourati, Z.; Delarue, M.
Deposited on : 2017-10-03
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

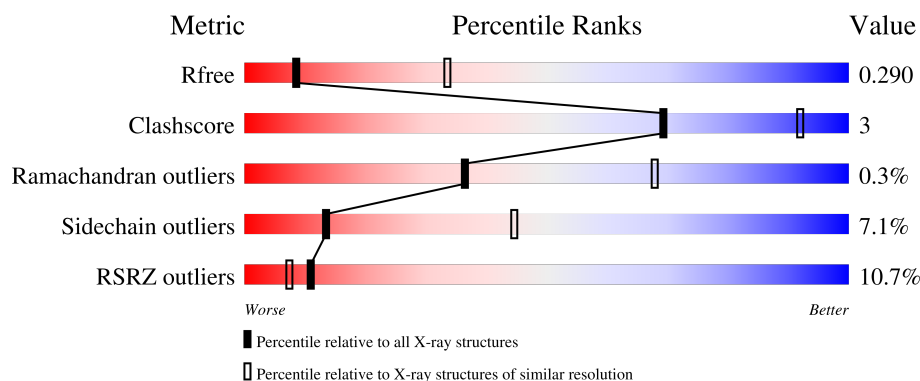
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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 $\leq 5\%$. 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	327	7% 80% 15% • 5%
1	B	327	9% 80% 15% • 5%
1	C	327	13% 80% 15% 5%
1	D	327	12% 80% 15% 5%
1	E	327	11% 82% 13% • 5%

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	NA	A	403	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12685 atoms, of which 6 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 Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2523	1663	403	452	5			
1	B	311	Total	C	N	O	S	0	0	0
			2523	1663	403	452	5			
1	C	311	Total	C	N	O	S	0	0	0
			2523	1663	403	452	5			
1	D	311	Total	C	N	O	S	0	0	0
			2523	1663	403	452	5			
1	E	311	Total	C	N	O	S	0	0	0
			2523	1663	403	452	5			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	CYS	ASN	engineered mutation	UNP Q7NDN8
A	318	GLY	-	expression tag	UNP Q7NDN8
A	319	TYR	-	expression tag	UNP Q7NDN8
A	320	PRO	-	expression tag	UNP Q7NDN8
A	321	TYR	-	expression tag	UNP Q7NDN8
A	322	ASP	-	expression tag	UNP Q7NDN8
A	323	VAL	-	expression tag	UNP Q7NDN8
A	324	PRO	-	expression tag	UNP Q7NDN8
A	325	ASP	-	expression tag	UNP Q7NDN8
A	326	TYR	-	expression tag	UNP Q7NDN8
A	327	ALA	-	expression tag	UNP Q7NDN8
B	239	CYS	ASN	engineered mutation	UNP Q7NDN8
B	318	GLY	-	expression tag	UNP Q7NDN8
B	319	TYR	-	expression tag	UNP Q7NDN8
B	320	PRO	-	expression tag	UNP Q7NDN8
B	321	TYR	-	expression tag	UNP Q7NDN8
B	322	ASP	-	expression tag	UNP Q7NDN8
B	323	VAL	-	expression tag	UNP Q7NDN8
B	324	PRO	-	expression tag	UNP Q7NDN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	325	ASP	-	expression tag	UNP Q7NDN8
B	326	TYR	-	expression tag	UNP Q7NDN8
B	327	ALA	-	expression tag	UNP Q7NDN8
C	239	CYS	ASN	engineered mutation	UNP Q7NDN8
C	318	GLY	-	expression tag	UNP Q7NDN8
C	319	TYR	-	expression tag	UNP Q7NDN8
C	320	PRO	-	expression tag	UNP Q7NDN8
C	321	TYR	-	expression tag	UNP Q7NDN8
C	322	ASP	-	expression tag	UNP Q7NDN8
C	323	VAL	-	expression tag	UNP Q7NDN8
C	324	PRO	-	expression tag	UNP Q7NDN8
C	325	ASP	-	expression tag	UNP Q7NDN8
C	326	TYR	-	expression tag	UNP Q7NDN8
C	327	ALA	-	expression tag	UNP Q7NDN8
D	239	CYS	ASN	engineered mutation	UNP Q7NDN8
D	318	GLY	-	expression tag	UNP Q7NDN8
D	319	TYR	-	expression tag	UNP Q7NDN8
D	320	PRO	-	expression tag	UNP Q7NDN8
D	321	TYR	-	expression tag	UNP Q7NDN8
D	322	ASP	-	expression tag	UNP Q7NDN8
D	323	VAL	-	expression tag	UNP Q7NDN8
D	324	PRO	-	expression tag	UNP Q7NDN8
D	325	ASP	-	expression tag	UNP Q7NDN8
D	326	TYR	-	expression tag	UNP Q7NDN8
D	327	ALA	-	expression tag	UNP Q7NDN8
E	239	CYS	ASN	engineered mutation	UNP Q7NDN8
E	318	GLY	-	expression tag	UNP Q7NDN8
E	319	TYR	-	expression tag	UNP Q7NDN8
E	320	PRO	-	expression tag	UNP Q7NDN8
E	321	TYR	-	expression tag	UNP Q7NDN8
E	322	ASP	-	expression tag	UNP Q7NDN8
E	323	VAL	-	expression tag	UNP Q7NDN8
E	324	PRO	-	expression tag	UNP Q7NDN8
E	325	ASP	-	expression tag	UNP Q7NDN8
E	326	TYR	-	expression tag	UNP Q7NDN8
E	327	ALA	-	expression tag	UNP Q7NDN8

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

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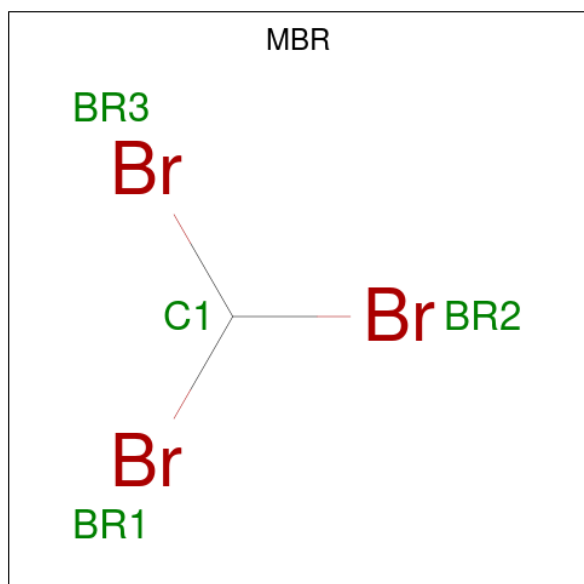
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is TRIBROMOMETHANE (CCD ID: MBR) (formula: CHBr_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	H	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	Br	C	H	0	0
			5	3	1	1		
4	C	1	Total	Br	C	H	0	0
			5	3	1	1		
4	D	1	Total	Br	C	H	0	0
			5	3	1	1		
4	E	1	Total	Br	C	H	0	0
			5	3	1	1		
4	E	1	Total	Br	C	H	0	0
			5	3	1	1		

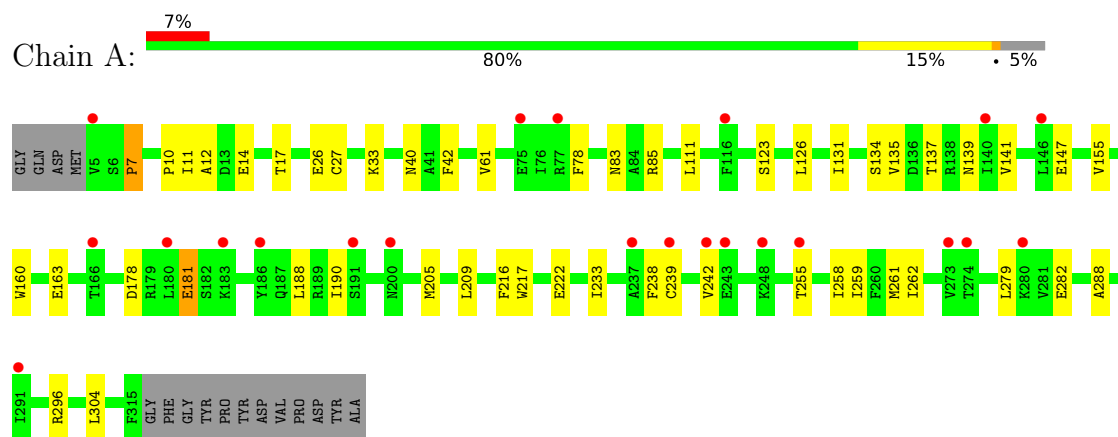
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	5	Total	O	0	0
			5	5		
5	C	4	Total	O	0	0
			4	4		
5	D	5	Total	O	0	0
			5	5		
5	E	11	Total	O	0	0
			11	11		

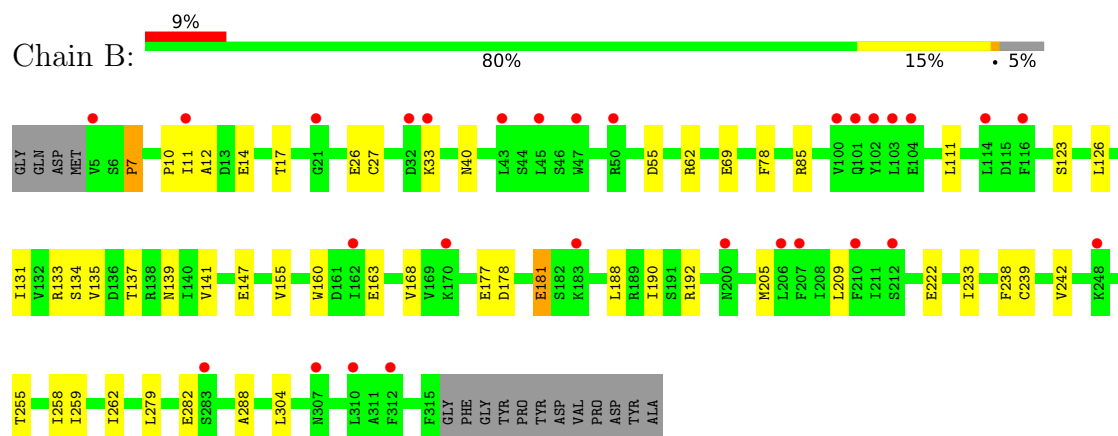
3 Residue-property plots [i](#)

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.

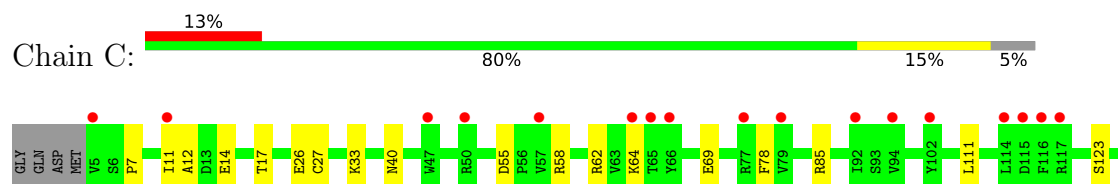
• Molecule 1: Proton-gated ion channel

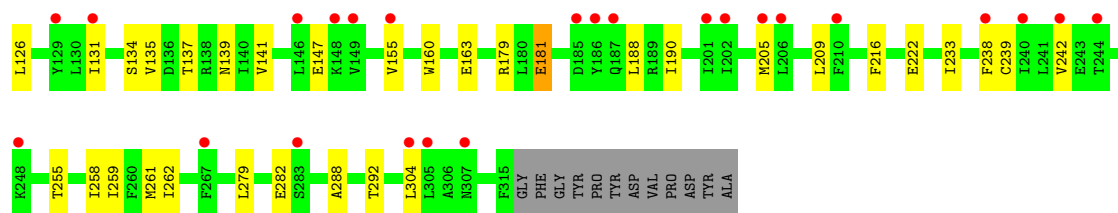


• Molecule 1: Proton-gated ion channel

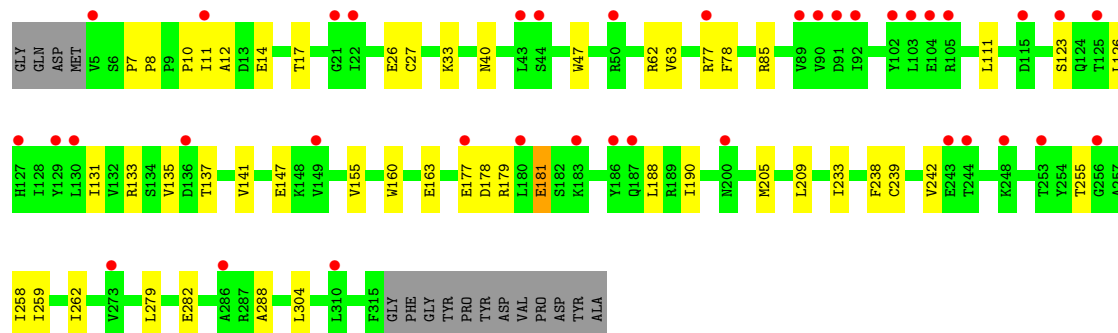
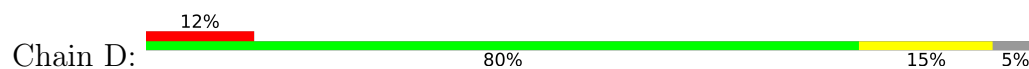


• Molecule 1: Proton-gated ion channel

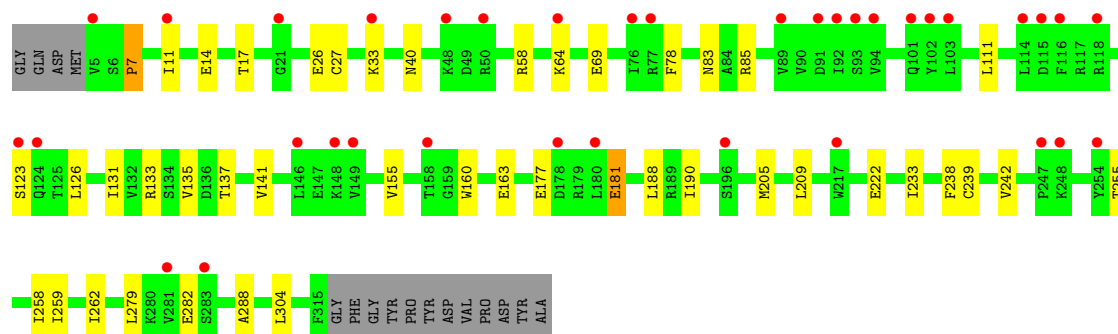
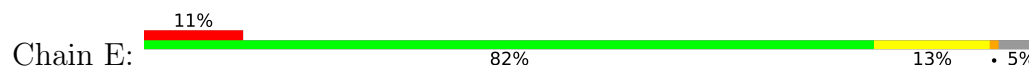




● Molecule 1: Proton-gated ion channel



● Molecule 1: Proton-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.79Å 133.32Å 158.77Å 90.00° 101.68° 90.00°	Depositor
Resolution (Å)	28.62 – 3.20 28.62 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.62-3.20) 98.7 (28.62-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.17Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.246 , 0.268 0.273 , 0.290	Depositor DCC
R_{free} test set	2914 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	103.6	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12685	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: NA, MBR, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/2591	1.22	4/3542 (0.1%)
1	B	0.76	0/2591	1.23	6/3542 (0.2%)
1	C	0.78	0/2591	1.23	4/3542 (0.1%)
1	D	0.77	0/2591	1.23	2/3542 (0.1%)
1	E	0.77	0/2591	1.23	3/3542 (0.1%)
All	All	0.77	0/12955	1.23	19/17710 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	258	ILE	CA-C-N	6.62	129.13	120.60
1	D	258	ILE	C-N-CA	6.62	129.13	120.60
1	A	258	ILE	CA-C-N	6.58	129.09	120.60
1	A	258	ILE	C-N-CA	6.58	129.09	120.60
1	E	258	ILE	CA-C-N	6.39	128.84	120.60
1	E	258	ILE	C-N-CA	6.39	128.84	120.60
1	C	258	ILE	CA-C-N	6.26	128.68	120.60
1	C	258	ILE	C-N-CA	6.26	128.68	120.60
1	B	258	ILE	CA-C-N	6.06	128.41	120.60
1	B	258	ILE	C-N-CA	6.06	128.41	120.60
1	B	55	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	12	ALA	CA-C-O	-5.38	114.89	121.78
1	B	7	PRO	N-CA-C	5.25	115.51	110.47
1	E	7	PRO	N-CA-C	5.14	115.40	110.47
1	A	42	PHE	CA-CB-CG	5.12	118.92	113.80
1	C	55	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	168	VAL	CA-C-N	5.05	127.37	120.46
1	B	168	VAL	C-N-CA	5.05	127.37	120.46
1	A	7	PRO	N-CA-C	5.01	115.28	110.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2523	0	2544	22	0
1	B	2523	0	2544	17	0
1	C	2523	0	2544	16	0
1	D	2523	0	2544	19	0
1	E	2523	0	2544	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	4	1	0	1	0
4	B	4	1	0	1	0
4	C	4	1	0	1	0
4	D	4	1	0	1	0
4	E	8	2	0	0	0
5	A	5	0	0	5	0
5	B	5	0	0	0	0
5	C	4	0	0	0	0
5	D	5	0	0	3	0
5	E	11	0	0	0	0
All	All	12679	6	12720	88	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 (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HG2	5:A:501:HOH:O	1.44	1.13
1:B:205:MET:HE2	1:B:238:PHE:HB3	1.69	0.74
1:A:205:MET:HE2	1:A:238:PHE:HB3	1.69	0.74
1:E:205:MET:HE2	1:E:238:PHE:HB3	1.70	0.73
1:C:205:MET:HE2	1:C:238:PHE:HB3	1.68	0.73
1:D:47:TRP:HD1	5:D:501:HOH:O	1.71	0.72
1:D:205:MET:HE2	1:D:238:PHE:HB3	1.71	0.72
1:B:78:PHE:HE2	1:B:85:ARG:HD3	1.65	0.62
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.64	0.62
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.65	0.62
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.65	0.60
1:B:26:GLU:HB2	1:B:40:ASN:HB3	1.85	0.58
1:C:26:GLU:HB2	1:C:40:ASN:HB3	1.86	0.58
1:A:134:SER:HB3	1:A:139:ASN:HA	1.84	0.58
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.39	0.58
1:E:26:GLU:HB2	1:E:40:ASN:HB3	1.86	0.57
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.68	0.57
1:D:26:GLU:HB2	1:D:40:ASN:HB3	1.85	0.57
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.41	0.56
1:A:26:GLU:HB2	1:A:40:ASN:HB3	1.87	0.56
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.41	0.56
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.89	0.55
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.41	0.55
1:A:216:PHE:CB	5:A:501:HOH:O	2.56	0.54
1:A:216:PHE:HB2	5:A:501:HOH:O	2.06	0.54
1:A:131:ILE:HG12	1:A:181:GLU:HG2	1.90	0.54
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.44	0.53
1:A:7:PRO:HG3	1:A:135:VAL:HG21	1.92	0.52
1:D:133:ARG:HH12	1:D:177:GLU:HB2	1.75	0.52
1:D:8:PRO:HG3	5:D:501:HOH:O	2.11	0.51
1:B:239:CYS:SG	1:B:259:ILE:HG23	2.50	0.51
1:D:47:TRP:CD1	5:D:501:HOH:O	2.56	0.51
1:B:131:ILE:HG12	1:B:181:GLU:HG2	1.92	0.50
1:D:7:PRO:HG3	1:D:135:VAL:HG21	1.92	0.50
1:E:7:PRO:HG3	1:E:135:VAL:HG21	1.94	0.50
1:A:126:LEU:HD12	1:A:188:LEU:HD23	1.93	0.50
1:C:131:ILE:HG12	1:C:181:GLU:HG2	1.94	0.49
1:E:131:ILE:HG12	1:E:181:GLU:HG2	1.93	0.49
1:A:216:PHE:C	5:A:501:HOH:O	2.54	0.49
1:D:239:CYS:SG	1:D:259:ILE:HG23	2.53	0.49
1:C:7:PRO:HG3	1:C:135:VAL:HG21	1.93	0.49
1:D:126:LEU:HD12	1:D:188:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:CYS:SG	1:E:259:ILE:HG23	2.53	0.48
1:D:131:ILE:HG12	1:D:181:GLU:HG2	1.95	0.48
1:E:126:LEU:HD12	1:E:188:LEU:HD23	1.95	0.48
1:B:126:LEU:HD12	1:B:188:LEU:HD23	1.94	0.47
1:C:126:LEU:HD12	1:C:188:LEU:HD23	1.96	0.47
1:A:239:CYS:SG	1:A:259:ILE:HG23	2.55	0.47
1:C:239:CYS:SG	1:C:259:ILE:HG23	2.54	0.47
1:A:217:TRP:CE3	5:A:501:HOH:O	2.68	0.47
1:C:238:PHE:O	1:C:242:VAL:HG23	2.15	0.47
1:E:238:PHE:O	1:E:242:VAL:HG23	2.14	0.47
1:C:134:SER:HB3	1:C:139:ASN:HA	1.98	0.47
1:B:10:PRO:HB2	1:B:12:ALA:O	2.16	0.46
1:C:255:THR:HG23	4:C:402:MBR:BR1	2.71	0.46
1:A:10:PRO:HB2	1:A:12:ALA:O	2.15	0.46
1:A:238:PHE:O	1:A:242:VAL:HG23	2.16	0.46
1:D:238:PHE:O	1:D:242:VAL:HG23	2.16	0.45
1:B:160:TRP:CE3	1:B:190:ILE:HD12	2.51	0.45
1:D:10:PRO:HB2	1:D:12:ALA:O	2.17	0.45
1:B:238:PHE:O	1:B:242:VAL:HG23	2.16	0.45
1:E:160:TRP:CE3	1:E:190:ILE:HD12	2.53	0.44
1:B:134:SER:HB3	1:B:139:ASN:HA	1.99	0.44
1:A:279:LEU:HB2	1:A:288:ALA:HB2	2.00	0.44
1:A:160:TRP:CE3	1:A:190:ILE:HD12	2.52	0.43
1:A:242:VAL:HG11	1:A:255:THR:HG21	2.00	0.43
1:A:261:MET:HE2	1:A:261:MET:HB3	1.92	0.43
1:C:160:TRP:CE3	1:C:190:ILE:HD12	2.52	0.43
1:C:261:MET:HE2	1:C:261:MET:HB3	1.90	0.43
1:D:160:TRP:CE3	1:D:190:ILE:HD12	2.53	0.43
1:B:133:ARG:HH12	1:B:177:GLU:HB2	1.82	0.43
1:B:209:LEU:HD13	1:B:262:ILE:HG23	2.01	0.43
1:B:279:LEU:HB2	1:B:288:ALA:HB2	1.99	0.43
1:E:209:LEU:HD13	1:E:262:ILE:HG23	2.00	0.43
1:D:242:VAL:HG11	1:D:255:THR:HG21	2.00	0.43
1:D:279:LEU:HB2	1:D:288:ALA:HB2	2.00	0.43
1:A:255:THR:HG23	4:A:404:MBR:BR1	2.74	0.42
1:E:133:ARG:HH12	1:E:177:GLU:HB2	1.84	0.42
1:D:255:THR:HG23	4:D:403:MBR:BR1	2.74	0.42
1:C:279:LEU:HB2	1:C:288:ALA:HB2	2.01	0.42
1:E:242:VAL:HG11	1:E:255:THR:HG21	2.00	0.42
1:E:279:LEU:HB2	1:E:288:ALA:HB2	2.00	0.42
1:B:255:THR:HG23	4:B:403:MBR:BR1	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HG11	1:B:255:THR:HG21	2.01	0.41
1:D:209:LEU:HD13	1:D:262:ILE:HG23	2.02	0.41
1:C:209:LEU:HD13	1:C:262:ILE:HG23	2.01	0.41
1:A:209:LEU:HD13	1:A:262:ILE:HG23	2.02	0.41
1:C:216:PHE:O	1:C:292:THR:HG22	2.22	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	309/327 (94%)	298 (96%)	10 (3%)	1 (0%)	36	68
1	B	309/327 (94%)	297 (96%)	11 (4%)	1 (0%)	36	68
1	C	309/327 (94%)	297 (96%)	11 (4%)	1 (0%)	36	68
1	D	309/327 (94%)	297 (96%)	11 (4%)	1 (0%)	36	68
1	E	309/327 (94%)	298 (96%)	10 (3%)	1 (0%)	36	68
All	All	1545/1635 (94%)	1487 (96%)	53 (3%)	5 (0%)	36	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	155	VAL
1	D	155	VAL
1	E	155	VAL
1	B	155	VAL
1	A	155	VAL

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	280/292 (96%)	261 (93%)	19 (7%)	14	46
1	B	280/292 (96%)	260 (93%)	20 (7%)	13	44
1	C	280/292 (96%)	259 (92%)	21 (8%)	12	42
1	D	280/292 (96%)	260 (93%)	20 (7%)	13	44
1	E	280/292 (96%)	261 (93%)	19 (7%)	14	46
All	All	1400/1460 (96%)	1301 (93%)	99 (7%)	13	44

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	14	GLU
1	A	17	THR
1	A	27	CYS
1	A	33	LYS
1	A	61	VAL
1	A	83	ASN
1	A	111	LEU
1	A	123	SER
1	A	137	THR
1	A	141	VAL
1	A	147	GLU
1	A	163	GLU
1	A	178	ASP
1	A	181	GLU
1	A	222	GLU
1	A	233	ILE
1	A	282	GLU
1	A	304	LEU
1	B	11	ILE
1	B	14	GLU
1	B	17	THR
1	B	27	CYS

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Mol	Chain	Res	Type
1	B	33	LYS
1	B	62	ARG
1	B	69	GLU
1	B	111	LEU
1	B	123	SER
1	B	137	THR
1	B	141	VAL
1	B	147	GLU
1	B	163	GLU
1	B	178	ASP
1	B	181	GLU
1	B	192	ARG
1	B	222	GLU
1	B	233	ILE
1	B	282	GLU
1	B	304	LEU
1	C	11	ILE
1	C	14	GLU
1	C	17	THR
1	C	27	CYS
1	C	33	LYS
1	C	58	ARG
1	C	62	ARG
1	C	64	LYS
1	C	69	GLU
1	C	111	LEU
1	C	123	SER
1	C	137	THR
1	C	141	VAL
1	C	147	GLU
1	C	163	GLU
1	C	179	ARG
1	C	181	GLU
1	C	222	GLU
1	C	233	ILE
1	C	282	GLU
1	C	304	LEU
1	D	11	ILE
1	D	14	GLU
1	D	17	THR
1	D	27	CYS
1	D	33	LYS

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Mol	Chain	Res	Type
1	D	62	ARG
1	D	63	VAL
1	D	77	ARG
1	D	111	LEU
1	D	123	SER
1	D	137	THR
1	D	141	VAL
1	D	147	GLU
1	D	163	GLU
1	D	178	ASP
1	D	179	ARG
1	D	181	GLU
1	D	233	ILE
1	D	282	GLU
1	D	304	LEU
1	E	11	ILE
1	E	14	GLU
1	E	17	THR
1	E	27	CYS
1	E	33	LYS
1	E	58	ARG
1	E	64	LYS
1	E	69	GLU
1	E	83	ASN
1	E	111	LEU
1	E	123	SER
1	E	137	THR
1	E	141	VAL
1	E	163	GLU
1	E	181	GLU
1	E	222	GLU
1	E	233	ILE
1	E	282	GLU
1	E	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	HIS
1	A	307	ASN
1	B	139	ASN
1	D	139	ASN

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Mol	Chain	Res	Type
1	E	83	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MBR	D	403	-	3,3,3	0.11	0	3,3,3	0.10	0
4	MBR	B	403	-	3,3,3	0.14	0	3,3,3	0.11	0
4	MBR	A	404	-	3,3,3	0.12	0	3,3,3	0.12	0
4	MBR	C	402	-	3,3,3	0.14	0	3,3,3	0.15	0
4	MBR	E	404	-	3,3,3	0.13	0	3,3,3	0.06	0
4	MBR	E	403	-	3,3,3	0.10	0	3,3,3	0.01	0

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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	MBR	1	0
4	B	403	MBR	1	0
4	A	404	MBR	1	0
4	C	402	MBR	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	311/327 (95%)	0.55	22 (7%) 22 14	110, 139, 199, 243	0
1	B	311/327 (95%)	0.61	29 (9%) 14 9	95, 134, 177, 216	0
1	C	311/327 (95%)	0.78	41 (13%) 7 6	117, 145, 205, 231	0
1	D	311/327 (95%)	0.81	38 (12%) 8 6	119, 149, 205, 253	0
1	E	311/327 (95%)	0.67	36 (11%) 9 7	112, 145, 202, 237	0
All	All	1555/1635 (95%)	0.68	166 (10%) 11 7	95, 142, 199, 253	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	115	ASP	11.4
1	B	102	TYR	7.0
1	D	102	TYR	6.9
1	D	21	GLY	6.7
1	C	66	TYR	6.5
1	D	89	VAL	6.2
1	D	104	GLU	6.1
1	C	115	ASP	5.7
1	D	43	LEU	5.5
1	B	104	GLU	5.5
1	A	248	LYS	5.4
1	E	283	SER	5.3
1	C	283	SER	5.2
1	E	248	LYS	5.0
1	E	102	TYR	4.9
1	E	124	GLN	4.8
1	D	129	TYR	4.7
1	C	129	TYR	4.7
1	E	114	LEU	4.7
1	B	43	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	5	VAL	4.6
1	E	116	PHE	4.6
1	C	146	LEU	4.5
1	C	248	LYS	4.4
1	C	102	TYR	4.3
1	E	217	TRP	4.3
1	D	92	ILE	4.2
1	E	123	SER	4.2
1	C	64	LYS	4.2
1	C	92	ILE	4.1
1	D	136	ASP	4.1
1	D	91	ASP	4.1
1	E	92	ILE	4.0
1	C	201	ILE	4.0
1	E	146	LEU	4.0
1	B	283	SER	4.0
1	D	186	TYR	4.0
1	C	187	GLN	3.9
1	E	76	ILE	3.9
1	B	312	PHE	3.9
1	B	103	LEU	3.9
1	B	210	PHE	3.9
1	A	242	VAL	3.8
1	E	33	LYS	3.8
1	C	65	THR	3.7
1	A	146	LEU	3.7
1	D	115	ASP	3.7
1	C	205	MET	3.7
1	B	47	TRP	3.6
1	E	48	LYS	3.6
1	E	50	ARG	3.6
1	C	202	ILE	3.5
1	C	149	VAL	3.5
1	D	127	HIS	3.5
1	D	103	LEU	3.4
1	D	123	SER	3.4
1	C	210	PHE	3.4
1	D	253	THR	3.3
1	C	242	VAL	3.3
1	C	79	VAL	3.3
1	E	89	VAL	3.3
1	D	11	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	114	LEU	3.3
1	D	244	THR	3.2
1	C	11	ILE	3.2
1	D	22	ILE	3.2
1	C	57	VAL	3.1
1	B	45	LEU	3.1
1	E	21	GLY	3.1
1	A	243	GLU	3.1
1	E	5	VAL	3.0
1	E	94	VAL	3.0
1	B	32	ASP	3.0
1	B	207	PHE	2.9
1	E	101	GLN	2.9
1	E	180	LEU	2.9
1	C	94	VAL	2.9
1	A	186	TYR	2.8
1	A	5	VAL	2.8
1	B	5	VAL	2.8
1	D	180	LEU	2.8
1	E	103	LEU	2.8
1	A	291	ILE	2.8
1	B	183	LYS	2.7
1	E	196	SER	2.7
1	D	50	ARG	2.7
1	A	280	LYS	2.7
1	E	149	VAL	2.7
1	C	117	ARG	2.7
1	C	50	ARG	2.6
1	D	248	LYS	2.6
1	B	21	GLY	2.6
1	D	256	GLY	2.6
1	C	240	ILE	2.6
1	D	77	ARG	2.6
1	A	116	PHE	2.6
1	A	239	CYS	2.6
1	C	47	TRP	2.5
1	B	116	PHE	2.5
1	D	90	VAL	2.5
1	B	11	ILE	2.5
1	C	244	THR	2.5
1	A	140	ILE	2.5
1	C	114	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	183	LYS	2.5
1	E	77	ARG	2.4
1	D	149	VAL	2.4
1	D	44	SER	2.4
1	C	131	ILE	2.4
1	D	130	LEU	2.4
1	C	307	ASN	2.4
1	D	125	THR	2.4
1	A	180	LEU	2.4
1	C	305	LEU	2.4
1	E	93	SER	2.4
1	E	281	VAL	2.4
1	B	200	ASN	2.3
1	C	116	PHE	2.3
1	B	50	ARG	2.3
1	C	77	ARG	2.3
1	A	75	GLU	2.3
1	E	254	TYR	2.3
1	A	183	LYS	2.3
1	C	155	VAL	2.3
1	E	91	ASP	2.3
1	C	148	LYS	2.2
1	E	178	ASP	2.2
1	C	206	LEU	2.2
1	A	255	THR	2.2
1	E	148	LYS	2.2
1	B	307	ASN	2.2
1	C	5	VAL	2.2
1	B	162	ILE	2.2
1	E	11	ILE	2.2
1	A	237	ALA	2.2
1	A	77	ARG	2.2
1	E	158	THR	2.2
1	B	206	LEU	2.2
1	D	243	GLU	2.2
1	E	64	LYS	2.2
1	C	267	PHE	2.2
1	D	273	VAL	2.1
1	D	310	LEU	2.1
1	A	191	SER	2.1
1	D	105	ARG	2.1
1	C	185	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	274	THR	2.1
1	B	33	LYS	2.1
1	B	310	LEU	2.1
1	C	186	TYR	2.1
1	D	286	ALA	2.1
1	B	248	LYS	2.1
1	B	101	GLN	2.1
1	C	238	PHE	2.1
1	A	273	VAL	2.1
1	B	100	VAL	2.1
1	B	170	LYS	2.1
1	C	304	LEU	2.1
1	D	177	GLU	2.1
1	D	200	ASN	2.0
1	A	166	THR	2.0
1	B	212	SER	2.0
1	A	200	ASN	2.0
1	D	187	GLN	2.0
1	E	247	PRO	2.0
1	E	118	ARG	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 oligosaccharides 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	NA	D	402	1/1	0.21	0.32	133,133,133,133	0
3	NA	B	402	1/1	0.34	0.37	152,152,152,152	0
3	NA	A	403	1/1	0.43	1.02	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	E	402	1/1	0.56	0.19	146,146,146,146	0
4	MBR	E	404	4/4	0.57	0.16	288,289,290,292	0
4	MBR	B	403	4/4	0.72	0.15	251,252,252,253	0
3	NA	A	402	1/1	0.72	0.16	145,145,145,145	0
4	MBR	D	403	4/4	0.75	0.12	289,289,289,289	0
4	MBR	A	404	4/4	0.77	0.13	252,254,255,255	0
4	MBR	E	403	4/4	0.78	0.20	282,285,286,286	0
4	MBR	C	402	4/4	0.78	0.13	254,256,256,258	0
3	NA	C	401	1/1	0.88	0.09	130,130,130,130	0
2	CL	D	401	1/1	0.89	0.14	126,126,126,126	0
2	CL	E	401	1/1	0.92	0.10	126,126,126,126	0
2	CL	B	401	1/1	0.93	0.10	119,119,119,119	0
2	CL	A	401	1/1	0.94	0.07	102,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.