



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:56 PM UTC

PDB ID : 4L8S / pdb_00004l8s
Title : Crystal structure of a human Valpha7.2/Vbeta13.3 MAIT TCR in complex with bovine MR1
Authors : Lopez-Sagaseta, J.; Adams, E.J.
Deposited on : 2013-06-17
Resolution : 2.90 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

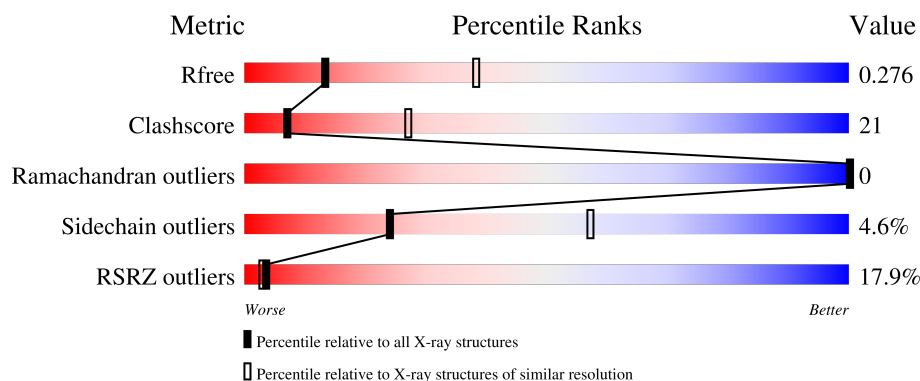
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	208	16% 65% 29% • 5%
2	B	252	12% 60% 33% • •
3	C	392	20% 59% 32% • 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
4	SO4	C	402	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6348 atoms, of which 4 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 Muccosal Associated Invariant T Cell Receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1507	951	238	309	9			

- Molecule 2 is a protein called Muccosal Associated Invariant T Cell Receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1855	1169	318	359	9			

- Molecule 3 is a protein called Beta-2-microglobulin, MHC class I-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	372	Total	C	N	O	S	0	0	0
			2950	1888	508	541	13			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	GLY	-	linker	UNP P01888
C	100	GLY	-	linker	UNP P01888
C	101	GLY	-	linker	UNP P01888
C	102	GLY	-	linker	UNP P01888
C	103	SER	-	linker	UNP P01888
C	104	GLY	-	linker	UNP P01888
C	105	GLY	-	linker	UNP P01888
C	107	SER	-	linker	UNP P01888
C	108	GLY	-	linker	UNP P01888
C	109	SER	-	linker	UNP P01888
C	110	GLY	-	linker	UNP P01888
C	111	GLY	-	linker	UNP P01888
C	112	GLY	-	linker	UNP P01888
C	113	GLY	-	linker	UNP P01888

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Chain	Residue	Modelled	Actual	Comment	Reference
C	114	SER	-	linker	UNP P01888

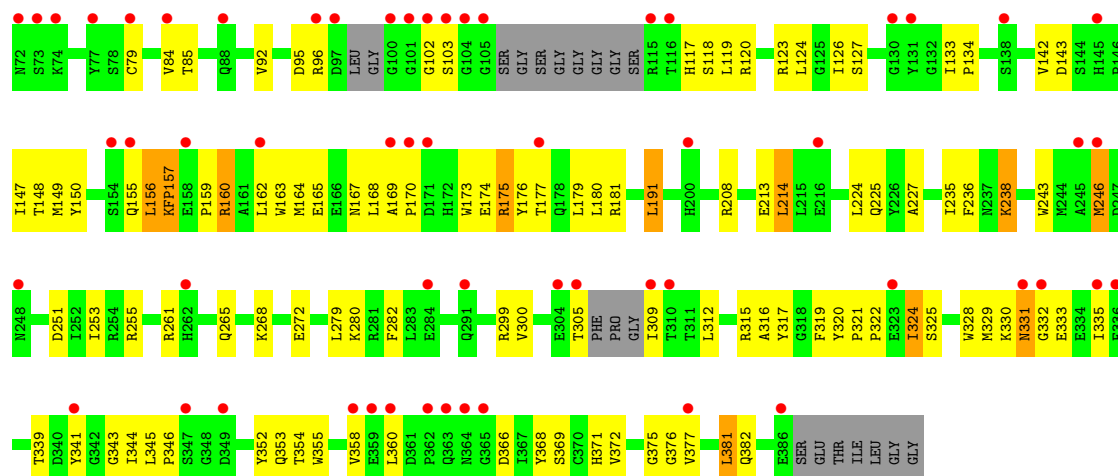
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	3	Total	O		0	0
			3	3			
5	B	1	Total	H	O	0	0
			3	2	1		
5	C	3	Total	H	O	0	0
			5	2	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.07Å 87.28Å 155.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.04 – 2.90 44.04 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (44.04-2.90) 95.8 (44.04-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.228 , 0.278 0.228 , 0.276	Depositor DCC
R_{free} test set	1251 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6348	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: SO4, KFP

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	0.28	0/1542	0.72	0/2101
2	B	0.29	0/1905	0.77	2/2603 (0.1%)
3	C	0.27	0/3016	0.73	2/4106 (0.0%)
All	All	0.28	0/6463	0.74	4/8810 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	375	GLY	N-CA-C	-6.22	106.63	114.16
3	C	331	ASN	N-CA-C	5.84	119.44	111.39
2	B	173	ASP	CA-C-N	5.07	124.67	119.05
2	B	173	ASP	C-N-CA	5.07	124.67	119.05

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	1507	0	1371	50	0
2	B	1855	0	1710	91	0
3	C	2950	0	2678	123	0
4	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
4	C	10	0	0	4	0
5	A	3	0	0	0	0
5	B	1	2	0	0	0
5	C	3	2	0	1	0
All	All	6344	4	5759	253	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 21.

All (253) 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:C:41:LYS:HB2	3:C:46:ILE:HD11	1.42	1.02
2:B:38:ASP:HB2	2:B:41:MET:HE3	1.47	0.95
2:B:3:GLY:HA2	2:B:27:MET:HE3	1.50	0.94
2:B:100:THR:HB	2:B:103:LEU:HD13	1.52	0.91
3:C:147:ILE:O	3:C:160:ARG:N	2.08	0.86
2:B:41:MET:SD	2:B:44:ARG:NH1	2.50	0.85
3:C:339:THR:HG22	3:C:358:VAL:HG22	1.56	0.85
1:A:59:ARG:NH2	1:A:82:ASP:OD2	2.09	0.84
1:A:158:VAL:HG23	2:B:174:PRO:HG3	1.60	0.84
3:C:23:LEU:HB2	3:C:70:THR:HG21	1.59	0.82
3:C:52:ASP:OD2	3:C:160:ARG:NH1	2.14	0.81
3:C:322:PRO:HG3	3:C:352:TYR:CE2	2.16	0.81
2:B:32:MET:HE3	2:B:74:PHE:HB2	1.62	0.80
2:B:49:SER:HB3	2:B:55:THR:HG22	1.62	0.80
2:B:49:SER:OG	2:B:68:ARG:HD2	1.84	0.77
1:A:165:ASP:HB3	1:A:166:PHE:HD2	1.50	0.77
1:A:36:GLN:HB2	1:A:46:LEU:HD11	1.67	0.77
3:C:344:ILE:HA	3:C:354:THR:HG22	1.68	0.74
2:B:86:THR:HG23	2:B:112:THR:HA	1.70	0.74
2:B:32:MET:CE	2:B:74:PHE:HB2	2.17	0.74
2:B:6:GLN:HE21	2:B:109:SER:HB2	1.52	0.73
3:C:305:THR:HA	3:C:309:ILE:HG22	1.70	0.72
3:C:369:SER:HB3	3:C:382:GLN:HA	1.74	0.70
2:B:32:MET:HE2	2:B:68:ARG:NH1	2.08	0.69
1:A:191:ILE:HG23	1:A:195:THR:HG21	1.75	0.69
3:C:159:PRO:HG3	3:C:173:TRP:CZ2	2.26	0.69
3:C:376:GLY:N	3:C:377:VAL:HB	2.08	0.69
1:A:95:TYR:HB3	2:B:98:PRO:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:MET:HE2	2:B:68:ARG:CZ	2.24	0.68
3:C:57:LYS:NZ	4:C:402:SO4:O4	2.24	0.68
2:B:28:ASN:OD1	2:B:71:LYS:NZ	2.24	0.67
3:C:147:ILE:HG21	3:C:164:MET:HE3	1.76	0.67
2:B:38:ASP:HB2	2:B:41:MET:CE	2.24	0.66
2:B:78:LEU:N	2:B:78:LEU:HD23	2.11	0.65
1:A:199:SER:OG	1:A:200:PRO:HD3	1.96	0.65
3:C:169:ALA:HB1	3:C:170:PRO:HD2	1.79	0.65
1:A:146:SER:HB2	1:A:153:ILE:HD11	1.78	0.64
2:B:172:THR:HG23	2:B:192:SER:HB2	1.80	0.64
1:A:191:ILE:HG23	1:A:192:PRO:HD2	1.80	0.63
3:C:32:PRO:HB2	3:C:33:PRO:HD2	1.80	0.62
2:B:135:ILE:HG23	2:B:198:ALA:HB1	1.81	0.62
2:B:196:VAL:HG21	2:B:200:PHE:CD1	2.35	0.61
3:C:23:LEU:HB2	3:C:70:THR:CG2	2.28	0.61
3:C:156:LEU:HD22	3:C:156:LEU:N	2.16	0.61
3:C:133:ILE:HG22	3:C:134:PRO:HD2	1.82	0.60
1:A:192:PRO:HG2	1:A:195:THR:CG2	2.32	0.60
2:B:9:LYS:HE2	2:B:107:GLU:HB2	1.83	0.60
2:B:218:SER:N	2:B:221:ASP:OD2	2.29	0.59
1:A:56:GLU:HG2	1:A:61:SER:HB3	1.84	0.59
2:B:37:GLN:HB2	2:B:43:LEU:CD2	2.33	0.58
3:C:300:VAL:HG23	3:C:381:LEU:HD13	1.86	0.58
3:C:329:MET:HE3	3:C:371:HIS:HB2	1.85	0.58
3:C:328:TRP:CD1	3:C:358:VAL:HG23	2.39	0.58
2:B:155:VAL:HA	2:B:213:GLN:O	2.04	0.58
2:B:202:GLN:HA	2:B:242:ARG:O	2.04	0.58
2:B:19:MET:HE1	2:B:111:LEU:HD21	1.86	0.57
2:B:97:ASP:OD1	2:B:98:PRO:HA	2.04	0.57
3:C:117:HIS:HA	3:C:143:ASP:OD1	2.04	0.57
1:A:52:ASP:H	1:A:66:ARG:HH21	1.50	0.57
2:B:135:ILE:HG23	2:B:198:ALA:CB	2.35	0.57
2:B:9:LYS:HE2	2:B:107:GLU:CB	2.34	0.56
1:A:157:CYS:HB3	2:B:193:ARG:NH2	2.19	0.56
3:C:119:LEU:HB2	3:C:279:LEU:HD13	1.87	0.56
3:C:148:THR:HG22	3:C:173:TRP:HZ3	1.70	0.56
2:B:211:GLN:HG3	2:B:234:ILE:HG23	1.87	0.56
3:C:299:ARG:NH2	4:C:401:SO4:O1	2.38	0.56
1:A:60:PHE:HD1	1:A:75:LEU:HD22	1.70	0.56
3:C:118:SER:CB	3:C:213:GLU:HB3	2.36	0.56
2:B:34:TRP:CH2	2:B:91:CYS:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:TRP:CE2	3:C:227:ALA:HB2	2.40	0.56
2:B:3:GLY:CA	2:B:27:MET:HE3	2.31	0.56
3:C:164:MET:HE1	3:C:282:PHE:CG	2.41	0.55
1:A:79:GLN:OE1	1:A:81:LYS:HE2	2.07	0.55
1:A:184:ASN:HA	1:A:187:ASN:ND2	2.22	0.55
3:C:324:ILE:HD13	3:C:325:SER:H	1.72	0.55
1:A:127:SER:HB2	2:B:126:ALA:CB	2.37	0.55
3:C:32:PRO:CB	3:C:33:PRO:HD2	2.37	0.55
2:B:130:PRO:HD2	2:B:201:TRP:CZ2	2.42	0.55
3:C:251:ASP:OD2	3:C:255:ARG:NH1	2.40	0.55
3:C:57:LYS:HE3	3:C:120:ARG:NH2	2.22	0.55
3:C:41:LYS:CB	3:C:46:ILE:HD11	2.28	0.54
1:A:36:GLN:HB2	1:A:46:LEU:CD1	2.36	0.54
3:C:147:ILE:CG2	3:C:164:MET:HE3	2.36	0.54
3:C:163:TRP:CZ3	3:C:164:MET:HE2	2.43	0.54
1:A:60:PHE:CD1	1:A:75:LEU:HD22	2.43	0.53
2:B:14:LYS:HA	2:B:114:LEU:O	2.09	0.53
3:C:224:LEU:HD22	3:C:243:TRP:HH2	1.73	0.53
3:C:341:TYR:HD2	3:C:343:GLY:H	1.54	0.53
3:C:324:ILE:HD11	3:C:372:VAL:HG13	1.89	0.53
1:A:165:ASP:HB3	1:A:166:PHE:CD2	2.37	0.53
2:B:6:GLN:NE2	2:B:109:SER:HB2	2.23	0.52
3:C:331:ASN:N	3:C:332:GLY:HA2	2.23	0.52
2:B:78:LEU:HD23	2:B:78:LEU:H	1.74	0.52
3:C:102:GLY:HA3	3:C:341:TYR:O	2.09	0.52
3:C:319:PHE:CE2	3:C:353:GLN:HA	2.44	0.52
3:C:329:MET:HE3	3:C:371:HIS:CG	2.45	0.52
2:B:27:MET:HE1	2:B:104:PHE:CD2	2.44	0.52
3:C:376:GLY:H	3:C:377:VAL:HB	1.73	0.52
1:A:34:TRP:O	1:A:46:LEU:HB2	2.10	0.52
2:B:34:TRP:CE2	2:B:76:LEU:HB2	2.44	0.52
3:C:118:SER:HB3	3:C:213:GLU:HB3	1.92	0.52
3:C:148:THR:HG21	3:C:157:KFP:H12	1.92	0.52
3:C:157:KFP:H16	3:C:180:LEU:HD21	1.91	0.52
2:B:214:PHE:O	2:B:232:THR:HG23	2.10	0.52
2:B:19:MET:HE1	2:B:21:LEU:HD21	1.91	0.51
1:A:45:PHE:HB3	2:B:102:GLU:HG3	1.92	0.51
3:C:118:SER:HA	3:C:213:GLU:HA	1.92	0.51
1:A:129:LYS:HD3	1:A:174:TRP:CD1	2.46	0.51
3:C:123:ARG:HB2	3:C:208:ARG:HB3	1.91	0.51
3:C:10:TYR:CE2	3:C:345:LEU:HD23	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:ILE:CG2	3:C:134:PRO:HD2	2.40	0.51
2:B:94:SER:HB3	2:B:103:LEU:HD12	1.92	0.51
3:C:315:ARG:HD3	3:C:355:TRP:HB3	1.93	0.51
3:C:177:THR:O	3:C:181:ARG:HG3	2.10	0.51
3:C:320:TYR:CG	3:C:321:PRO:HA	2.46	0.51
2:B:34:TRP:CE3	2:B:76:LEU:HD12	2.46	0.50
2:B:196:VAL:HG22	2:B:197:SER:N	2.26	0.50
3:C:79:CYS:HB3	3:C:92:VAL:HG23	1.93	0.50
3:C:174:GLU:O	3:C:177:THR:HG22	2.11	0.50
2:B:34:TRP:HB3	2:B:46:ILE:HD11	1.94	0.50
3:C:175:ARG:O	3:C:175:ARG:HD3	2.12	0.50
3:C:214:LEU:HD11	3:C:280:LYS:HE2	1.93	0.50
3:C:34:GLN:CD	3:C:133:ILE:HD11	2.36	0.50
2:B:34:TRP:O	2:B:46:ILE:HG12	2.12	0.50
3:C:95:ASP:OD1	3:C:96:ARG:N	2.44	0.50
2:B:19:MET:CE	2:B:111:LEU:HD21	2.41	0.50
2:B:127:VAL:HG13	2:B:237:ALA:HB3	1.93	0.50
3:C:236:PHE:HB2	3:C:243:TRP:CH2	2.46	0.50
3:C:331:ASN:HD21	3:C:366:ASP:HA	1.77	0.50
3:C:329:MET:HE3	3:C:371:HIS:CB	2.41	0.50
1:A:18:VAL:HG12	1:A:78:LEU:HD21	1.94	0.49
3:C:253:ILE:HD12	3:C:253:ILE:N	2.28	0.49
2:B:36:ARG:NH2	2:B:85:GLN:HA	2.27	0.49
2:B:192:SER:C	2:B:193:ARG:HD3	2.38	0.49
3:C:31:HIS:ND1	3:C:32:PRO:HA	2.27	0.49
3:C:330:LYS:HB2	3:C:335:ILE:HD11	1.94	0.49
3:C:12:ARG:HD2	3:C:22:TYR:CD1	2.47	0.49
1:A:18:VAL:HG12	1:A:75:LEU:HB2	1.94	0.48
3:C:324:ILE:HD13	3:C:325:SER:N	2.27	0.48
1:A:17:ILE:N	1:A:17:ILE:HD12	2.27	0.48
1:A:59:ARG:HH22	1:A:82:ASP:CG	2.21	0.48
2:B:211:GLN:NE2	2:B:234:ILE:HD13	2.28	0.48
2:B:41:MET:CE	2:B:44:ARG:HH12	2.27	0.48
3:C:25:CYS:HB2	3:C:39:LEU:HD21	1.95	0.48
3:C:35:ILE:HG21	3:C:63:LEU:HD12	1.94	0.48
1:A:131:VAL:HG12	1:A:174:TRP:HB3	1.95	0.48
2:B:25:GLN:HG2	2:B:27:MET:H	1.79	0.48
1:A:6:GLN:OE1	1:A:102:GLY:HA2	2.14	0.48
3:C:148:THR:HG22	3:C:173:TRP:CZ3	2.48	0.48
3:C:236:PHE:HB2	3:C:243:TRP:CZ3	2.48	0.48
3:C:322:PRO:HG3	3:C:352:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:O	1:A:173:ALA:HA	2.14	0.47
1:A:153:ILE:HA	1:A:172:VAL:O	2.15	0.47
3:C:57:LYS:HE3	3:C:120:ARG:CZ	2.44	0.47
1:A:146:SER:HB2	1:A:153:ILE:CD1	2.45	0.47
2:B:36:ARG:HH21	2:B:85:GLN:HA	1.79	0.47
2:B:52:GLU:OE2	2:B:52:GLU:N	2.44	0.47
1:A:192:PRO:HD2	1:A:195:THR:HG21	1.95	0.47
2:B:157:LEU:C	2:B:157:LEU:HD23	2.39	0.47
1:A:54:LEU:HD11	1:A:61:SER:HB2	1.97	0.47
3:C:315:ARG:HB3	3:C:317:TYR:CE1	2.49	0.47
3:C:49:GLU:HB2	3:C:66:HIS:CE1	2.50	0.46
1:A:158:VAL:CG2	2:B:174:PRO:HG3	2.39	0.46
3:C:10:TYR:CD2	3:C:345:LEU:HD23	2.50	0.46
2:B:177:LEU:HD23	2:B:177:LEU:H	1.80	0.46
3:C:148:THR:CG2	3:C:157:KFP:H12	2.44	0.46
1:A:192:PRO:HG2	1:A:195:THR:HG22	1.97	0.46
2:B:101:GLY:HA2	2:B:103:LEU:N	2.30	0.46
2:B:190:LEU:HD13	2:B:191:SER:N	2.31	0.46
3:C:124:LEU:HD11	3:C:126:ILE:HD11	1.98	0.45
3:C:150:TYR:HE2	3:C:155:GLN:O	1.99	0.45
2:B:13:LEU:HD11	2:B:19:MET:HB2	1.99	0.45
2:B:46:ILE:HG22	2:B:60:VAL:O	2.16	0.45
3:C:4:PRO:HA	3:C:85:THR:OG1	2.16	0.45
3:C:225:GLN:HG2	3:C:235:ILE:HG23	1.97	0.45
1:A:91:MET:HE1	2:B:99:ASN:HA	1.98	0.45
2:B:37:GLN:HB2	2:B:43:LEU:HD21	1.98	0.45
3:C:176:TYR:O	3:C:180:LEU:HD23	2.16	0.45
1:A:95:TYR:CG	2:B:98:PRO:HG3	2.51	0.45
2:B:49:SER:CB	2:B:68:ARG:HD2	2.46	0.45
3:C:159:PRO:HG2	3:C:165:GLU:HB2	1.98	0.45
1:A:191:ILE:HG22	1:A:192:PRO:O	2.17	0.45
3:C:53:LEU:HA	3:C:63:LEU:HD21	1.98	0.45
2:B:110:ARG:HD3	2:B:154:HIS:CE1	2.52	0.44
3:C:103:SER:HA	3:C:341:TYR:HB3	1.99	0.44
1:A:33:PHE:HE2	2:B:101:GLY:HA3	1.83	0.44
1:A:42:ALA:HB2	2:B:106:GLY:O	2.18	0.44
2:B:150:PHE:CE1	2:B:188:TYR:HB2	2.52	0.44
2:B:196:VAL:HG22	2:B:200:PHE:HB3	1.99	0.44
2:B:153:ASP:O	2:B:154:HIS:ND1	2.50	0.44
3:C:175:ARG:HD3	3:C:175:ARG:C	2.43	0.44
3:C:261:ARG:O	3:C:265:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:TYR:OH	3:C:346:PRO:O	2.31	0.44
3:C:56:SER:HB3	4:C:402:SO4:O2	2.18	0.44
3:C:329:MET:HB3	3:C:332:GLY:O	2.18	0.44
3:C:343:GLY:O	3:C:354:THR:HG22	2.17	0.44
2:B:193:ARG:HD3	2:B:193:ARG:N	2.33	0.44
3:C:35:ILE:HG21	3:C:63:LEU:CD1	2.48	0.44
3:C:40:LEU:HA	3:C:44:GLU:O	2.18	0.44
3:C:147:ILE:HG13	3:C:148:THR:H	1.83	0.44
1:A:192:PRO:O	1:A:195:THR:HG23	2.18	0.44
3:C:102:GLY:O	3:C:103:SER:HB2	2.17	0.44
3:C:369:SER:CB	3:C:382:GLN:HA	2.43	0.44
2:B:25:GLN:OE1	2:B:29:HIS:N	2.49	0.44
3:C:312:LEU:CD1	3:C:360:LEU:HD11	2.47	0.44
3:C:147:ILE:C	3:C:160:ARG:HB2	2.43	0.43
2:B:60:VAL:O	2:B:60:VAL:HG22	2.18	0.43
3:C:157:KFP:H14	3:C:157:KFP:H21	1.55	0.43
3:C:344:ILE:N	3:C:344:ILE:HD12	2.33	0.43
2:B:38:ASP:HB3	2:B:39:PRO:HD2	2.01	0.43
3:C:57:LYS:NZ	5:C:502:HOH:O	2.52	0.43
3:C:149:MET:HG3	3:C:160:ARG:NH1	2.33	0.43
2:B:78:LEU:N	2:B:78:LEU:CD2	2.81	0.43
2:B:46:ILE:HG22	2:B:60:VAL:HG13	2.00	0.43
3:C:167:ASN:C	3:C:168:LEU:HD22	2.44	0.43
3:C:31:HIS:HA	3:C:32:PRO:C	2.44	0.43
2:B:173:ASP:HA	2:B:174:PRO:HD3	1.88	0.43
3:C:316:ALA:O	3:C:353:GLN:HB2	2.19	0.43
3:C:344:ILE:HA	3:C:354:THR:CG2	2.42	0.43
2:B:92:ALA:HA	2:B:104:PHE:O	2.19	0.42
1:A:12:ALA:O	1:A:107:ILE:HA	2.18	0.42
2:B:172:THR:CG2	2:B:190:LEU:HD11	2.48	0.42
2:B:196:VAL:HG22	2:B:197:SER:H	1.83	0.42
2:B:19:MET:HE3	2:B:19:MET:HB3	1.94	0.42
2:B:229:LYS:HG2	2:B:231:VAL:HG13	2.01	0.42
2:B:157:LEU:HD23	2:B:158:SER:N	2.35	0.42
3:C:246:MET:HE3	3:C:246:MET:HB3	1.78	0.42
3:C:118:SER:HB2	3:C:213:GLU:HB3	2.02	0.42
3:C:127:SER:HA	3:C:191:LEU:HD13	2.02	0.42
3:C:156:LEU:N	3:C:156:LEU:CD2	2.83	0.42
3:C:160:ARG:HA	3:C:160:ARG:HD3	1.68	0.42
1:A:32:LEU:C	1:A:32:LEU:HD23	2.45	0.42
2:B:86:THR:HG23	2:B:111:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:LYS:HG3	4:C:402:SO4:S	2.60	0.42
1:A:26:THR:HB	1:A:92:ASP:OD1	2.19	0.42
3:C:330:LYS:N	3:C:333:GLU:O	2.40	0.42
2:B:49:SER:HB2	2:B:54:THR:O	2.20	0.41
2:B:87:SER:OG	2:B:88:VAL:N	2.52	0.41
3:C:175:ARG:HH11	3:C:179:LEU:HD11	1.84	0.41
1:A:124:SER:C	1:A:126:SER:H	2.28	0.41
3:C:238:LYS:HE3	3:C:272:GLU:OE2	2.20	0.41
1:A:4:ILE:HD11	1:A:88:CYS:SG	2.60	0.41
1:A:45:PHE:CB	2:B:102:GLU:HG3	2.51	0.41
3:C:34:GLN:H	3:C:34:GLN:HG2	1.69	0.41
3:C:117:HIS:O	3:C:214:LEU:N	2.45	0.41
1:A:16:ALA:C	1:A:17:ILE:HD12	2.46	0.41
3:C:19:LYS:HA	3:C:20:PRO:HD3	1.97	0.41
3:C:27:VAL:HG21	3:C:37:ILE:HD13	2.01	0.41
3:C:159:PRO:HG3	3:C:173:TRP:CE2	2.55	0.41
3:C:268:LYS:HE3	3:C:272:GLU:OE2	2.21	0.40
3:C:341:TYR:HE2	3:C:343:GLY:HA2	1.86	0.40
1:A:38:HIS:CD2	1:A:84:ALA:HB2	2.56	0.40
3:C:360:LEU:HD22	3:C:368:TYR:CZ	2.56	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	196/208 (94%)	188 (96%)	8 (4%)	0	100	100
2	B	240/252 (95%)	234 (98%)	6 (2%)	0	100	100
3	C	363/392 (93%)	349 (96%)	14 (4%)	0	100	100
All	All	799/852 (94%)	771 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	164/183 (90%)	156 (95%)	8 (5%)	22	54
2	B	195/216 (90%)	186 (95%)	9 (5%)	24	57
3	C	295/341 (86%)	282 (96%)	13 (4%)	25	59
All	All	654/740 (88%)	624 (95%)	30 (5%)	24	57

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	25	GLN
1	A	50	VAL
1	A	96	GLN
1	A	143	VAL
1	A	165	ASP
1	A	194	ASP
1	A	195	THR
2	B	19	MET
2	B	25	GLN
2	B	36	ARG
2	B	66	VAL
2	B	76	LEU
2	B	78	LEU
2	B	110	ARG
2	B	111	LEU
2	B	184	ASN
3	C	23	LEU
3	C	84	VAL
3	C	142	VAL
3	C	156	LEU
3	C	160	ARG
3	C	162	LEU

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Mol	Chain	Res	Type
3	C	175	ARG
3	C	191	LEU
3	C	214	LEU
3	C	238	LYS
3	C	246	MET
3	C	324	ILE
3	C	381	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	94	ASN
1	A	142	ASN
2	B	99	ASN
3	C	13	HIS
3	C	66	HIS
3	C	167	ASN
3	C	301	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	KFP	C	157	3	22,23,24	1.76	4 (18%)	20,30,32	1.80	5 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KFP	C	157	3	-	1/10/11/13	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	157	KFP	CAF-C6	-5.23	1.39	1.50
3	C	157	KFP	C4A-C4	-3.93	1.39	1.47
3	C	157	KFP	C7-N8	2.82	1.40	1.34
3	C	157	KFP	CAF-NAL	-2.53	1.34	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	157	KFP	C6-C7-N8	-3.75	119.55	123.14
3	C	157	KFP	CAF-NAL-CAJ	3.27	124.70	113.20
3	C	157	KFP	C2-N3-C4	-3.11	119.41	125.11
3	C	157	KFP	CAF-C6-N5	2.38	121.06	116.56
3	C	157	KFP	C4A-C4-N3	2.36	118.56	114.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	157	KFP	CAH-CAJ-NAL-CAF

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	157	KFP	4	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.13	0
4	SO4	A	301	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	C	402	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	C	401	-	4,4,4	0.24	0	6,6,6	0.09	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	SO4	3	0
4	C	401	SO4	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	198/208 (95%)	1.09	34 (17%) 4 3	42, 68, 110, 140	0
2	B	242/252 (96%)	0.98	31 (12%) 7 6	40, 70, 101, 128	0
3	C	371/392 (94%)	1.23	80 (21%) 2 2	43, 75, 125, 158	0
All	All	811/852 (95%)	1.12	145 (17%) 3 3	40, 72, 119, 158	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	105	GLY	6.5
3	C	305	THR	5.4
2	B	100	THR	5.3
3	C	69	PHE	5.0
3	C	97	ASP	4.8
1	A	200	PRO	4.7
3	C	17	ASP	4.6
3	C	309	ILE	4.6
2	B	99	ASN	4.6
1	A	150	ASP	4.4
3	C	21	ASN	4.2
1	A	183	ALA	4.0
1	A	184	ASN	4.0
1	A	156	LYS	3.9
2	B	226	ASP	3.9
3	C	18	GLY	3.8
3	C	71	PRO	3.7
3	C	364	ASN	3.7
1	A	190	ILE	3.7
1	A	199	SER	3.7
3	C	72	ASN	3.7
3	C	158	GLU	3.6
2	B	118	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	100	GLY	3.6
3	C	20	PRO	3.6
1	A	144	SER	3.5
2	B	111	LEU	3.5
3	C	248	ASN	3.5
3	C	362	PRO	3.5
2	B	101	GLY	3.4
1	A	138	ASP	3.4
1	A	169	ASN	3.4
2	B	69	LEU	3.4
3	C	349	ASP	3.4
1	A	101	ALA	3.3
3	C	245	ALA	3.3
3	C	363	GLN	3.3
3	C	70	THR	3.3
3	C	96	ARG	3.3
3	C	155	GLN	3.3
2	B	95	GLU	3.2
2	B	98	PRO	3.2
2	B	46	ILE	3.2
1	A	3	ASN	3.1
3	C	15	PRO	3.1
1	A	162	ARG	3.1
3	C	360	LEU	3.1
2	B	2	ALA	3.1
1	A	188	ASN	3.1
3	C	115	ARG	3.1
1	A	157	CYS	3.0
3	C	23	LEU	3.0
2	B	219	GLU	3.0
3	C	145	HIS	3.0
3	C	67	ALA	3.0
2	B	222	GLU	2.9
3	C	43	GLY	2.9
2	B	153	ASP	2.9
3	C	101	GLY	2.8
1	A	164	MET	2.8
3	C	169	ALA	2.8
2	B	116	ASP	2.8
2	B	187	ARG	2.7
3	C	34	GLN	2.7
2	B	70	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	171	ASP	2.7
3	C	386	GLU	2.7
1	A	166	PHE	2.7
1	A	159	LEU	2.7
3	C	103	SER	2.7
1	A	158	VAL	2.6
2	B	182	ALA	2.6
2	B	243	ALA	2.6
3	C	22	TYR	2.6
3	C	365	GLY	2.6
3	C	84	VAL	2.6
3	C	347	SER	2.5
3	C	52	ASP	2.5
2	B	97	ASP	2.5
3	C	154	SER	2.5
3	C	359	GLU	2.5
3	C	310	THR	2.5
1	A	191	ILE	2.5
2	B	131	SER	2.5
3	C	170	PRO	2.5
3	C	46	ILE	2.5
3	C	104	GLY	2.5
3	C	323	GLU	2.5
3	C	130	GLY	2.4
3	C	336	PHE	2.4
1	A	177	LYS	2.4
3	C	341	TYR	2.4
3	C	335	ILE	2.4
3	C	138	SER	2.4
3	C	246	MET	2.4
3	C	304	GLU	2.4
2	B	13	LEU	2.4
3	C	42	ASN	2.4
3	C	331	ASN	2.4
3	C	216	GLU	2.4
3	C	8	GLN	2.4
2	B	27	MET	2.3
3	C	73	SER	2.3
3	C	131	TYR	2.3
3	C	9	VAL	2.3
3	C	88	GLN	2.3
2	B	112	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	102	GLY	2.3
1	A	187	ASN	2.3
1	A	176	ASN	2.3
3	C	291	GLN	2.3
3	C	16	GLU	2.2
1	A	27	SER	2.2
3	C	77	TYR	2.2
1	A	181	ALA	2.2
2	B	177	LEU	2.2
2	B	175	GLN	2.2
3	C	332	GLY	2.2
3	C	162	LEU	2.2
1	A	146	SER	2.2
3	C	200	HIS	2.2
2	B	185	ASP	2.1
3	C	74	LYS	2.1
3	C	116	THR	2.1
2	B	109	SER	2.1
1	A	179	ASP	2.1
2	B	3	GLY	2.1
2	B	96	THR	2.1
1	A	98	ILE	2.1
1	A	178	SER	2.1
3	C	79	CYS	2.1
3	C	358	VAL	2.1
1	A	198	PRO	2.1
3	C	177	THR	2.1
1	A	92	ASP	2.1
3	C	284	GLU	2.1
3	C	66	HIS	2.0
1	A	143	VAL	2.0
1	A	151	VAL	2.0
3	C	262	HIS	2.0
3	C	377	VAL	2.0
1	A	197	PHE	2.0
3	C	55	PHE	2.0
3	C	1	ILE	2.0
2	B	79	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	KFP	C	157	22/23	0.84	0.19	67,72,78,81	0

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
4	SO4	C	402	5/5	0.76	0.18	127,128,129,129	0
4	SO4	A	302	5/5	0.81	0.11	129,130,131,132	0
4	SO4	A	301	5/5	0.84	0.14	100,102,102,103	0
4	SO4	C	401	5/5	0.89	0.14	73,73,75,77	0
4	SO4	B	301	5/5	0.90	0.14	86,87,88,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.