



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:45 PM GMT

PDB ID : 4G1E
Title : Crystal structure of integrin alpha V beta 3 with coil-coiled tag.
Authors : Dong, X.; Mi, L.; Zhu, J.; Wang, W.; Luo, B.; Springer, T.A.
Deposited on : 2012-07-10
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

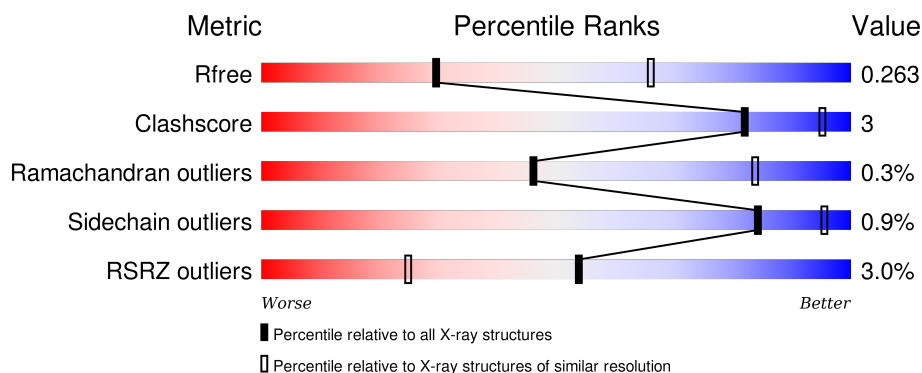
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	998	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>••</div> </div>
2	B	738	<div> <div>4%</div> <div>88%</div> <div>8%</div> <div>•</div> </div>

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	CA	A	2005	-	-	-	X
7	NAG	A	2039	-	-	-	X
9	MAN	A	2034	-	-	-	X
9	MAN	A	2036	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13732 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	964	7512	4752	1271	1453	36	0	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	960	MET	-	EXPRESSION TAG	UNP P06756
A	961	GLY	-	EXPRESSION TAG	UNP P06756
A	962	SER	-	EXPRESSION TAG	UNP P06756
A	963	GLY	-	EXPRESSION TAG	UNP P06756
A	964	GLY	-	EXPRESSION TAG	UNP P06756
A	965	GLU	-	EXPRESSION TAG	UNP P06756
A	966	ASN	-	EXPRESSION TAG	UNP P06756
A	967	ALA	-	EXPRESSION TAG	UNP P06756
A	968	GLN	-	EXPRESSION TAG	UNP P06756
A	969	CYS	-	EXPRESSION TAG	UNP P06756
A	970	GLU	-	EXPRESSION TAG	UNP P06756
A	971	LYS	-	EXPRESSION TAG	UNP P06756
A	972	GLU	-	EXPRESSION TAG	UNP P06756
A	973	LEU	-	EXPRESSION TAG	UNP P06756
A	974	GLN	-	EXPRESSION TAG	UNP P06756
A	975	ALA	-	EXPRESSION TAG	UNP P06756
A	976	LEU	-	EXPRESSION TAG	UNP P06756
A	977	GLU	-	EXPRESSION TAG	UNP P06756
A	978	LYS	-	EXPRESSION TAG	UNP P06756
A	979	GLU	-	EXPRESSION TAG	UNP P06756
A	980	ASN	-	EXPRESSION TAG	UNP P06756
A	981	ALA	-	EXPRESSION TAG	UNP P06756
A	982	GLN	-	EXPRESSION TAG	UNP P06756
A	983	LEU	-	EXPRESSION TAG	UNP P06756
A	984	GLU	-	EXPRESSION TAG	UNP P06756
A	985	TRP	-	EXPRESSION TAG	UNP P06756
A	986	GLU	-	EXPRESSION TAG	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
A	987	LEU	-	EXPRESSION TAG	UNP P06756
A	988	GLN	-	EXPRESSION TAG	UNP P06756
A	989	ALA	-	EXPRESSION TAG	UNP P06756
A	990	LEU	-	EXPRESSION TAG	UNP P06756
A	991	GLU	-	EXPRESSION TAG	UNP P06756
A	992	LYS	-	EXPRESSION TAG	UNP P06756
A	993	GLU	-	EXPRESSION TAG	UNP P06756
A	994	LEU	-	EXPRESSION TAG	UNP P06756
A	995	GLN	-	EXPRESSION TAG	UNP P06756
A	996	ALA	-	EXPRESSION TAG	UNP P06756
A	997	LEU	-	EXPRESSION TAG	UNP P06756
A	998	CYS	-	EXPRESSION TAG	UNP P06756

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	709	Total	C	N	O	S	0	0	0
			5454	3359	933	1091	71			

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	692	GLU	-	EXPRESSION TAG	UNP P05106
B	693	SER	-	EXPRESSION TAG	UNP P05106
B	694	MET	-	EXPRESSION TAG	UNP P05106
B	695	GLU	-	EXPRESSION TAG	UNP P05106
B	696	ASN	-	EXPRESSION TAG	UNP P05106
B	697	LEU	-	EXPRESSION TAG	UNP P05106
B	698	TYR	-	EXPRESSION TAG	UNP P05106
B	699	PHE	-	EXPRESSION TAG	UNP P05106
B	700	GLN	-	EXPRESSION TAG	UNP P05106
B	701	SER	-	EXPRESSION TAG	UNP P05106
B	702	GLY	-	EXPRESSION TAG	UNP P05106
B	703	GLY	-	EXPRESSION TAG	UNP P05106
B	704	LYS	-	EXPRESSION TAG	UNP P05106
B	705	ASN	-	EXPRESSION TAG	UNP P05106
B	706	ALA	-	EXPRESSION TAG	UNP P05106
B	707	GLN	-	EXPRESSION TAG	UNP P05106
B	708	CYS	-	EXPRESSION TAG	UNP P05106
B	709	LYS	-	EXPRESSION TAG	UNP P05106
B	710	LYS	-	EXPRESSION TAG	UNP P05106
B	711	LYS	-	EXPRESSION TAG	UNP P05106

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Chain	Residue	Modelled	Actual	Comment	Reference
B	712	LEU	-	EXPRESSION TAG	UNP P05106
B	713	GLN	-	EXPRESSION TAG	UNP P05106
B	714	ALA	-	EXPRESSION TAG	UNP P05106
B	715	LEU	-	EXPRESSION TAG	UNP P05106
B	716	LYS	-	EXPRESSION TAG	UNP P05106
B	717	LYS	-	EXPRESSION TAG	UNP P05106
B	718	LYS	-	EXPRESSION TAG	UNP P05106
B	719	ASN	-	EXPRESSION TAG	UNP P05106
B	720	ALA	-	EXPRESSION TAG	UNP P05106
B	721	GLN	-	EXPRESSION TAG	UNP P05106
B	722	LEU	-	EXPRESSION TAG	UNP P05106
B	723	LYS	-	EXPRESSION TAG	UNP P05106
B	724	TRP	-	EXPRESSION TAG	UNP P05106
B	725	LYS	-	EXPRESSION TAG	UNP P05106
B	726	LEU	-	EXPRESSION TAG	UNP P05106
B	727	GLN	-	EXPRESSION TAG	UNP P05106
B	728	ALA	-	EXPRESSION TAG	UNP P05106
B	729	LEU	-	EXPRESSION TAG	UNP P05106
B	730	CYS	-	EXPRESSION TAG	UNP P05106
B	731	THR	-	EXPRESSION TAG	UNP P05106
B	732	GLY	-	EXPRESSION TAG	UNP P05106
B	733	HIS	-	EXPRESSION TAG	UNP P05106
B	734	HIS	-	EXPRESSION TAG	UNP P05106
B	735	HIS	-	EXPRESSION TAG	UNP P05106
B	736	HIS	-	EXPRESSION TAG	UNP P05106
B	737	HIS	-	EXPRESSION TAG	UNP P05106
B	738	HIS	-	EXPRESSION TAG	UNP P05106

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	5	Total Ca 5 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total C N O 50 28 2 20	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			50	28	2	20		
4	B	4	Total	C	N	O	0	0
			50	28	2	20		
4	B	4	Total	C	N	O	0	0
			50	28	2	20		

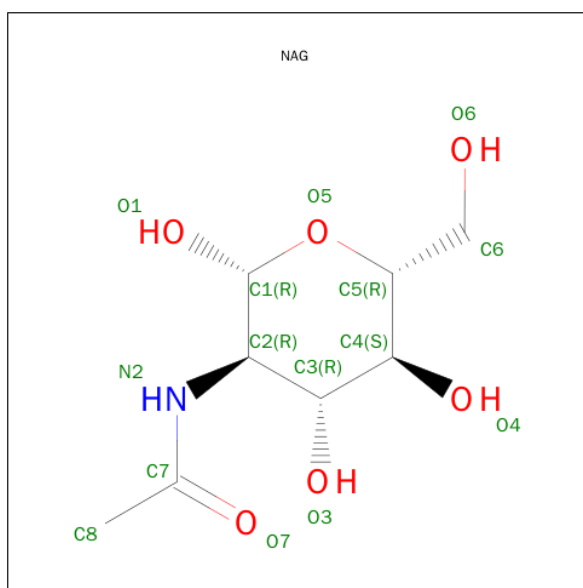
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

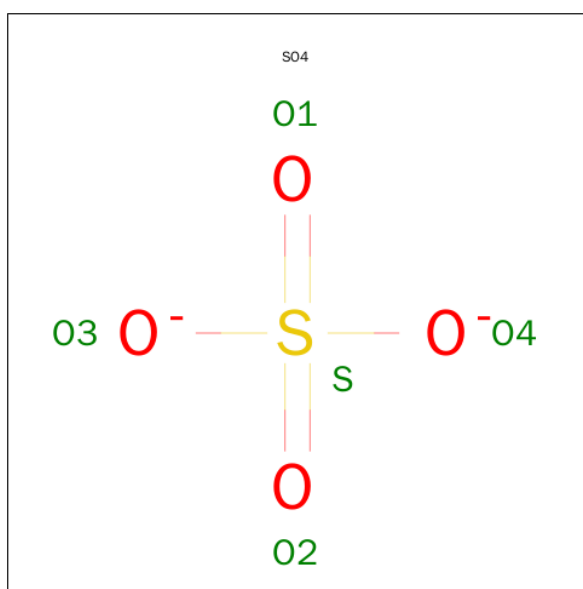
- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	2	Total	C	N	O	0	0
			28	16	2	10		
8	A	2	Total	C	N	O	0	0
			28	16	2	10		
8	B	2	Total	C	N	O	0	0
			28	16	2	10		
8	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	B	1	Total O S 5 4 1	0	0
10	B	1	Total O S 5 4 1	0	0
10	B	1	Total O S 5 4 1	0	0

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	3	Total Cl 3 3	0	0
11	A	4	Total Cl 4 4	0	0

- Molecule 12 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Ni 1 1	0	0

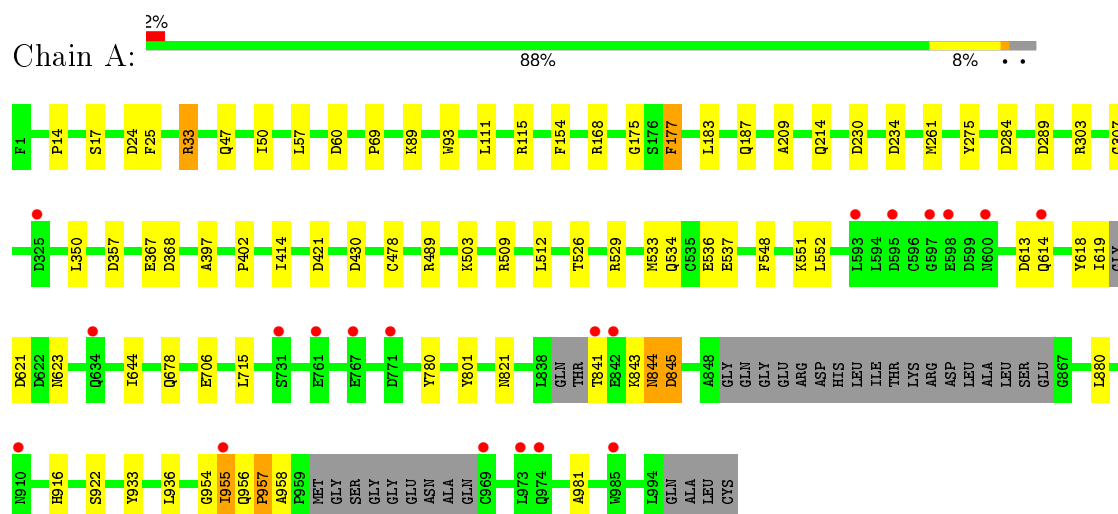
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	60	Total O 60 60	0	0
13	B	39	Total O 39 39	0	0

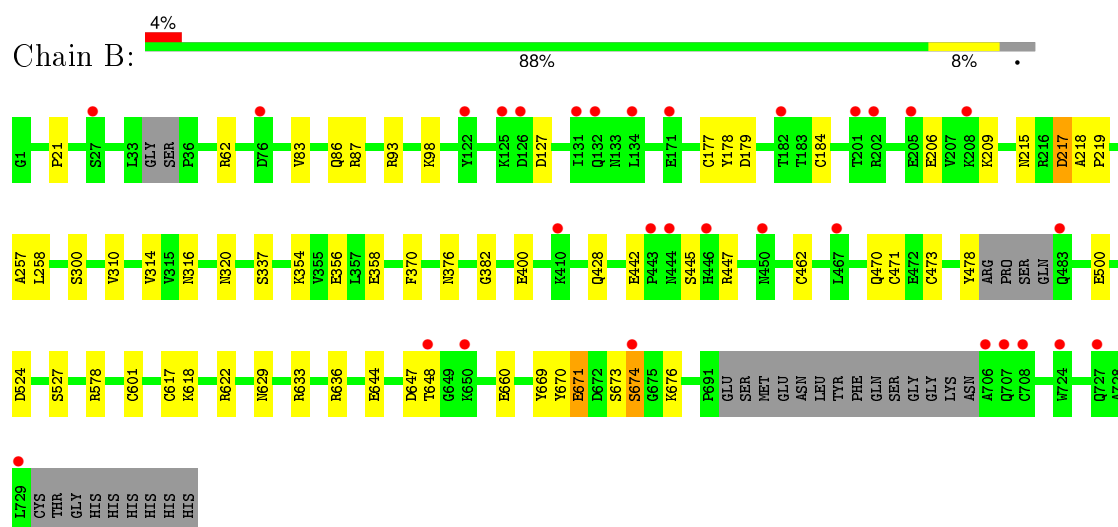
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: Integrin alpha-V



• Molecule 2: Integrin beta-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.56Å 128.56Å 352.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.52 – 3.00 47.52 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.52-3.00) 100.0 (47.52-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.241 , 0.261 0.242 , 0.263	Depositor DCC
R_{free} test set	1002 reflections (1.46%)	DCC
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.0	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 79656 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13732	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, BMA, NAG, CL, CA, SO4, MAN

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	0.21	0/7669	0.37	0/10392
2	B	0.22	0/5549	0.36	0/7493
All	All	0.21	0/13218	0.37	0/17885

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

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	7512	0	7319	44	1
2	B	5454	0	5220	35	1
3	A	5	0	0	0	0
3	B	1	0	0	0	0
4	A	100	0	86	5	0
4	B	100	0	86	3	0
5	A	78	0	68	0	0
5	B	39	0	34	0	0
6	A	94	0	79	2	0
7	A	28	0	26	0	0
8	A	56	0	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	56	0	50	0	0
9	A	72	0	61	4	0
10	A	15	0	0	0	0
10	B	15	0	0	0	0
11	A	4	0	0	0	0
11	B	3	0	0	0	0
12	A	1	0	0	0	0
13	A	60	0	0	1	0
13	B	39	0	0	1	0
All	All	13732	0	13079	86	1

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.

The worst 5 of 86 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)
2:B:177:CYS:N	2:B:184:CYS:SG	2.62	0.73
1:A:503:LYS:O	1:A:509:ARG:NH1	2.21	0.73
4:A:2023:BMA:H4	4:A:2024:MAN:H2	1.71	0.71
1:A:618:TYR:O	1:A:623:ASN:ND2	2.25	0.70
2:B:87:ARG:NH1	2:B:428:GLN:OE1	2.25	0.69

All (1) 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)
1:A:958:ALA:O	2:B:62:ARG:NH1[4_555]	2.17	0.03

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	954/998 (96%)	900 (94%)	50 (5%)	4 (0%)	39	80
2	B	701/738 (95%)	669 (95%)	31 (4%)	1 (0%)	56	90
All	All	1655/1736 (95%)	1569 (95%)	81 (5%)	5 (0%)	46	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	843	LYS
2	B	217	ASP
1	A	957	PRO
1	A	955	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	819/844 (97%)	812 (99%)	7 (1%)	84	95
2	B	628/653 (96%)	622 (99%)	6 (1%)	82	95
All	All	1447/1497 (97%)	1434 (99%)	13 (1%)	84	95

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	844	ASN
1	A	845	ASP
2	B	671	GLU
1	A	841	THR
2	B	217	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	623	ASN

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Mol	Chain	Res	Type
2	B	376	ASN
2	B	629	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 ⓘ

47 carbohydrates 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	A	2006	1,4	14,14,15	0.49	0	15,19,21	0.66	0
4	NAG	A	2007	4	14,14,15	0.60	0	15,19,21	1.35	3 (20%)
4	BMA	A	2008	4	11,11,12	0.47	0	14,15,17	1.20	1 (7%)
4	MAN	A	2009	4	11,11,12	0.62	0	14,15,17	0.64	0
5	NAG	A	2010	1,5	14,14,15	0.51	0	15,19,21	0.64	0
5	NAG	A	2011	5	14,14,15	0.52	0	15,19,21	0.64	0
5	BMA	A	2012	5	11,11,12	0.68	0	14,15,17	0.64	0
6	NAG	A	2013	1,6	14,14,15	0.55	0	15,19,21	0.72	0
6	NAG	A	2014	6	14,14,15	0.47	0	15,19,21	0.75	0
6	BMA	A	2015	6	11,11,12	0.81	0	14,15,17	0.92	0
6	MAN	A	2016	6	11,11,12	0.59	0	14,15,17	1.45	4 (28%)
6	MAN	A	2017	6	11,11,12	0.57	0	14,15,17	1.42	3 (21%)
6	MAN	A	2018	6	11,11,12	0.62	0	14,15,17	1.12	1 (7%)
6	MAN	A	2019	6	11,11,12	0.64	0	14,15,17	0.78	1 (7%)
6	MAN	A	2020	6	11,11,12	0.60	0	14,15,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2021	1,4	14,14,15	0.53	0	15,19,21	0.60	0
4	NAG	A	2022	4	14,14,15	0.59	0	15,19,21	0.97	0
4	BMA	A	2023	4	11,11,12	0.98	1 (9%)	14,15,17	1.29	2 (14%)
4	MAN	A	2024	4	11,11,12	0.64	0	14,15,17	1.31	1 (7%)
8	NAG	A	2026	1,8	14,14,15	0.51	0	15,19,21	0.62	0
8	NAG	A	2027	8	14,14,15	0.49	0	15,19,21	0.60	0
5	NAG	A	2028	1,5	14,14,15	0.50	0	15,19,21	0.71	0
5	NAG	A	2029	5	14,14,15	0.54	0	15,19,21	0.89	0
5	BMA	A	2030	5	11,11,12	0.68	0	14,15,17	0.65	0
9	NAG	A	2031	1,9	14,14,15	0.55	0	15,19,21	0.65	0
9	NAG	A	2032	9	14,14,15	0.56	0	15,19,21	0.74	0
9	BMA	A	2033	9	11,11,12	0.68	0	14,15,17	0.88	0
9	MAN	A	2034	9	11,11,12	0.63	0	14,15,17	0.73	0
9	MAN	A	2035	9	11,11,12	0.63	0	14,15,17	1.18	2 (14%)
9	MAN	A	2036	9	11,11,12	0.60	0	14,15,17	0.65	0
8	NAG	A	2037	1,8	14,14,15	0.52	0	15,19,21	0.69	0
8	NAG	A	2038	8	14,14,15	0.49	0	15,19,21	0.69	0
8	NAG	B	2002	8,2	14,14,15	0.53	0	15,19,21	0.60	0
8	NAG	B	2003	8	14,14,15	0.50	0	15,19,21	0.74	0
8	NAG	B	2004	8,2	14,14,15	0.58	0	15,19,21	0.65	0
8	NAG	B	2005	8	14,14,15	0.48	0	15,19,21	0.60	0
4	NAG	B	2006	2,4	14,14,15	0.49	0	15,19,21	0.75	0
4	NAG	B	2007	4	14,14,15	0.53	0	15,19,21	0.74	0
4	BMA	B	2008	4	11,11,12	0.57	0	14,15,17	0.69	0
4	MAN	B	2009	4	11,11,12	0.64	0	14,15,17	0.79	0
5	NAG	B	2010	2,5	14,14,15	0.50	0	15,19,21	0.65	0
5	NAG	B	2011	5	14,14,15	0.53	0	15,19,21	0.65	0
5	BMA	B	2012	5	11,11,12	0.61	0	14,15,17	0.72	0
4	NAG	B	2013	2,4	14,14,15	0.57	0	15,19,21	0.64	0
4	NAG	B	2014	4	14,14,15	0.57	0	15,19,21	0.77	0
4	BMA	B	2015	4	11,11,12	0.70	0	14,15,17	0.72	0
4	MAN	B	2016	4	11,11,12	0.63	0	14,15,17	0.72	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	A	2006	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2007	4	-	0/6/23/26	0/1/1/1
4	BMA	A	2008	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	2009	4	-	0/2/19/22	0/1/1/1
5	NAG	A	2010	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2011	5	-	0/6/23/26	0/1/1/1
5	BMA	A	2012	5	-	0/2/19/22	0/1/1/1
6	NAG	A	2013	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2014	6	-	0/6/23/26	0/1/1/1
6	BMA	A	2015	6	-	0/2/19/22	0/1/1/1
6	MAN	A	2016	6	-	0/2/19/22	0/1/1/1
6	MAN	A	2017	6	-	0/2/19/22	0/1/1/1
6	MAN	A	2018	6	-	0/2/19/22	0/1/1/1
6	MAN	A	2019	6	-	0/2/19/22	0/1/1/1
6	MAN	A	2020	6	-	0/2/19/22	0/1/1/1
4	NAG	A	2021	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2022	4	-	0/6/23/26	0/1/1/1
4	BMA	A	2023	4	-	0/2/19/22	0/1/1/1
4	MAN	A	2024	4	-	0/2/19/22	0/1/1/1
8	NAG	A	2026	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	2027	8	-	0/6/23/26	0/1/1/1
5	NAG	A	2028	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2029	5	-	0/6/23/26	0/1/1/1
5	BMA	A	2030	5	-	0/2/19/22	0/1/1/1
9	NAG	A	2031	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	2032	9	-	0/6/23/26	0/1/1/1
9	BMA	A	2033	9	-	0/2/19/22	0/1/1/1
9	MAN	A	2034	9	-	0/2/19/22	0/1/1/1
9	MAN	A	2035	9	-	0/2/19/22	0/1/1/1
9	MAN	A	2036	9	-	0/2/19/22	0/1/1/1
8	NAG	A	2037	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	2038	8	-	0/6/23/26	0/1/1/1
8	NAG	B	2002	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	2003	8	-	0/6/23/26	0/1/1/1
8	NAG	B	2004	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	2005	8	-	0/6/23/26	0/1/1/1
4	NAG	B	2006	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2007	4	-	0/6/23/26	0/1/1/1
4	BMA	B	2008	4	-	0/2/19/22	0/1/1/1
4	MAN	B	2009	4	-	0/2/19/22	0/1/1/1
5	NAG	B	2010	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2011	5	-	0/6/23/26	0/1/1/1
5	BMA	B	2012	5	-	0/2/19/22	0/1/1/1
4	NAG	B	2013	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2014	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	B	2015	4	-	0/2/19/22	0/1/1/1
4	MAN	B	2016	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2023	BMA	C2-C3	2.01	1.55	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2024	MAN	O5-C1-C2	-4.10	104.20	110.86
6	A	2016	MAN	C1-C2-C3	-3.54	105.36	109.54
6	A	2018	MAN	O5-C1-C2	-3.16	105.72	110.86
6	A	2016	MAN	O5-C1-C2	-2.38	107.00	110.86
6	A	2017	MAN	C1-C2-C3	-2.35	106.76	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2007	NAG	1	0
4	A	2008	BMA	1	0
6	A	2017	MAN	2	0
6	A	2018	MAN	2	0
4	A	2023	BMA	4	0
4	A	2024	MAN	4	0
9	A	2031	NAG	1	0
9	A	2033	BMA	3	0
9	A	2034	MAN	1	0
9	A	2035	MAN	2	0
4	B	2006	NAG	1	0
4	B	2014	NAG	2	0

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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	$\# Z > 2$
7	NAG	A	2025	1	14,14,15	0.54	0	15,19,21	0.58	0
7	NAG	A	2039	1	14,14,15	0.49	0	15,19,21	0.59	0
10	SO4	A	2040	-	4,4,4	0.23	0	6,6,6	0.08	0
10	SO4	A	2041	-	4,4,4	0.23	0	6,6,6	0.08	0
10	SO4	A	2042	-	4,4,4	0.24	0	6,6,6	0.08	0
10	SO4	B	2017	-	4,4,4	0.23	0	6,6,6	0.10	0
10	SO4	B	2018	-	4,4,4	0.22	0	6,6,6	0.08	0
10	SO4	B	2019	-	4,4,4	0.24	0	6,6,6	0.08	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
7	NAG	A	2025	1	-	0/6/23/26	0/1/1/1
7	NAG	A	2039	1	-	0/6/23/26	0/1/1/1
10	SO4	A	2040	-	-	0/0/0/0	0/0/0/0
10	SO4	A	2041	-	-	0/0/0/0	0/0/0/0
10	SO4	A	2042	-	-	0/0/0/0	0/0/0/0
10	SO4	B	2017	-	-	0/0/0/0	0/0/0/0
10	SO4	B	2018	-	-	0/0/0/0	0/0/0/0
10	SO4	B	2019	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	964/998 (96%)	0.18	20 (2%) 67 36	74, 119, 180, 268	0
2	B	709/738 (96%)	0.19	30 (4%) 40 16	81, 126, 177, 254	0
All	All	1673/1736 (96%)	0.18	50 (2%) 54 25	74, 122, 178, 268	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	598	GLU	5.5
1	A	974	GLN	5.3
2	B	446	HIS	5.3
2	B	706	ALA	5.1
2	B	648	THR	4.3

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. 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
9	MAN	A	2034	11/12	0.66	0.42	5.52	191,208,215,217	0
9	MAN	A	2036	11/12	0.55	0.54	3.99	186,196,206,206	0
9	MAN	A	2035	11/12	0.68	0.34	1.73	180,192,207,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	2028	14/15	0.76	0.24	0.98	98,150,168,170	0
4	NAG	A	2021	14/15	0.91	0.27	0.71	121,147,175,176	0
9	BMA	A	2033	11/12	0.76	0.28	0.57	195,200,203,207	0
9	NAG	A	2032	14/15	0.72	0.31	0.55	165,190,195,196	0
8	NAG	B	2004	14/15	0.80	0.24	0.14	122,155,172,186	0
5	NAG	A	2010	14/15	0.92	0.25	0.07	97,120,152,152	0
9	NAG	A	2031	14/15	0.72	0.25	-0.02	167,179,191,198	0
4	NAG	B	2006	14/15	0.94	0.20	-0.41	85,121,133,133	0
6	NAG	A	2013	14/15	0.94	0.20	-0.49	75,85,110,117	0
5	NAG	B	2010	14/15	0.93	0.16	-0.59	102,123,128,136	0
4	NAG	A	2006	14/15	0.95	0.18	-0.87	78,98,114,119	0
4	NAG	B	2013	14/15	0.92	0.20	-0.91	87,119,143,159	0
4	NAG	A	2022	14/15	0.74	0.18	-2.13	97,164,173,174	0
4	NAG	A	2007	14/15	0.76	0.23	-	123,144,158,160	0
6	NAG	A	2014	14/15	0.94	0.15	-	87,102,133,135	0
5	BMA	A	2012	11/12	0.48	0.49	-	162,180,184,184	0
8	NAG	B	2003	14/15	0.73	0.41	-	172,182,191,192	0
8	NAG	A	2026	14/15	0.91	0.24	-	136,163,178,192	0
4	BMA	B	2015	11/12	0.56	0.36	-	155,172,179,184	0
8	NAG	A	2037	14/15	0.73	0.21	-	101,150,165,181	0
4	MAN	A	2009	11/12	0.72	0.41	-	148,158,171,173	0
6	MAN	A	2018	11/12	0.80	0.23	-	122,159,167,186	0
4	BMA	A	2023	11/12	0.91	0.22	-	162,173,180,180	0
8	NAG	A	2027	14/15	0.75	0.40	-	181,197,204,205	0
4	NAG	B	2014	14/15	0.78	0.35	-	174,183,191,193	0
5	NAG	A	2029	14/15	0.74	0.34	-	141,166,172,175	0
4	BMA	B	2008	11/12	0.54	0.35	-	164,178,186,187	0
4	BMA	A	2008	11/12	0.68	0.28	-	157,163,167,172	0
5	NAG	B	2011	14/15	0.79	0.19	-	136,145,162,176	0
6	BMA	A	2015	11/12	0.81	0.15	-	133,145,155,165	0
4	MAN	B	2016	11/12	0.84	0.42	-	160,174,181,183	0
5	BMA	A	2030	11/12	0.50	0.51	-	131,166,172,175	0
8	NAG	B	2002	14/15	0.90	0.25	-	116,140,152,166	0
6	MAN	A	2019	11/12	0.65	0.44	-	175,184,191,191	0
4	MAN	A	2024	11/12	0.80	0.23	-	150,162,176,179	0
6	MAN	A	2017	11/12	0.91	0.17	-	146,156,163,166	0
5	BMA	B	2012	11/12	0.73	0.27	-	148,170,176,178	0
4	MAN	B	2009	11/12	0.66	0.42	-	130,156,162,163	0
6	MAN	A	2016	11/12	0.90	0.23	-	132,167,174,179	0
5	NAG	A	2011	14/15	0.87	0.38	-	144,176,189,189	0
8	NAG	A	2038	14/15	0.75	0.37	-	171,179,183,184	0
4	NAG	B	2007	14/15	0.89	0.26	-	143,151,168,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NAG	B	2005	14/15	0.75	0.30	-	143,198,213,218	0
6	MAN	A	2020	11/12	0.78	0.35	-	184,194,202,207	0

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(\AA^2)	Q<0.9
7	NAG	A	2039	14/15	0.77	0.29	2.63	128,152,160,163	0
3	CA	A	2005	1/1	0.80	0.45	1.77	267,267,267,267	0
10	SO4	B	2018	5/5	0.92	0.20	-0.34	123,128,144,146	0
10	SO4	A	2042	5/5	0.94	0.16	-0.44	135,139,141,142	0
3	CA	B	2001	1/1	0.59	0.18	-1.14	302,302,302,302	0
10	SO4	A	2041	5/5	0.96	0.15	-1.24	126,129,132,134	0
3	CA	A	2004	1/1	0.96	0.12	-1.36	115,115,115,115	0
10	SO4	B	2017	5/5	0.97	0.14	-1.75	103,108,116,122	0
3	CA	A	2002	1/1	0.97	0.05	-1.89	121,121,121,121	0
3	CA	A	2003	1/1	0.92	0.10	-1.92	117,117,117,117	0
10	SO4	A	2040	5/5	0.95	0.16	-2.20	108,121,128,142	0
3	CA	A	2001	1/1	0.95	0.06	-2.33	124,124,124,124	0
12	NI	A	2047	1/1	0.97	0.12	-3.60	128,128,128,128	0
7	NAG	A	2025	14/15	0.76	0.25	-	136,151,161,163	0
11	CL	B	2022	1/1	0.91	0.10	-	109,109,109,109	0
11	CL	A	2046	1/1	0.92	0.07	-	88,88,88,88	0
11	CL	A	2043	1/1	0.90	0.21	-	100,100,100,100	0
11	CL	A	2045	1/1	0.26	0.40	-	141,141,141,141	0
11	CL	B	2021	1/1	0.91	0.14	-	89,89,89,89	0
10	SO4	B	2019	5/5	0.90	0.17	-	171,174,175,178	0
11	CL	B	2020	1/1	0.75	0.19	-	106,106,106,106	0
11	CL	A	2044	1/1	0.96	0.21	-	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.