



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 10:12 AM EDT

PDB ID : 9Z9F / pdb_00009z9f
Title : Structure of FabS1CE2_ER-2a in complex with the extracellular region of EGFR
Authors : Mallette, E.; Singer, A.U.; Bruce, H.A.; Blazer, L.L.; Adams, J.J.; Suits, M.D.L.; Sidhu, S.S.
Deposited on : 2025-11-18
Resolution : 3.06 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

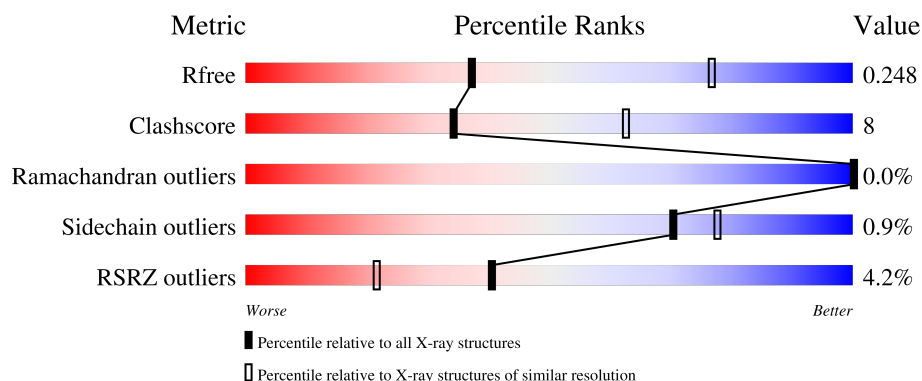
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	237	<div> <div>2%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	C	237	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	B	212	<div> <div>89%</div> <div>11%</div> </div>
2	D	212	<div> <div>%</div> <div>85%</div> <div>15%</div> </div>
3	G	625	<div> <div>10%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	K	625	<div><div></div><div>3%</div><div>79%</div><div>19%</div><div></div></div>
4	E	2	<div><div></div><div>100%</div><div></div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15825 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1758	1127	288	335	8			
1	C	232	Total	C	N	O	S	0	1	0
			1747	1115	288	336	8			

- Molecule 2 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1628	1019	269	334	6			
2	D	212	Total	C	N	O	S	0	2	0
			1643	1027	271	339	6			

- Molecule 3 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	601	Total	C	N	O	S	0	1	0
			4295	2632	755	848	60			
3	K	613	Total	C	N	O	S	0	0	0
			4570	2814	808	888	60			

There are 8 discrepancies between the modelled and reference sequences:

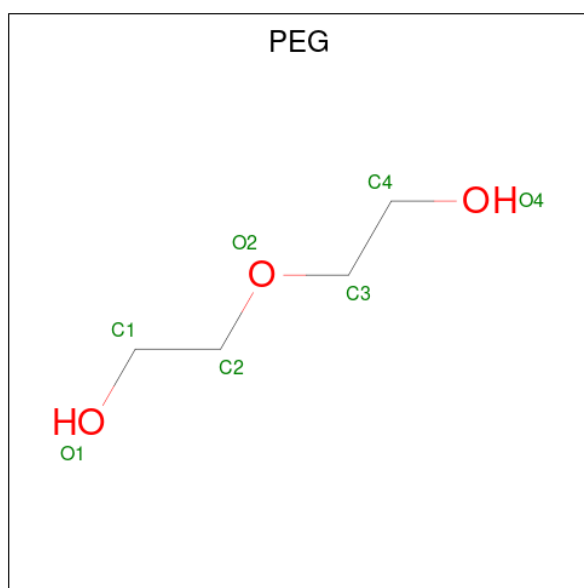
Chain	Residue	Modelled	Actual	Comment	Reference
G	622	LEU	-	expression tag	UNP P00533
G	623	VAL	-	expression tag	UNP P00533
G	624	PRO	-	expression tag	UNP P00533
G	625	ARG	-	expression tag	UNP P00533
K	622	LEU	-	expression tag	UNP P00533
K	623	VAL	-	expression tag	UNP P00533
K	624	PRO	-	expression tag	UNP P00533
K	625	ARG	-	expression tag	UNP P00533

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			14	8	6		
5	A	1	Total	C	O	0	1
			14	8	6		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		
6	B	2	Total	Na	0	0
			2	2		
6	D	4	Total	Na	0	0
			4	4		

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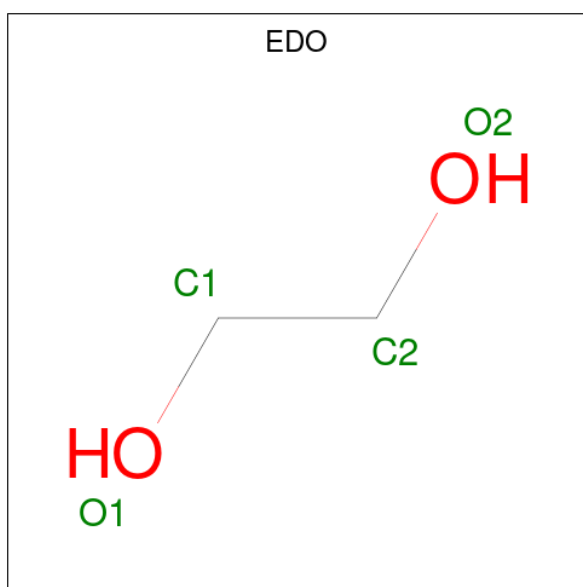
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Na	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

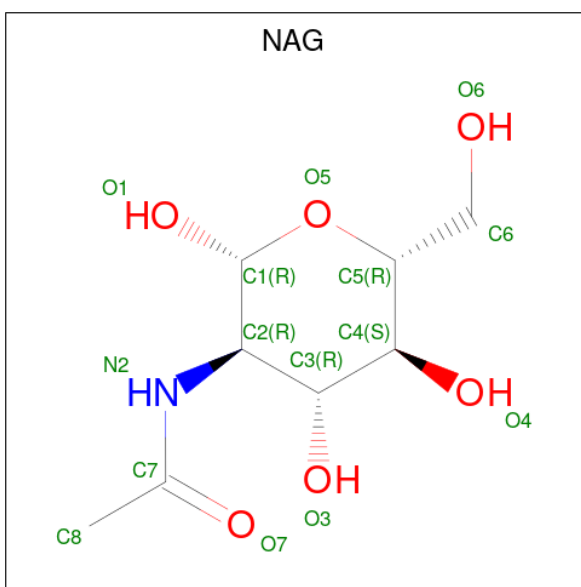
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	D	2	Total	Cl	0	0
			2	2		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	1	Total	C	N	O	0	0
			14	8	1	5		
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	K	1	Total	C	N	O	0	0
			14	8	1	5		

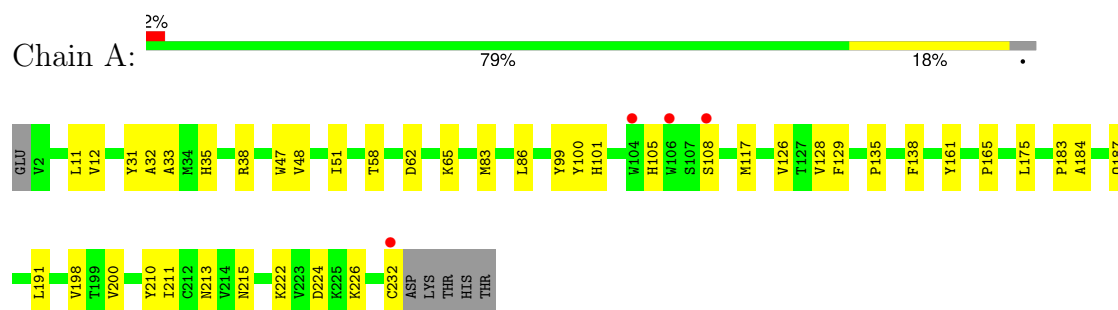
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	O	0	0
			1	1		
10	C	3	Total	O	0	0
			3	3		
10	D	5	Total	O	0	0
			5	5		
10	G	1	Total	O	0	0
			1	1		

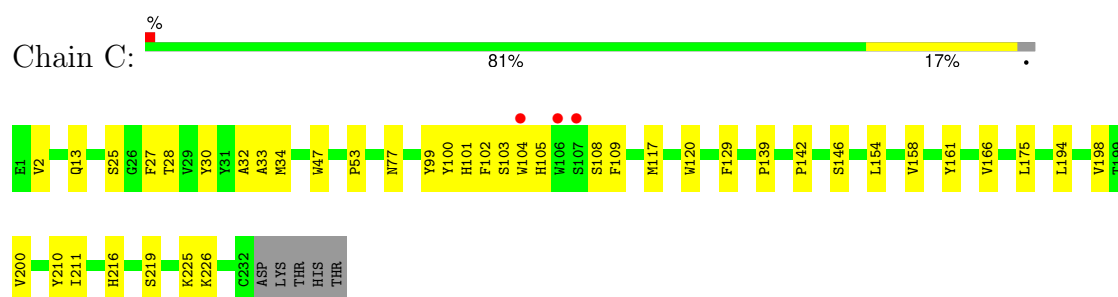
3 Residue-property plots [i](#)

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.

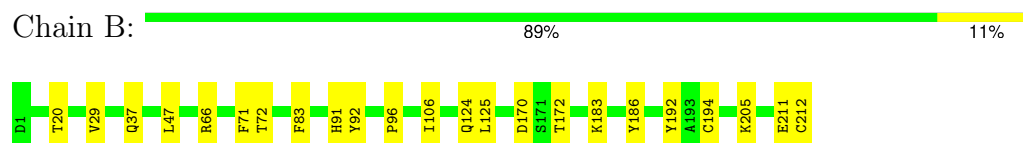
- Molecule 1: heavy chain



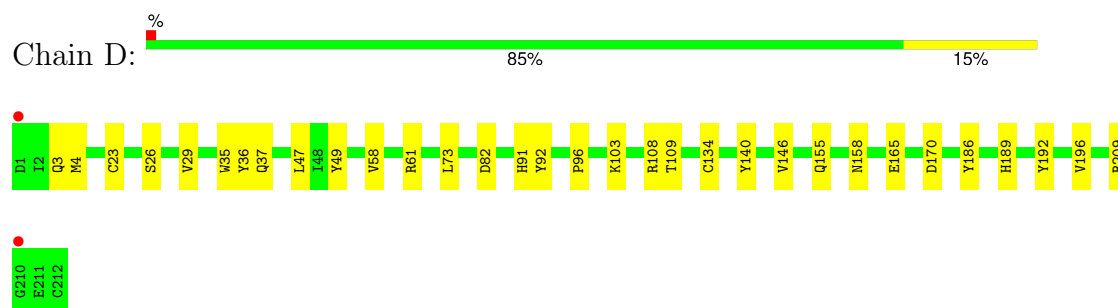
- Molecule 1: heavy chain



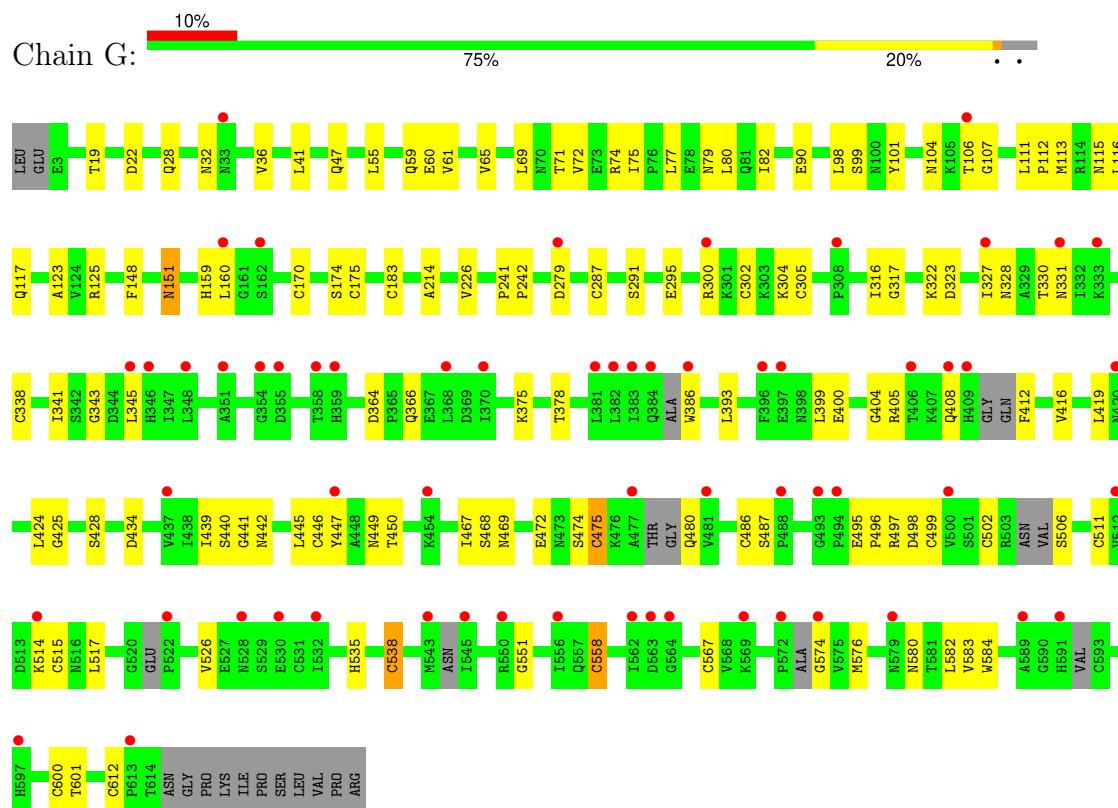
- Molecule 2: light chain



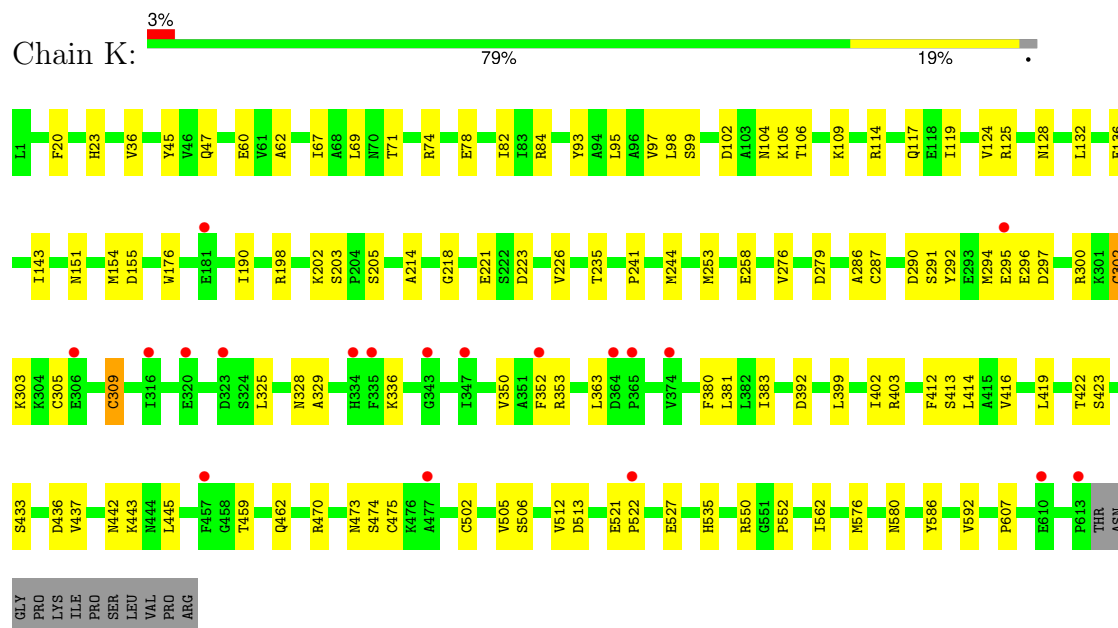
- Molecule 2: light chain



- Molecule 3: Epidermal growth factor receptor



- Molecule 3: Epidermal growth factor receptor



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.53Å 113.85Å 118.77Å 114.16° 95.24° 104.88°	Depositor
Resolution (Å)	34.42 – 3.06 34.42 – 3.06	Depositor EDS
% Data completeness (in resolution range)	91.4 (34.42-3.06) 91.3 (34.42-3.06)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.213 , 0.249 0.212 , 0.248	Depositor DCC
R_{free} test set	2602 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15825	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, EDO, NA, PEG

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	0.13	0/1813	0.35	0/2477
1	C	0.13	0/1799	0.37	0/2457
2	B	0.15	0/1664	0.38	0/2264
2	D	0.14	0/1679	0.38	0/2285
3	G	0.17	0/4367	0.42	0/5946
3	K	0.13	0/4660	0.38	0/6333
All	All	0.14	0/15982	0.39	0/21762

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1758	0	1677	30	0
1	C	1747	0	1662	28	0
2	B	1628	0	1568	14	0
2	D	1643	0	1573	20	0
3	G	4295	0	3790	79	1
3	K	4570	0	4237	73	2
4	E	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	40	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	4	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	D	2	0	0	0	0
8	B	8	0	12	0	0
9	G	14	0	13	0	1
9	K	84	0	78	4	0
10	B	1	0	0	0	0
10	C	3	0	0	0	0
10	D	5	0	0	0	0
10	G	1	0	0	0	0
All	All	15825	0	14675	232	2

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 8.

All (232) 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)
3:G:475:CYS:SG	3:G:480:GLN:NE2	2.54	0.78
3:G:323:ASP:HB2	4:E:2:NAG:H3	1.68	0.76
3:G:90:GLU:OE2	3:G:580:ASN:ND2	2.20	0.74
3:G:441:GLY:H	3:G:468:SER:HB2	1.52	0.74
3:K:104:ASN:HB2	3:K:106:THR:HG23	1.70	0.74
1:A:105:HIS:HA	3:K:279:ASP:HB3	1.71	0.72
3:G:496:PRO:HB2	3:G:511:CYS:HB2	1.71	0.72
3:G:495:GLU:HG3	3:G:497:ARG:H	1.55	0.71
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.73	0.70
3:G:47:GLN:HA	3:G:71:THR:HG23	1.74	0.69
3:K:392:ASP:HB3	3:K:423:SER:HB2	1.75	0.69
3:K:190:ILE:HD12	3:K:202:LYS:HG2	1.75	0.68
1:A:213:ASN:ND2	1:A:224:ASP:OD1	2.25	0.68
1:C:33:ALA:HB3	1:C:99:TYR:HB2	1.75	0.68
3:G:79:ASN:HA	3:G:115:ASN:HD22	1.59	0.68
3:K:521:GLU:HB3	3:K:522:PRO:HD3	1.77	0.67
3:G:82:ILE:HG21	3:G:226:VAL:HG11	1.77	0.66
3:G:446:CYS:O	3:G:449:ASN:ND2	2.30	0.64
3:K:328:ASN:HD22	9:K:703:NAG:H83	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:341:ILE:HG22	3:G:343:GLY:H	1.61	0.64
3:G:424:LEU:HG	3:G:445:LEU:HD11	1.81	0.63
2:D:189:HIS:O	2:D:209:ARG:NH1	2.33	0.62
3:K:221:GLU:HG3	3:K:235:THR:HG23	1.80	0.62
1:A:33:ALA:HB3	1:A:99:TYR:HB2	1.80	0.62
3:G:316:ILE:HD12	3:G:345:LEU:HA	1.81	0.61
1:C:139:PRO:HD3	1:C:225:LYS:HE2	1.82	0.61
1:A:11:LEU:HB3	1:A:129:PHE:CE2	2.36	0.61
3:G:408:GLN:HB3	3:G:412:PHE:HB2	1.83	0.60
1:C:30:TYR:HA	1:C:53:PRO:HB2	1.84	0.60
3:K:292:TYR:HD1	3:K:305:CYS:HB2	1.67	0.60
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.83	0.59
3:G:317:GLY:HA2	3:G:322:LYS:HA	1.84	0.59
3:G:517:LEU:HD21	3:G:526:VAL:HG23	1.84	0.59
3:G:19:THR:HG23	3:G:22:ASP:H	1.68	0.59
3:G:36:VAL:HG22	3:G:60:GLU:HB2	1.85	0.58
1:C:216:HIS:ND1	1:C:219:SER:OG	2.30	0.58
1:C:104:TRP:CD1	2:D:49:TYR:HH	2.21	0.58
3:K:95:LEU:HB3	3:K:124:VAL:HG13	1.86	0.58
3:G:117:GLN:HB2	3:G:214:ALA:HB1	1.85	0.57
3:K:292:TYR:CD1	3:K:305:CYS:HB2	2.39	0.57
3:G:440:SER:HA	3:G:467:ILE:O	2.05	0.56
3:G:295:GLU:HG2	3:G:300:ARG:HA	1.86	0.56
2:B:125:LEU:HD12	2:B:183:LYS:HG3	1.87	0.56
1:C:32:ALA:HB2	1:C:100:TYR:HD2	1.70	0.56
2:B:211:GLU:HG2	2:B:212:CYS:H	1.71	0.56
3:K:295:GLU:HA	3:K:300:ARG:HA	1.88	0.55
2:D:146:VAL:HG22	2:D:196:VAL:HG22	1.87	0.55
3:K:218:GLY:H	3:K:223:ASP:HB3	1.71	0.55
3:K:290:ASP:O	3:K:305:CYS:HB3	2.07	0.55
3:K:329:ALA:HA	3:K:363:LEU:HD13	1.87	0.54
2:D:4:MET:HE3	2:D:23:CYS:SG	2.48	0.54
3:G:287:CYS:HB3	3:G:291:SER:HB2	1.90	0.54
1:A:83:MET:HE1	1:A:126:VAL:HG11	1.90	0.53
1:A:105:HIS:H	1:A:108:SER:HB2	1.72	0.53
3:G:316:ILE:HD11	3:G:327:ILE:HG23	1.91	0.53
1:A:11:LEU:HB3	1:A:129:PHE:HE2	1.72	0.53
3:G:447:TYR:O	3:G:450:THR:HG22	2.09	0.53
1:C:142:PRO:HG3	1:C:154:LEU:HB3	1.91	0.53
3:K:294:MET:HG2	3:K:296:GLU:HG2	1.90	0.52
3:G:496:PRO:HA	3:G:499:CYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:412:PHE:CD1	3:K:436:ASP:HB2	2.44	0.52
3:K:381:LEU:HG	3:K:383:ILE:HD11	1.92	0.52
3:K:99:SER:HA	3:K:128:ASN:O	2.09	0.52
2:B:91:HIS:CD2	2:B:96:PRO:HG3	2.44	0.52
1:A:47:TRP:CE3	2:B:96:PRO:HD2	2.44	0.52
3:G:104:ASN:HB3	3:G:106:THR:HG22	1.93	0.51
1:C:101:HIS:CE1	1:C:104:TRP:H	2.28	0.51
3:K:117:GLN:HB2	3:K:214:ALA:HB1	1.92	0.51
3:K:67:ILE:HB	3:K:97:VAL:HG22	1.91	0.51
3:G:59:GLN:HA	3:G:80:LEU:HA	1.93	0.51
3:G:416:VAL:HG13	3:G:419:LEU:HD12	1.92	0.51
1:C:105:HIS:HB2	1:C:108:SER:O	2.10	0.51
3:K:71:THR:HG21	3:K:102:ASP:HB3	1.92	0.51
2:B:29:VAL:HG13	2:B:92:TYR:HB2	1.93	0.50
1:C:109:PHE:HZ	3:G:279:ASP:HA	1.76	0.50
3:K:586:TYR:CE2	3:K:607:PRO:HD3	2.46	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.92	0.50
3:G:291:SER:HB3	3:G:302:CYS:HB3	1.94	0.50
3:G:72:VAL:HG12	3:G:74:ARG:H	1.75	0.50
3:K:422:THR:HA	3:K:445:LEU:HA	1.94	0.50
1:A:31:TYR:OH	3:K:258:GLU:OE1	2.27	0.50
1:A:175:LEU:HD21	1:A:198:VAL:HG21	1.93	0.50
3:K:114:ARG:HA	3:K:176:TRP:CD1	2.47	0.50
1:A:62:ASP:HA	1:A:65:LYS:HD2	1.93	0.50
1:A:215:ASN:HD21	1:A:222:LYS:HE3	1.77	0.50
3:K:505:VAL:HG23	3:K:512:VAL:HG23	1.93	0.50
3:G:487:SER:OG	3:G:502:CYS:O	2.30	0.49
1:A:32:ALA:HB2	1:A:100:TYR:HD1	1.77	0.49
3:K:412:PHE:HD1	3:K:436:ASP:HB2	1.77	0.49
1:C:101:HIS:CE1	1:C:105:HIS:HD2	2.31	0.49
1:A:138:PHE:CE2	2:B:124:GLN:HG3	2.48	0.49
3:K:419:LEU:N	3:K:442:ASN:OD1	2.43	0.49
1:C:175:LEU:HD21	1:C:198:VAL:HG21	1.95	0.49
3:K:328:ASN:HD22	9:K:703:NAG:C8	2.26	0.48
1:A:101:HIS:HB2	3:K:253:MET:HE3	1.95	0.48
2:D:3:GLN:N	2:D:26:SER:OG	2.41	0.48
3:G:574:GLY:N	3:G:583:VAL:O	2.46	0.48
3:G:558:CYS:HB3	3:G:567:CYS:HB3	1.73	0.48
3:G:61:VAL:HG23	3:G:80:LEU:HD11	1.95	0.48
3:G:502:CYS:SG	3:G:506:SER:HB2	2.54	0.48
3:G:123:ALA:HB2	3:G:148:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:498:ASP:OD1	3:G:498:ASP:N	2.45	0.48
2:D:186:TYR:HA	2:D:192:TYR:OH	2.15	0.47
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.96	0.47
3:G:386:TRP:HB3	3:G:419:LEU:HD22	1.96	0.47
3:G:378:THR:HG23	3:G:405[A]:ARG:HD3	1.97	0.47
3:G:514:LYS:HG3	3:G:515:CYS:H	1.78	0.47
3:K:399:LEU:HD21	3:K:402:ILE:HD11	1.97	0.47
3:G:28:GLN:O	3:G:32:ASN:HB2	2.14	0.47
3:G:600:CYS:SG	3:G:612:CYS:HB2	2.55	0.47
3:K:119:ILE:HG13	3:K:143:ILE:HG22	1.96	0.47
1:C:101:HIS:CE1	1:C:105:HIS:CD2	3.03	0.47
3:K:535:HIS:CD2	3:K:552:PRO:HG3	2.50	0.47
1:A:51:ILE:HG13	1:A:58:THR:HG22	1.96	0.47
1:A:165:PRO:HA	5:A:302[B]:PEG:H11	1.97	0.47
3:K:36:VAL:HG13	3:K:60:GLU:HB2	1.97	0.47
3:K:98:LEU:HD13	3:K:580:ASN:HB3	1.96	0.46
3:G:170:CYS:N	3:G:183:CYS:SG	2.89	0.46
3:G:295:GLU:HA	3:G:300:ARG:HA	1.97	0.46
3:K:82:ILE:HG21	3:K:226:VAL:HG21	1.97	0.46
1:A:211:ILE:HD11	1:A:226:LYS:HD3	1.97	0.46
1:A:101:HIS:CG	3:K:244:MET:HB2	2.50	0.46
1:A:187:GLN:HG3	1:A:191:LEU:O	2.15	0.46
3:G:55:LEU:HB3	3:G:77:LEU:HD23	1.97	0.46
3:G:538:CYS:HA	3:G:558:CYS:HA	1.97	0.46
3:K:416:VAL:HG13	3:K:419:LEU:HD22	1.98	0.46
1:C:47:TRP:CE3	2:D:96:PRO:HD2	2.50	0.46
3:K:151:ASN:OD1	9:K:701:NAG:O5	2.33	0.46
1:C:211:ILE:HG12	1:C:226:LYS:HG3	1.96	0.46
2:D:29:VAL:HA	2:D:92:TYR:CD2	2.51	0.46
3:K:352:PHE:CD1	3:K:363:LEU:HB3	2.51	0.46
2:D:108:ARG:HG2	2:D:140:TYR:CG	2.51	0.45
3:G:439:ILE:HG23	3:G:442:ASN:HD22	1.81	0.45
1:C:117:MET:O	2:D:36:TYR:HE2	1.98	0.45
1:C:200:VAL:HG11	1:C:210:TYR:CZ	2.51	0.45
3:G:375:LYS:HA	3:G:399:LEU:HA	1.98	0.45
3:G:439:ILE:HG23	3:G:442:ASN:ND2	2.31	0.45
1:A:200:VAL:HG11	1:A:210:TYR:CZ	2.51	0.45
3:G:472:GLU:C	3:G:474:SER:H	2.24	0.45
3:K:380:PHE:HB2	3:K:413:SER:HA	1.98	0.45
3:G:328:ASN:HB2	3:G:331:ASN:N	2.32	0.45
2:D:108:ARG:HG3	2:D:109:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:328:ASN:HB2	3:G:331:ASN:H	1.81	0.45
3:G:576:MET:HB3	3:G:576:MET:HE2	1.64	0.45
3:K:527:GLU:OE1	3:K:550:ARG:NH1	2.50	0.45
3:K:136:GLU:OE1	3:K:136:GLU:N	2.48	0.45
3:K:336:LYS:HB2	3:K:336:LYS:HE3	1.71	0.45
1:C:120:TRP:H	1:C:120:TRP:CD1	2.35	0.45
2:D:35:TRP:CD2	2:D:73:LEU:HB2	2.52	0.45
1:A:184:ALA:HB3	5:A:302[B]:PEG:H32	1.98	0.44
3:G:99:SER:HB3	3:G:582:LEU:HD11	1.99	0.44
3:G:291:SER:HA	3:G:304:LYS:O	2.18	0.44
3:K:350:VAL:HA	3:K:353:ARG:HD3	2.00	0.44
3:G:69:LEU:HD23	3:G:99:SER:O	2.16	0.44
3:K:276:VAL:HG23	3:K:286:ALA:HB2	1.99	0.44
2:B:20:THR:HG23	2:B:72:THR:HG23	2.00	0.44
3:G:495:GLU:CD	3:G:496:PRO:HD2	2.42	0.44
3:K:403:ARG:O	3:K:433:SER:HB2	2.17	0.44
2:D:91:HIS:NE2	2:D:96:PRO:HG3	2.33	0.44
3:K:562:ILE:HD12	3:K:592:VAL:HG22	1.99	0.44
1:C:13:GLN:HA	1:C:129:PHE:O	2.18	0.44
3:K:328:ASN:HD22	9:K:703:NAG:C7	2.31	0.44
3:K:23:HIS:HD1	3:K:23:HIS:C	2.27	0.43
1:A:31:TYR:CE2	3:K:241:PRO:HB3	2.53	0.43
2:D:108:ARG:NE	2:D:170:ASP:O	2.50	0.43
2:D:155:GLN:OE1	2:D:158:ASN:ND2	2.44	0.43
3:G:113:MET:HE3	3:G:116:LEU:HD22	1.99	0.43
3:G:576:MET:CE	3:G:580:ASN:HA	2.49	0.43
1:C:28:THR:HG22	1:C:30:TYR:H	1.84	0.43
3:G:328:ASN:HB3	3:G:330:THR:H	1.82	0.43
1:C:47:TRP:CD2	2:D:96:PRO:HD2	2.53	0.43
3:G:101:TYR:HA	3:G:107:GLY:HA3	2.00	0.43
3:G:364:ASP:C	3:G:366:GLN:H	2.27	0.43
3:G:424:LEU:HD23	3:G:424:LEU:HA	1.85	0.43
2:B:186:TYR:O	2:B:192:TYR:OH	2.31	0.43
2:D:103:LYS:HZ3	2:D:165:GLU:CD	2.27	0.43
3:K:69:LEU:HD11	3:K:576:MET:HE2	2.01	0.43
3:G:41:LEU:HB3	3:G:65:VAL:HG22	2.00	0.43
3:G:576:MET:HE3	3:G:580:ASN:HA	2.00	0.43
2:B:66:ARG:HG3	2:B:71:PHE:CE2	2.53	0.42
3:K:436:ASP:OD1	3:K:462:GLN:HA	2.18	0.42
3:K:513:ASP:OD1	3:K:513:ASP:N	2.52	0.42
1:C:34:MET:HE3	1:C:34:MET:HB3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:584:TRP:NE1	3:G:601:THR:O	2.53	0.42
3:G:393:LEU:H	3:G:425:GLY:H	1.67	0.42
3:K:291:SER:HB3	3:K:303:LYS:HA	2.01	0.42
1:C:161:TYR:OH	1:C:194:LEU:HD23	2.19	0.42
3:K:292:TYR:HB3	3:K:309:CYS:SG	2.59	0.42
1:C:158:VAL:HG11	1:C:166:VAL:HG11	2.02	0.42
1:A:35:HIS:CG	1:A:117:MET:HE2	2.55	0.42
3:K:203:SER:OG	3:K:205:SER:OG	2.36	0.42
1:A:38:ARG:HG2	1:A:48:VAL:HG23	2.02	0.42
3:G:404:GLY:HA3	3:G:434:ASP:O	2.20	0.42
3:K:294:MET:HB3	3:K:302:CYS:HA	2.02	0.42
1:A:183:PRO:HA	5:A:302[A]:PEG:H12	2.02	0.41
1:C:27:PHE:O	1:C:77:ASN:ND2	2.37	0.41
1:C:146:SER:O	1:C:146:SER:OG	2.38	0.41
3:G:535:HIS:HB2	3:G:551:GLY:H	1.85	0.41
3:K:20:PHE:CD2	3:K:47:GLN:HG3	2.55	0.41
2:B:211:GLU:HG2	2:B:212:CYS:N	2.35	0.41
1:C:102:PHE:O	1:C:103:SER:C	2.63	0.41
3:K:62:ALA:HA	3:K:84:ARG:HB2	2.02	0.41
3:K:325:LEU:HD23	3:K:325:LEU:H	1.84	0.41
3:K:109:LYS:HA	3:K:132:LEU:HA	2.01	0.41
3:K:414:LEU:HB3	3:K:437:VAL:HG22	2.02	0.41
3:K:433:SER:O	3:K:459:THR:HG22	2.20	0.41
3:K:93:TYR:CE1	3:K:125:ARG:HB2	2.56	0.41
3:K:443:LYS:O	3:K:470:ARG:HD3	2.20	0.41
2:B:205:LYS:HA	2:B:205:LYS:HD2	1.93	0.41
2:D:61:ARG:NE	2:D:82:ASP:OD2	2.42	0.41
3:G:400:GLU:HA	3:G:428:SER:O	2.21	0.41
3:K:502:CYS:SG	3:K:506:SER:HB3	2.60	0.41
3:G:98:LEU:HD21	3:G:125:ARG:HG2	2.02	0.41
3:G:241:PRO:HA	3:G:242:PRO:HD3	1.91	0.41
3:K:45:TYR:HE1	3:K:69:LEU:HD22	1.85	0.41
3:K:74:ARG:NH2	3:K:78:GLU:OE2	2.54	0.41
2:B:83:PHE:CD1	2:B:106:ILE:HG13	2.56	0.41
2:B:170:ASP:OD1	2:B:172:THR:OG1	2.38	0.41
3:G:170:CYS:HB3	3:G:174:SER:O	2.21	0.41
3:K:291:SER:HA	3:K:305:CYS:HB3	2.02	0.41
3:G:75:ILE:O	3:G:112:PRO:HD2	2.21	0.40
1:A:83:MET:HE1	1:A:126:VAL:HG21	2.03	0.40
3:K:198:ARG:H	3:K:198:ARG:HG2	1.66	0.40
1:A:12:VAL:O	1:A:128:VAL:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:VAL:HA	1:C:25:SER:O	2.22	0.40
3:G:159:HIS:O	3:G:160:LEU:HB3	2.20	0.40
3:K:104:ASN:O	3:K:105:LYS:HB2	2.21	0.40
3:K:473:ASN:OD1	3:K:474:SER:N	2.55	0.40
1:A:135:PRO:HB3	1:A:161:TYR:HB3	2.02	0.40
3:G:75:ILE:HB	3:G:111:LEU:HD12	2.03	0.40
3:G:439:ILE:CG2	3:G:445:LEU:HD23	2.52	0.40
3:G:467:ILE:C	3:G:469:ASN:H	2.29	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:151:ASN:OD1	3:K:154:MET:O[1_554]	1.61	0.59
3:K:155:ASP:OD2	9:G:701:NAG:O6[1_556]	1.83	0.37

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	230/237 (97%)	224 (97%)	6 (3%)	0	100	100
1	C	231/237 (98%)	224 (97%)	7 (3%)	0	100	100
2	B	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
2	D	211/212 (100%)	202 (96%)	9 (4%)	0	100	100
3	G	584/625 (93%)	528 (90%)	56 (10%)	0	100	100
3	K	611/625 (98%)	564 (92%)	46 (8%)	1 (0%)	43	70
All	All	2077/2148 (97%)	1945 (94%)	131 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	297	ASP

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	190/196 (97%)	189 (100%)	1 (0%)	81	82
1	C	188/196 (96%)	188 (100%)	0	100	100
2	B	186/187 (100%)	185 (100%)	1 (0%)	81	82
2	D	187/187 (100%)	186 (100%)	1 (0%)	81	82
3	G	442/546 (81%)	434 (98%)	8 (2%)	51	70
3	K	498/546 (91%)	494 (99%)	4 (1%)	73	79
All	All	1691/1858 (91%)	1676 (99%)	15 (1%)	70	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	CYS
2	B	194	CYS
2	D	134	CYS
3	G	151	ASN
3	G	175	CYS
3	G	305	CYS
3	G	338	CYS
3	G	475	CYS
3	G	486	CYS
3	G	538	CYS
3	G	558	CYS
3	K	287	CYS
3	K	302	CYS
3	K	309	CYS
3	K	475	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	138	ASN
1	C	180	HIS
2	D	79	GLN
2	D	138	ASN
2	D	189	HIS
3	G	47	GLN
3	G	115	ASN
3	G	121	HIS
3	G	211	GLN
3	G	408	GLN
3	G	480	GLN
3	G	541	GLN
3	K	139	GLN
3	K	469	ASN
3	K	528	ASN
3	K	566	HIS
3	K	597	HIS

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 ⓘ

2 monosaccharides 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	$\# Z > 2$
4	NAG	E	1	3,4	14,14,15	0.61	1 (7%)	17,19,21	0.73	0
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	0.42	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
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	O5-C1	-2.04	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

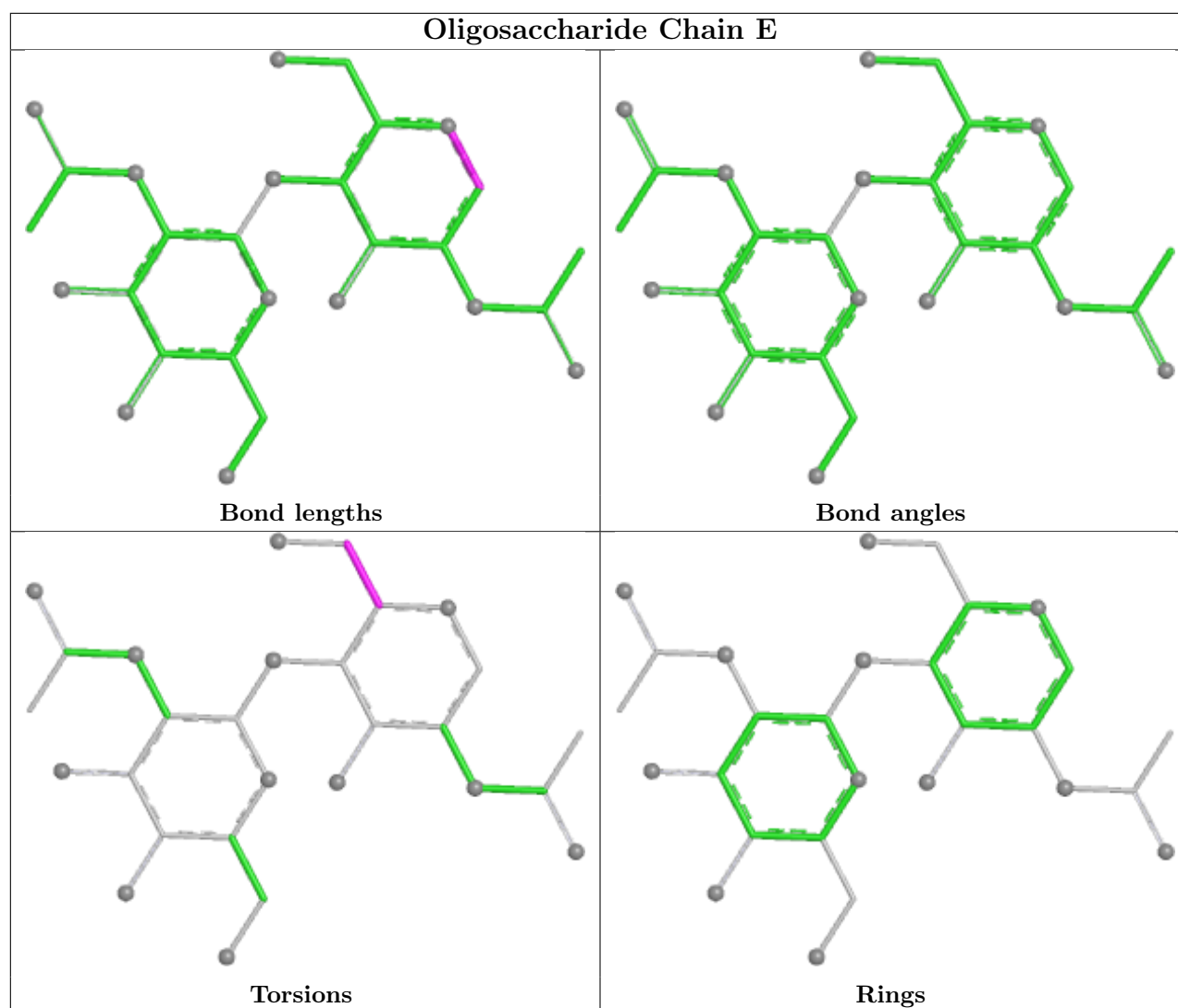
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	$\# Z > 2$
5	PEG	A	302[A]	-	6,6,6	0.11	0	5,5,5	0.09	0
9	NAG	K	701	3	14,14,15	0.98	1 (7%)	17,19,21	1.44	1 (5%)
9	NAG	K	705	3	14,14,15	1.34	1 (7%)	17,19,21	1.28	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	A	301[A]	-	6,6,6	0.13	0	5,5,5	0.08	0
8	EDO	B	302	-	3,3,3	0.44	0	2,2,2	0.39	0
9	NAG	K	703	3	14,14,15	0.29	0	17,19,21	0.33	0
8	EDO	B	301	-	3,3,3	0.46	0	2,2,2	0.27	0
9	NAG	K	706	3	14,14,15	0.18	0	17,19,21	0.45	0
9	NAG	G	701	3	14,14,15	0.45	0	17,19,21	1.02	2 (11%)
9	NAG	K	704	3	14,14,15	0.26	0	17,19,21	0.65	1 (5%)
5	PEG	A	302[B]	-	6,6,6	0.10	0	5,5,5	0.10	0
5	PEG	A	301[B]	-	6,6,6	0.09	0	5,5,5	0.11	0
9	NAG	K	702	3	14,14,15	0.32	0	17,19,21	0.63	1 (5%)

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
5	PEG	A	302[A]	-	-	3/4/4/4	-
9	NAG	K	701	3	-	2/6/23/26	0/1/1/1
9	NAG	K	705	3	-	4/6/23/26	0/1/1/1
5	PEG	A	301[A]	-	-	2/4/4/4	-
8	EDO	B	302	-	-	1/1/1/1	-
9	NAG	K	703	3	-	3/6/23/26	0/1/1/1
8	EDO	B	301	-	-	0/1/1/1	-
9	NAG	K	706	3	-	0/6/23/26	0/1/1/1
9	NAG	G	701	3	-	2/6/23/26	0/1/1/1
9	NAG	K	704	3	-	4/6/23/26	0/1/1/1
5	PEG	A	302[B]	-	-	3/4/4/4	-
5	PEG	A	301[B]	-	-	2/4/4/4	-
9	NAG	K	702	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	705	NAG	O5-C1	4.85	1.51	1.43
9	K	701	NAG	O5-C1	3.03	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	701	NAG	C1-O5-C5	5.58	119.66	112.19
9	K	705	NAG	C1-O5-C5	4.69	118.47	112.19
9	K	704	NAG	C1-O5-C5	2.25	115.20	112.19
9	K	702	NAG	C1-O5-C5	2.20	115.14	112.19
9	G	701	NAG	O5-C1-C2	-2.17	107.93	111.29
9	G	701	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	701	NAG	C4-C5-C6-O6
9	K	705	NAG	O5-C5-C6-O6
9	K	704	NAG	O5-C5-C6-O6
9	K	704	NAG	C4-C5-C6-O6
9	K	701	NAG	O5-C5-C6-O6
9	K	705	NAG	C4-C5-C6-O6
9	G	701	NAG	C8-C7-N2-C2
9	G	701	NAG	O7-C7-N2-C2
9	K	702	NAG	C8-C7-N2-C2
9	K	702	NAG	O7-C7-N2-C2
9	K	703	NAG	C8-C7-N2-C2
9	K	703	NAG	O7-C7-N2-C2
9	K	704	NAG	C8-C7-N2-C2
9	K	704	NAG	O7-C7-N2-C2
9	K	705	NAG	C8-C7-N2-C2
9	K	705	NAG	O7-C7-N2-C2
5	A	302[A]	PEG	O2-C3-C4-O4
5	A	302[A]	PEG	O1-C1-C2-O2
5	A	302[B]	PEG	O2-C3-C4-O4
9	K	703	NAG	O5-C5-C6-O6
5	A	302[B]	PEG	C1-C2-O2-C3
5	A	301[B]	PEG	C4-C3-O2-C2
5	A	301[A]	PEG	O1-C1-C2-O2
5	A	301[B]	PEG	O1-C1-C2-O2
5	A	301[A]	PEG	C1-C2-O2-C3
8	B	302	EDO	O1-C1-C2-O2
5	A	302[A]	PEG	C1-C2-O2-C3
5	A	302[B]	PEG	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	302[A]	PEG	1	0
9	K	701	NAG	1	0
9	K	703	NAG	3	0
9	G	701	NAG	0	1
5	A	302[B]	PEG	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	231/237 (97%)	-0.20	4 (1%) 69 46	20, 28, 42, 82	1 (0%)
1	C	232/237 (97%)	-0.19	3 (1%) 75 53	11, 27, 44, 91	1 (0%)
2	B	212/212 (100%)	-0.25	0 100 100	20, 31, 44, 58	0
2	D	212/212 (100%)	-0.23	2 (0%) 81 61	11, 30, 42, 60	2 (0%)
3	G	601/625 (96%)	0.87	61 (10%) 12 6	25, 110, 148, 160	1 (0%)
3	K	613/625 (98%)	0.50	19 (3%) 51 29	22, 79, 115, 130	0
All	All	2101/2148 (97%)	0.31	89 (4%) 40 21	11, 58, 140, 160	5 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106[A]	TRP	4.2
3	G	591	HIS	4.1
1	C	106	TRP	4.0
1	C	104	TRP	3.9
3	G	522	PRO	3.8
1	C	107	SER	3.6
3	G	437	VAL	3.5
3	G	351	ALA	3.4
3	G	613	PRO	3.3
3	K	610	GLU	3.2
3	G	545	ILE	3.2
2	D	210	GLY	3.1
3	G	409	HIS	3.1
3	G	572	PRO	3.1
3	G	562	ILE	3.1
3	K	347	ILE	3.1
3	G	345	LEU	3.0
3	G	579	ASN	3.0
3	G	556	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	G	543	MET	3.0
3	G	368	LEU	3.0
3	G	589	ALA	3.0
3	K	334	HIS	3.0
3	K	477	ALA	2.9
1	A	104	TRP	2.9
3	G	494	PRO	2.9
3	G	33	ASN	2.8
3	G	384	GLN	2.8
3	G	386	TRP	2.7
3	G	355	ASP	2.7
3	G	512	VAL	2.7
3	K	352	PHE	2.7
3	G	346	HIS	2.6
3	G	528	ASN	2.6
3	G	327	ILE	2.6
2	D	1[A]	ASP	2.6
3	K	323	ASP	2.6
3	K	320	GLU	2.6
3	G	477	ALA	2.6
3	G	481	VAL	2.6
3	K	613	PRO	2.6
3	G	381	LEU	2.6
3	G	106	THR	2.5
3	G	160	LEU	2.4
3	K	522	PRO	2.4
3	G	348	LEU	2.4
3	G	359	HIS	2.4
3	K	316	ILE	2.4
3	G	396	PHE	2.4
3	G	308	PRO	2.4
3	K	364	ASP	2.4
3	K	365	PRO	2.4
3	G	564	GLY	2.3
3	G	447	TYR	2.3
3	K	335	PHE	2.3
3	G	514	LYS	2.3
1	A	232	CYS	2.3
3	G	563	ASP	2.3
3	G	569	LYS	2.3
3	K	374	VAL	2.3
1	A	108	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	K	306	GLU	2.2
3	G	358	THR	2.2
3	G	408	GLN	2.2
3	G	420	ASN	2.2
3	G	550	ARG	2.2
3	G	370	ILE	2.2
3	G	532	ILE	2.2
3	G	397	GLU	2.2
3	G	493	GLY	2.2
3	K	343	GLY	2.2
3	G	500	VAL	2.1
3	G	162	SER	2.1
3	G	454	LYS	2.1
3	G	354	GLY	2.1
3	K	457	PHE	2.1
3	G	333	LYS	2.1
3	G	331	ASN	2.1
3	G	383	ILE	2.1
3	G	279	ASP	2.1
3	G	406	THR	2.1
3	G	574	GLY	2.1
3	G	488	PRO	2.1
3	G	530	GLU	2.1
3	K	181	GLU	2.0
3	K	295	GLU	2.0
3	G	300	ARG	2.0
3	G	382	LEU	2.0
3	G	597	HIS	2.0

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

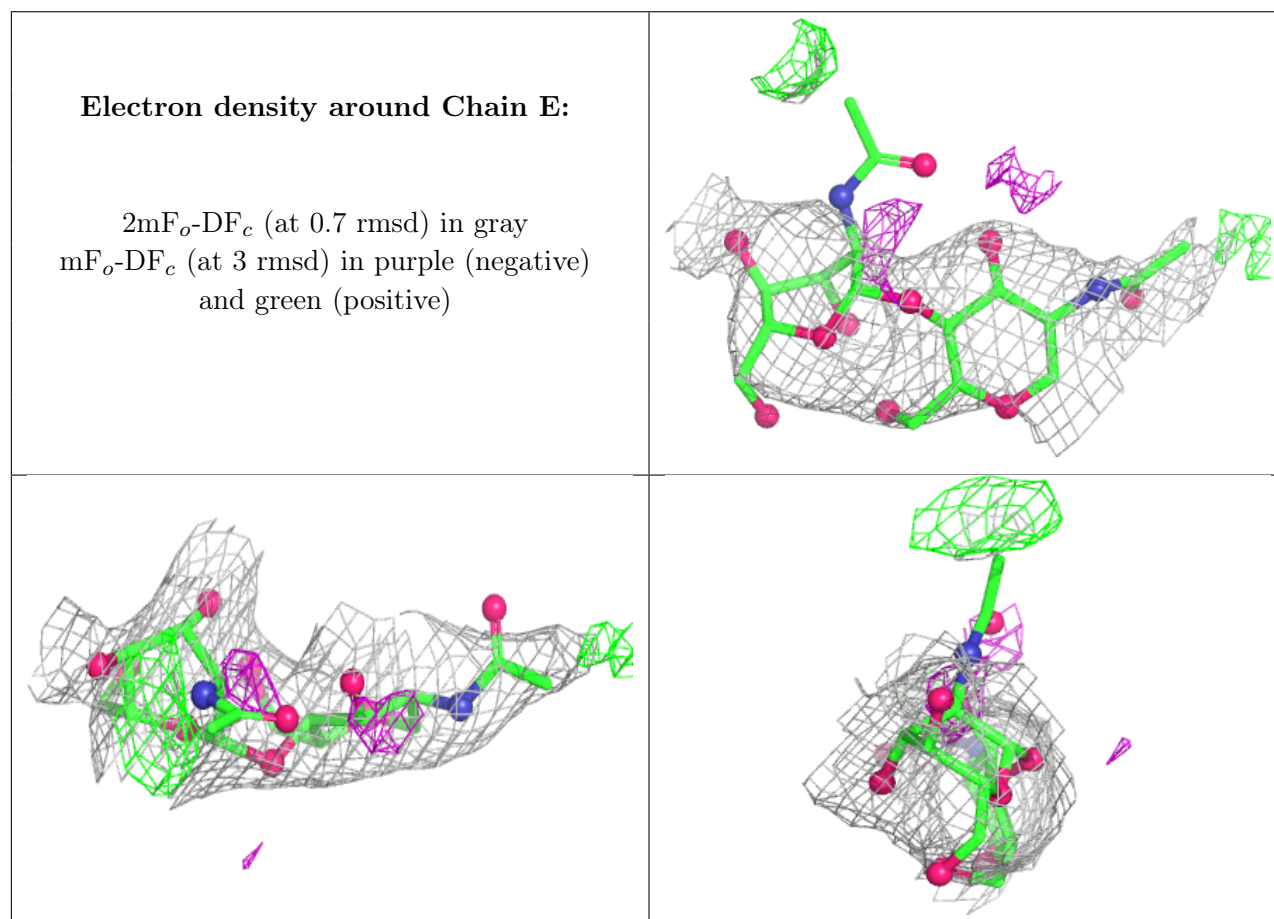
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
4	NAG	E	1	14/15	-	-	129,129,129,129	0
4	NAG	E	2	14/15	-	-	132,132,132,132	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
9	NAG	K	702	14/15	0.62	0.15	88,88,88,88	0
9	NAG	K	705	14/15	0.62	0.17	104,104,104,104	0
9	NAG	K	703	14/15	0.67	0.15	112,112,112,112	0
9	NAG	K	704	14/15	0.68	0.15	100,100,100,100	0
5	PEG	A	302[A]	7/7	0.78	0.32	23,23,23,23	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	302[B]	7/7	0.78	0.32	23,23,23,23	7
6	NA	B	303	1/1	0.79	0.16	27,27,27,27	0
9	NAG	K	701	14/15	0.79	0.14	58,58,58,58	0
9	NAG	K	706	14/15	0.79	0.14	94,94,94,94	0
5	PEG	A	301[B]	7/7	0.83	0.35	25,25,25,25	7
5	PEG	A	301[A]	7/7	0.83	0.35	25,25,25,25	7
8	EDO	B	301	4/4	0.85	0.14	37,37,37,37	0
9	NAG	G	701	14/15	0.85	0.12	60,60,60,60	0
8	EDO	B	302	4/4	0.88	0.13	41,41,41,41	0
6	NA	G	702	1/1	0.88	0.18	40,40,40,40	0
6	NA	D	302	1/1	0.90	0.08	28,28,28,28	0
7	CL	D	306	1/1	0.91	0.08	52,52,52,52	0
6	NA	D	304	1/1	0.91	0.17	35,35,35,35	0
6	NA	A	303	1/1	0.94	0.07	25,25,25,25	0
6	NA	D	301	1/1	0.95	0.08	26,26,26,26	0
6	NA	A	304	1/1	0.95	0.07	29,29,29,29	0
6	NA	D	303	1/1	0.95	0.07	33,33,33,33	0
7	CL	A	305	1/1	0.96	0.07	40,40,40,40	0
7	CL	D	305	1/1	0.96	0.10	47,47,47,47	0
6	NA	B	304	1/1	0.96	0.07	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.