



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:31 AM UTC

PDB ID : 4L9L / pdb_00004l9l
Title : Crystal structure of a human Valpha7.2/Vbeta13.2 MAIT TCR in complex with bovine MR1
Authors : Lopez-Sagaseta, J.; Adams, E.J.
Deposited on : 2013-06-18
Resolution : 3.40 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

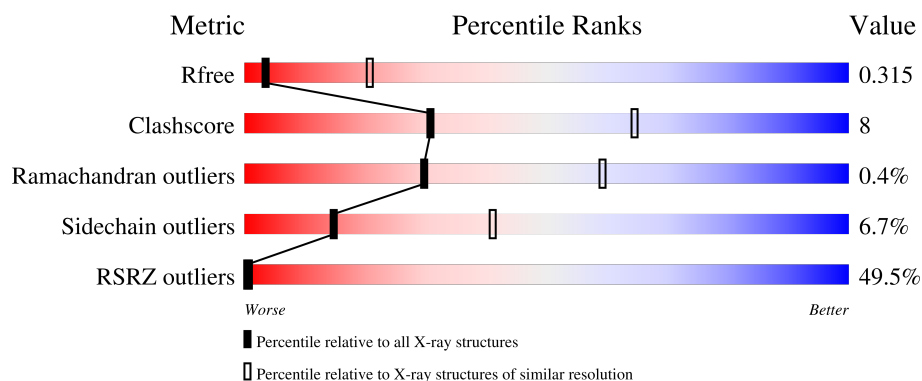
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	C	392	42% 65% 16% • 16%
2	A	208	40% 80% 14% 6%
3	B	252	51% 69% 20% 5% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6041 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 Beta-2-microglobulin, MHC class I-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	329	Total	C	N	O	S	0	0	0
			2684	1723	466	482	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	106	SER	-	linker	UNP P01888
C	107	GLY	-	linker	UNP P01888
C	108	SER	-	linker	UNP P01888
C	109	GLY	-	linker	UNP P01888
C	110	GLY	-	linker	UNP P01888
C	111	GLY	-	linker	UNP P01888
C	112	GLY	-	linker	UNP P01888
C	113	SER	-	linker	UNP P01888

- Molecule 2 is a protein called Human MAIT TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	196	Total	C	N	O	S	0	0	0
			1492	945	239	300	8			

- Molecule 3 is a protein called Human MAIT TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	239	Total	C	N	O	S	0	0	0
			1854	1178	317	350	9			

- 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	B	1	Total	O	S	0	0
			5	4	1		

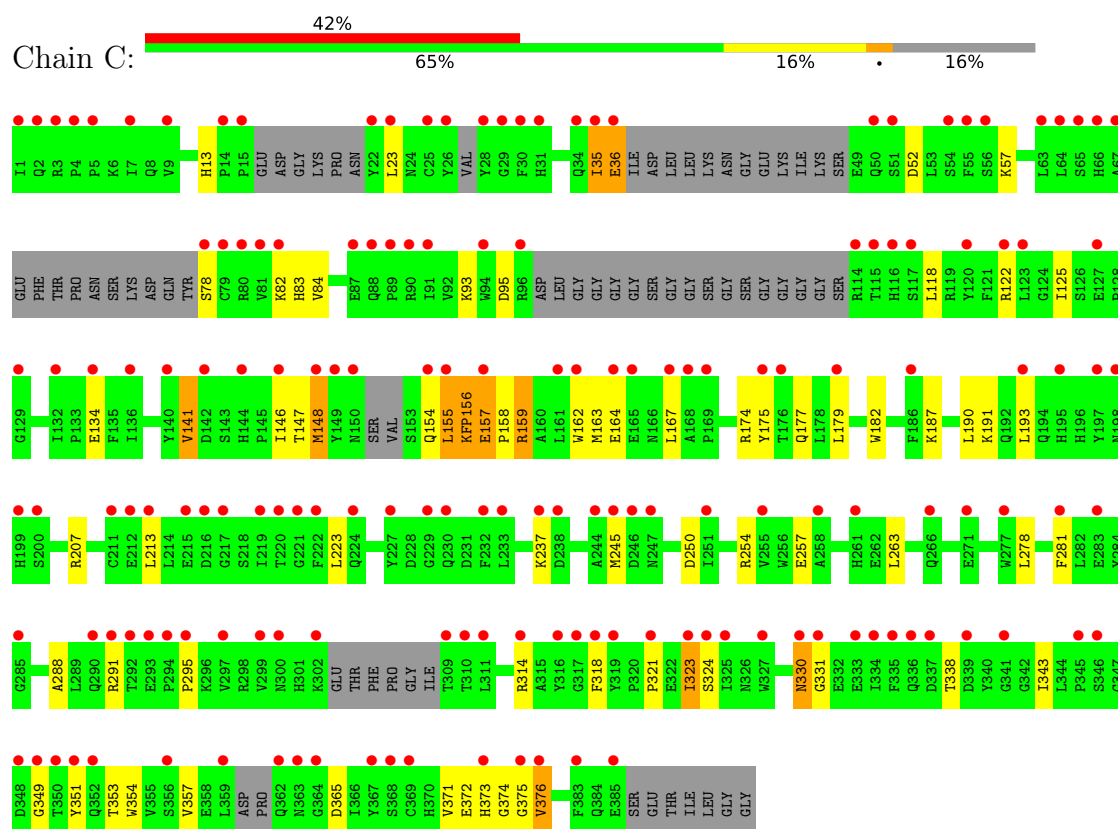
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			1	1		

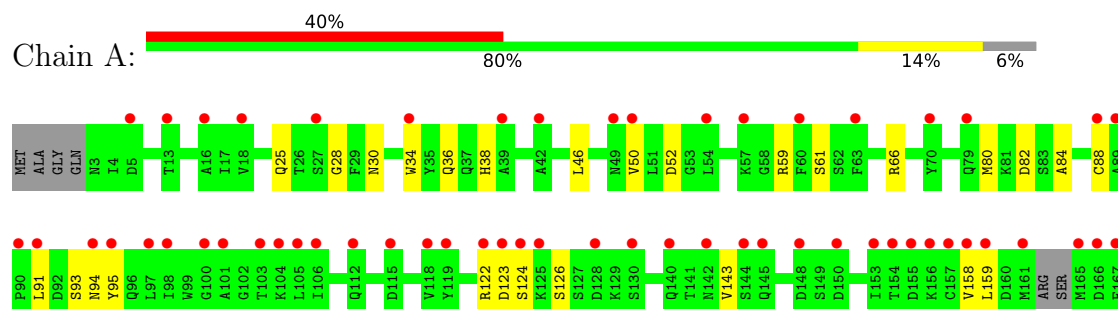
3 Residue-property plots

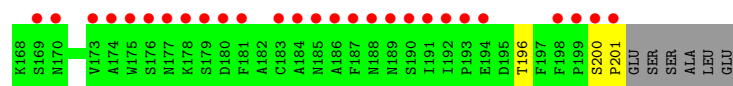
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-2-microglobulin, MHC class I-related protein

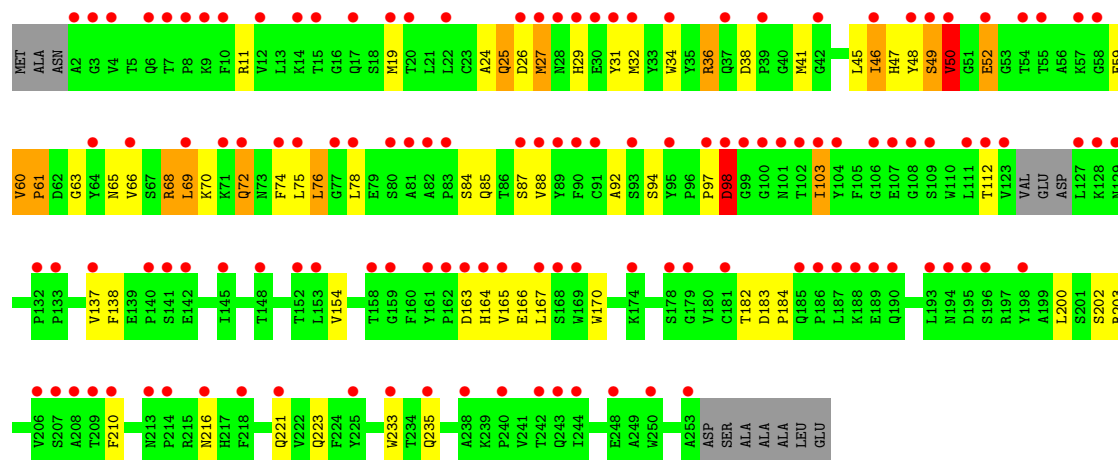


- Molecule 2: Human MAIT TCR alpha chain





● Molecule 3: Human MAIT TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.77Å 86.98Å 156.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.58 – 3.40 47.58 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.58-3.40) 97.9 (47.58-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.58 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.254 , 0.312 0.258 , 0.315	Depositor DCC
R_{free} test set	806 reflections (3.02%)	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)	0.33 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	6041	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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	C	0.36	1/2740 (0.0%)	0.75	6/3717 (0.2%)
2	A	0.31	0/1526	0.75	1/2078 (0.0%)
3	B	0.37	0/1908	0.86	5/2606 (0.2%)
All	All	0.35	1/6174 (0.0%)	0.79	12/8401 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	157	GLU	C-N	6.24	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	60	VAL	CA-C-N	-7.13	110.93	119.84
3	B	60	VAL	C-N-CA	-7.13	110.93	119.84
1	C	157	GLU	CA-C-N	-7.08	113.37	120.31
1	C	157	GLU	C-N-CA	-7.08	113.37	120.31
3	B	98	ASP	N-CA-C	-6.81	100.08	110.30
3	B	50	VAL	CB-CA-C	-6.28	103.79	112.02
3	B	26	ASP	N-CA-C	-6.02	105.69	113.16
1	C	330	ASN	N-CA-C	5.73	119.30	111.39
1	C	349	GLY	N-CA-C	-5.55	107.70	114.92
1	C	374	GLY	N-CA-C	-5.42	108.23	115.32
1	C	148	MET	N-CA-C	5.31	116.10	107.23
2	A	94	ASN	N-CA-C	-5.16	103.71	110.53

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	C	2684	0	2463	38	0
2	A	1492	0	1374	17	0
3	B	1854	0	1730	47	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
5	C	1	0	0	0	0
All	All	6041	0	5567	96	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 8.

All (96) 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:B:92:ALA:HB1	3:B:103:ILE:HD11	1.67	0.76
1:C:36:GLU:O	1:C:82:LYS:N	2.12	0.71
1:C:122:ARG:HB2	1:C:207:ARG:HB3	1.74	0.69
3:B:11:ARG:HG2	3:B:19:MET:HE2	1.74	0.69
3:B:59:GLU:HG2	3:B:60:VAL:HG13	1.74	0.68
2:A:80:MET:HE2	2:A:159:LEU:HD12	1.78	0.65
3:B:163:ASP:O	3:B:164:HIS:ND1	2.30	0.64
3:B:154:VAL:HG22	3:B:203:ARG:HG3	1.81	0.63
1:C:177:GLN:O	3:B:50:VAL:HG11	1.99	0.62
1:C:343:ILE:HA	1:C:353:THR:HG22	1.81	0.62
1:C:147:THR:HB	1:C:156:KFP:H12	1.82	0.62
1:C:118:LEU:HB2	1:C:278:LEU:HD13	1.81	0.62
2:A:59:ARG:NH2	2:A:82:ASP:OD2	2.32	0.61
3:B:36:ARG:NH1	3:B:38:ASP:OD1	2.35	0.60
3:B:63:GLY:HA3	3:B:85:GLN:NE2	2.17	0.59
1:C:158:PRO:HG3	1:C:164:GLU:HB2	1.85	0.59
3:B:31:TYR:HB2	3:B:94:SER:O	2.04	0.58
3:B:94:SER:HB2	3:B:103:ILE:HA	1.85	0.58
1:C:338:THR:HG22	1:C:357:VAL:HG22	1.85	0.58
2:A:158:VAL:HG23	3:B:184:PRO:HG3	1.85	0.58
1:C:122:ARG:HD2	1:C:207:ARG:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:GLU:HA	1:C:36:GLU:OE1	2.03	0.57
1:C:182:TRP:NE1	3:B:98:ASP:OD1	2.37	0.57
1:C:146:ILE:O	1:C:159:ARG:N	2.37	0.57
2:A:123:ASP:CB	2:A:124:SER:HA	2.34	0.57
3:B:27:MET:HB3	3:B:29:HIS:NE2	2.20	0.57
1:C:321:PRO:HG3	1:C:351:TYR:CE1	2.40	0.57
2:A:36:GLN:HB2	2:A:46:LEU:HD11	1.87	0.56
3:B:47:HIS:CE1	3:B:61:PRO:HB2	2.41	0.56
3:B:36:ARG:NH2	3:B:84:SER:O	2.37	0.56
3:B:49:SER:OG	3:B:68:ARG:HD2	2.06	0.56
3:B:52:GLU:HA	3:B:68:ARG:HD3	1.88	0.56
3:B:92:ALA:HB1	3:B:103:ILE:CD1	2.35	0.56
3:B:66:VAL:HG22	3:B:76:LEU:HD23	1.87	0.56
1:C:141:VAL:HG12	1:C:146:ILE:HD13	1.88	0.56
3:B:66:VAL:HG13	3:B:75:LEU:O	2.06	0.55
2:A:52:ASP:H	2:A:66:ARG:HH21	1.55	0.55
1:C:250:ASP:OD2	1:C:254:ARG:NH1	2.40	0.54
3:B:47:HIS:HE1	3:B:61:PRO:HB2	1.72	0.53
2:A:38:HIS:CD2	2:A:84:ALA:HB2	2.43	0.53
1:C:78:SER:HA	1:C:93:LYS:HA	1.90	0.53
2:A:59:ARG:NH1	4:A:301:SO4:O3	2.42	0.53
1:C:52:ASP:OD2	1:C:159:ARG:NH1	2.41	0.53
1:C:330:ASN:N	1:C:331:GLY:HA2	2.23	0.53
1:C:318:PHE:HZ	1:C:353:THR:HG23	1.76	0.51
1:C:35:ILE:HG13	1:C:83:HIS:HD2	1.76	0.51
2:A:122:ARG:HG2	2:A:123:ASP:H	1.76	0.50
1:C:154:GLN:O	1:C:155:LEU:HD22	2.11	0.50
1:C:187:LYS:HE2	1:C:191:LYS:HE2	1.95	0.49
3:B:72:GLN:OE1	3:B:72:GLN:N	2.46	0.49
2:A:95:TYR:HB3	3:B:97:PRO:HB2	1.93	0.49
1:C:295:PRO:HD3	1:C:373:HIS:CD2	2.48	0.49
3:B:32:MET:HB3	3:B:74:PHE:CD2	2.48	0.49
3:B:46:ILE:O	3:B:61:PRO:HB3	2.13	0.48
2:A:28:GLY:N	2:A:93:SER:HB2	2.29	0.47
2:A:34:TRP:CH2	2:A:88:CYS:HB2	2.50	0.47
3:B:34:TRP:HB3	3:B:46:ILE:HD11	1.95	0.47
3:B:233:TRP:CE2	3:B:235:GLN:HB2	2.50	0.46
2:A:124:SER:C	2:A:126:SER:H	2.23	0.46
1:C:330:ASN:HD21	1:C:365:ASP:HA	1.81	0.46
2:A:158:VAL:N	3:B:182:THR:O	2.48	0.46
3:B:38:ASP:HB2	3:B:41:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:TRP:H	1:C:162:TRP:CD1	2.34	0.45
3:B:27:MET:HB3	3:B:29:HIS:CD2	2.52	0.45
3:B:210:PHE:O	3:B:216:ASN:ND2	2.48	0.45
3:B:24:ALA:HA	3:B:72:GLN:O	2.17	0.45
2:A:124:SER:HB2	3:B:138:PHE:CE2	2.52	0.44
3:B:170:TRP:NE1	3:B:221:GLN:OE1	2.49	0.44
1:C:125:ILE:HB	1:C:134:GLU:HA	2.00	0.44
1:C:163:MET:HE1	1:C:281:PHE:CG	2.53	0.44
1:C:323:ILE:HD11	1:C:371:VAL:HG13	2.00	0.43
3:B:45:LEU:HD21	3:B:48:TYR:HB3	1.99	0.43
1:C:257:GLU:HA	1:C:263:LEU:HD11	2.00	0.43
3:B:25:GLN:NE2	3:B:32:MET:HE2	2.33	0.43
1:C:288:ALA:O	1:C:291:ARG:NH1	2.52	0.43
3:B:25:GLN:OE1	3:B:29:HIS:N	2.50	0.43
1:C:175:TYR:O	1:C:179:LEU:HD23	2.19	0.43
3:B:166:GLU:HB2	3:B:223:GLN:HB3	2.01	0.43
1:C:375:GLY:N	1:C:376:VAL:HB	2.34	0.42
3:B:167:LEU:HA	3:B:221:GLN:O	2.19	0.42
2:A:200:SER:OG	2:A:201:PRO:HD3	2.20	0.41
3:B:34:TRP:O	3:B:45:LEU:HD12	2.20	0.41
2:A:30:ASN:HB2	2:A:91:LEU:HB3	2.03	0.41
1:C:372:GLU:HG3	1:C:375:GLY:HA2	2.02	0.41
3:B:183:ASP:HB2	3:B:200:LEU:CD2	2.50	0.41
3:B:69:LEU:HB2	3:B:70:LYS:H	1.79	0.41
3:B:87:SER:OG	3:B:88:VAL:N	2.54	0.41
1:C:146:ILE:O	1:C:158:PRO:HA	2.21	0.41
1:C:179:LEU:HD22	1:C:182:TRP:CE3	2.55	0.41
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.89	0.41
3:B:34:TRP:CE2	3:B:76:LEU:HB2	2.56	0.41
1:C:323:ILE:HD13	1:C:324:SER:H	1.85	0.40
3:B:49:SER:OG	3:B:68:ARG:NH2	2.53	0.40
1:C:314:ARG:HD3	1:C:354:TRP:HB3	2.03	0.40
3:B:63:GLY:HA3	3:B:85:GLN:HE21	1.84	0.40
3:B:182:THR:HG23	3:B:202:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

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	C	310/392 (79%)	300 (97%)	9 (3%)	1 (0%)	36	65
2	A	192/208 (92%)	183 (95%)	9 (5%)	0	100	100
3	B	235/252 (93%)	225 (96%)	8 (3%)	2 (1%)	14	42
All	All	737/852 (86%)	708 (96%)	26 (4%)	3 (0%)	30	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	61	PRO
3	B	69	LEU
1	C	376	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	273/341 (80%)	253 (93%)	20 (7%)	13	39
2	A	161/183 (88%)	156 (97%)	5 (3%)	35	59
3	B	195/213 (92%)	178 (91%)	17 (9%)	9	32
All	All	629/737 (85%)	587 (93%)	42 (7%)	15	41

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	13	HIS
1	C	23	LEU
1	C	35	ILE
1	C	36	GLU
1	C	57	LYS
1	C	84	VAL
1	C	95	ASP
1	C	141	VAL
1	C	148	MET
1	C	155	LEU
1	C	157	GLU
1	C	159	ARG
1	C	167	LEU
1	C	174	ARG
1	C	190	LEU
1	C	213	LEU
1	C	223	LEU
1	C	237	LYS
1	C	245	MET
1	C	323	ILE
2	A	25	GLN
2	A	50	VAL
2	A	61	SER
2	A	143	VAL
2	A	196	THR
3	B	25	GLN
3	B	27	MET
3	B	36	ARG
3	B	46	ILE
3	B	49	SER
3	B	50	VAL
3	B	52	GLU
3	B	65	ASN
3	B	68	ARG
3	B	72	GLN
3	B	76	LEU
3	B	78	LEU
3	B	98	ASP
3	B	103	ILE
3	B	112	THR
3	B	137	VAL
3	B	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	171	HIS
1	C	199	HIS
1	C	224	GLN
1	C	300	ASN
1	C	326	ASN
1	C	373	HIS
2	A	21	ASN
2	A	113	ASN
3	B	25	GLN
3	B	65	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	$\# Z > 2$
1	KFP	C	156	1	22,23,24	1.92	4 (18%)	20,30,32	1.86	6 (30%)

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
1	KFP	C	156	1	-	0/10/11/13	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	156	KFP	C4A-C4	-5.39	1.36	1.47
1	C	156	KFP	CAF-C6	-5.22	1.39	1.50
1	C	156	KFP	C7-N8	2.62	1.39	1.34
1	C	156	KFP	CAF-NAL	-2.40	1.35	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	156	KFP	C7-C6-N5	-4.55	117.92	120.87
1	C	156	KFP	CAF-NAL-CAJ	3.54	125.64	113.20
1	C	156	KFP	CAF-C6-N5	2.53	121.35	116.56
1	C	156	KFP	C6-C7-N8	-2.47	120.77	123.14
1	C	156	KFP	C2-N3-C4	-2.30	120.90	125.11
1	C	156	KFP	C4A-C4-N3	2.07	118.03	114.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	156	KFP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	301	-	4,4,4	0.24	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	301	-	4,4,4	0.27	0	6,6,6	0.15	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	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	C	328/392 (83%)	2.06	165 (50%)  	24, 97, 130, 152	0
2	A	196/208 (94%)	1.98	84 (42%)  	53, 87, 141, 174	0
3	B	239/252 (94%)	2.07	129 (53%)  	54, 92, 128, 155	0
All	All	763/852 (89%)	2.04	378 (49%)  	24, 92, 132, 174	0

All (378) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	247	ASN	5.7
1	C	309	THR	5.0
1	C	385	GLU	4.9
2	A	184	ALA	4.5
1	C	67	ALA	4.4
3	B	69	LEU	4.4
2	A	157	CYS	4.3
1	C	82	LYS	4.2
2	A	156	LYS	4.2
3	B	169	TRP	4.2
2	A	154	THR	4.1
2	A	183	CYS	4.1
3	B	107	GLU	4.0
1	C	195	HIS	4.0
3	B	208	ALA	4.0
3	B	123	VAL	4.0
1	C	114	ARG	4.0
2	A	60	PHE	4.0
1	C	65	SER	4.0
1	C	88	GLN	3.9
2	A	145	GLN	3.9
2	A	190	SER	3.9
1	C	79	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	A	161	MET	3.8
2	A	123	ASP	3.8
3	B	28	ASN	3.8
1	C	14	PRO	3.8
3	B	187	LEU	3.7
3	B	189	GLU	3.7
1	C	363	ASN	3.7
2	A	105	LEU	3.7
2	A	191	ILE	3.7
3	B	77	GLY	3.7
2	A	201	PRO	3.6
3	B	248	GLU	3.6
2	A	166	ASP	3.6
2	A	90	PRO	3.6
1	C	310	THR	3.6
2	A	179	SER	3.6
1	C	150	ASN	3.5
3	B	31	TYR	3.5
1	C	89	PRO	3.5
3	B	153	LEU	3.5
2	A	104	LYS	3.5
1	C	213	LEU	3.5
1	C	9	VAL	3.4
3	B	194	ASN	3.4
1	C	335	PHE	3.4
2	A	186	ALA	3.4
2	A	198	PHE	3.4
1	C	36	GLU	3.4
1	C	233	LEU	3.3
3	B	42	GLY	3.3
1	C	334	ILE	3.3
1	C	336	GLN	3.3
3	B	164	HIS	3.3
2	A	150	ASP	3.3
2	A	153	ILE	3.3
3	B	163	ASP	3.3
3	B	240	PRO	3.3
1	C	55	PHE	3.3
2	A	142	ASN	3.3
1	C	245	MET	3.3
1	C	294	PRO	3.3
3	B	185	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	50	GLN	3.2
3	B	235	GLN	3.2
3	B	133	PRO	3.2
3	B	109	SER	3.2
2	A	192	ILE	3.2
2	A	167	PHE	3.2
3	B	132	PRO	3.2
1	C	142	ASP	3.1
3	B	91	CYS	3.1
1	C	162	TRP	3.1
3	B	81	ALA	3.1
2	A	175	TRP	3.1
3	B	210	PHE	3.1
2	A	106	ILE	3.1
3	B	46	ILE	3.1
3	B	29	HIS	3.1
1	C	224	GLN	3.1
3	B	238	ALA	3.1
1	C	56	SER	3.1
1	C	87	GLU	3.1
2	A	101	ALA	3.1
3	B	72	GLN	3.1
1	C	28	TYR	3.1
2	A	91	LEU	3.0
3	B	54	THR	3.0
2	A	27	SER	3.0
3	B	22	LEU	3.0
1	C	116	HIS	3.0
1	C	3	ARG	3.0
2	A	170	ASN	3.0
3	B	71	LYS	3.0
3	B	87	SER	3.0
1	C	345	PRO	3.0
3	B	8	PRO	3.0
1	C	375	GLY	3.0
2	A	57	LYS	3.0
2	A	118	VAL	3.0
1	C	251	ILE	3.0
3	B	145	ILE	3.0
1	C	314	ARG	3.0
2	A	180	ASP	3.0
1	C	350	THR	3.0

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Mol	Chain	Res	Type	RSRZ
3	B	178	SER	3.0
2	A	155	ASP	3.0
1	C	129	GLY	3.0
2	A	165	MET	3.0
2	A	100	GLY	2.9
2	A	181	PHE	2.9
1	C	351	TYR	2.9
2	A	200	SER	2.9
1	C	331	GLY	2.9
1	C	238	ASP	2.9
3	B	27	MET	2.9
2	A	130	SER	2.9
2	A	148	ASP	2.9
1	C	291	ARG	2.9
1	C	179	LEU	2.9
1	C	324	SER	2.9
3	B	141	SER	2.9
1	C	25	CYS	2.9
3	B	4	VAL	2.9
3	B	3	GLY	2.9
1	C	78	SER	2.8
3	B	98	ASP	2.8
1	C	176	THR	2.8
1	C	215	GLU	2.8
2	A	177	ASN	2.8
3	B	181	CYS	2.8
3	B	80	SER	2.8
1	C	169	PRO	2.8
3	B	198	TYR	2.8
3	B	6	GLN	2.8
1	C	81	VAL	2.8
1	C	115	THR	2.8
1	C	123	LEU	2.8
2	A	159	LEU	2.8
1	C	362	GLN	2.8
2	A	193	PRO	2.8
3	B	78	LEU	2.8
3	B	250	TRP	2.8
2	A	16	ALA	2.8
1	C	237	LYS	2.8
1	C	281	PHE	2.7
2	A	63	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	187	PHE	2.7
1	C	94	TRP	2.7
2	A	189	ASN	2.7
1	C	117	SER	2.7
1	C	327	TRP	2.7
3	B	100	GLY	2.7
1	C	339	ASP	2.7
2	A	128	ASP	2.7
3	B	174	LYS	2.7
1	C	352	GLN	2.7
1	C	217	GLY	2.7
1	C	220	THR	2.7
2	A	185	ASN	2.7
1	C	167	LEU	2.7
3	B	193	LEU	2.7
3	B	9	LYS	2.7
1	C	311	LEU	2.7
2	A	158	VAL	2.7
3	B	190	GLN	2.7
3	B	10	PHE	2.7
1	C	369	CYS	2.7
3	B	34	TRP	2.7
1	C	161	LEU	2.7
3	B	95	TYR	2.7
3	B	195	ASP	2.7
1	C	15	PRO	2.6
1	C	222	PHE	2.6
1	C	164	GLU	2.6
1	C	64	LEU	2.6
1	C	368	SER	2.6
1	C	197	TYR	2.6
1	C	348	ASP	2.6
1	C	96	ARG	2.6
1	C	271	GLU	2.6
1	C	244	ALA	2.6
1	C	346	SER	2.6
1	C	91	ILE	2.6
1	C	290	GLN	2.6
1	C	29	GLY	2.6
3	B	108	GLY	2.6
1	C	63	LEU	2.6
2	A	173	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	140	TYR	2.6
2	A	144	SER	2.6
1	C	321	PRO	2.6
1	C	337	ASP	2.6
3	B	129	ASN	2.6
1	C	297	VAL	2.6
1	C	136	ILE	2.6
1	C	146	ILE	2.6
2	A	98	ILE	2.6
3	B	49	SER	2.6
2	A	5	ASP	2.6
3	B	52	GLU	2.6
3	B	242	THR	2.6
1	C	26	TYR	2.5
1	C	295	PRO	2.5
3	B	39	PRO	2.5
1	C	200	SER	2.5
3	B	58	GLY	2.5
3	B	106	GLY	2.5
1	C	300	ASN	2.5
1	C	292	THR	2.5
1	C	66	HIS	2.5
1	C	367	TYR	2.5
3	B	161	TYR	2.5
2	A	125	LYS	2.5
3	B	137	VAL	2.5
1	C	168	ALA	2.5
3	B	148	THR	2.5
2	A	122	ARG	2.5
2	A	112	GLN	2.5
3	B	82	ALA	2.5
3	B	20	THR	2.5
1	C	120	TYR	2.5
3	B	162	PRO	2.5
3	B	57	LYS	2.5
1	C	258	ALA	2.5
1	C	356	SER	2.5
1	C	35	ILE	2.5
1	C	333	GLU	2.5
1	C	148	MET	2.5
1	C	30	PHE	2.5
3	B	216	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	55	THR	2.5
1	C	5	PRO	2.5
1	C	23	LEU	2.5
1	C	229	GLY	2.5
2	A	42	ALA	2.4
3	B	2	ALA	2.4
1	C	155	LEU	2.4
1	C	4	PRO	2.4
2	A	199	PRO	2.4
1	C	144	HIS	2.4
1	C	299	VAL	2.4
1	C	325	ILE	2.4
3	B	30	GLU	2.4
3	B	74	PHE	2.4
1	C	283	GLU	2.4
1	C	383	PHE	2.4
2	A	13	THR	2.4
1	C	330	ASN	2.4
2	A	39	ALA	2.4
3	B	14	LYS	2.4
3	B	19	MET	2.4
1	C	266	GLN	2.4
1	C	293	GLU	2.4
3	B	253	ALA	2.3
3	B	99	GLY	2.3
3	B	244	ILE	2.3
1	C	198	ASN	2.3
2	A	49	ASN	2.3
3	B	104	TYR	2.3
3	B	12	VAL	2.3
3	B	66	VAL	2.3
3	B	188	LYS	2.3
2	A	169	SER	2.3
3	B	159	GLY	2.3
2	A	174	ALA	2.3
3	B	15	THR	2.3
3	B	152	THR	2.3
3	B	196	SER	2.3
2	A	50	VAL	2.3
3	B	83	PRO	2.3
1	C	285	GLY	2.3
2	A	103	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	207	SER	2.3
1	C	359	LEU	2.3
1	C	22	TYR	2.3
1	C	319	TYR	2.3
1	C	232	PHE	2.3
2	A	188	ASN	2.3
1	C	34	GLN	2.3
1	C	212	GLU	2.3
1	C	154	GLN	2.3
3	B	37	GLN	2.3
2	A	18	VAL	2.3
1	C	127	GLU	2.2
1	C	165	GLU	2.2
1	C	186	PHE	2.2
1	C	373	HIS	2.2
3	B	89	TYR	2.2
1	C	255	VAL	2.2
1	C	376	VAL	2.2
2	A	140	GLN	2.2
3	B	213	ASN	2.2
1	C	216	ASP	2.2
3	B	26	ASP	2.2
2	A	95	TYR	2.2
3	B	206	VAL	2.2
1	C	134	GLU	2.2
3	B	128	LYS	2.2
1	C	261	HIS	2.2
1	C	175	TYR	2.2
1	C	2	GLN	2.2
2	A	79	GLN	2.2
3	B	179	GLY	2.2
1	C	302	LYS	2.2
1	C	277	TRP	2.2
3	B	233	TRP	2.2
1	C	31	HIS	2.2
1	C	132	ILE	2.2
1	C	193	LEU	2.2
2	A	194	GLU	2.2
3	B	142	GLU	2.2
1	C	316	TYR	2.1
1	C	1	ILE	2.1
2	A	54	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	127	LEU	2.1
2	A	178	LYS	2.1
2	A	94	ASN	2.1
3	B	101	ASN	2.1
3	B	90	PHE	2.1
3	B	165	VAL	2.1
3	B	103	ILE	2.1
1	C	230	GLN	2.1
3	B	168	SER	2.1
3	B	186	PRO	2.1
1	C	318	PHE	2.1
2	A	88	CYS	2.1
2	A	115	ASP	2.1
3	B	50	VAL	2.1
3	B	111	LEU	2.1
3	B	112	THR	2.1
3	B	209	THR	2.1
1	C	227	TYR	2.1
1	C	80	ARG	2.1
3	B	32	MET	2.1
1	C	341	GLY	2.1
1	C	364	GLY	2.1
2	A	124	SER	2.1
2	A	34	TRP	2.1
1	C	211	CYS	2.1
3	B	75	LEU	2.1
2	A	119	TYR	2.1
3	B	48	TYR	2.1
3	B	221	GLN	2.1
1	C	317	GLY	2.1
1	C	54	SER	2.1
3	B	88	VAL	2.1
1	C	90	ARG	2.1
1	C	323	ILE	2.1
1	C	199	HIS	2.1
3	B	102	THR	2.1
3	B	158	THR	2.1
3	B	225	TYR	2.1
1	C	349	GLY	2.1
3	B	140	PRO	2.1
3	B	214	PRO	2.1
1	C	51	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	122	ARG	2.0
3	B	167	LEU	2.0
1	C	246	ASP	2.0
3	B	64	TYR	2.0
1	C	221	GLY	2.0
3	B	97	PRO	2.0
1	C	7	ILE	2.0
2	A	176	SER	2.0
3	B	93	SER	2.0
2	A	89	ALA	2.0
1	C	149	TYR	2.0
2	A	70	TYR	2.0
3	B	7	THR	2.0
3	B	218	PHE	2.0
3	B	17	GLN	2.0
3	B	243	GLN	2.0
1	C	157	GLU	2.0
2	A	97	LEU	2.0
1	C	219	ILE	2.0

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

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
1	KFP	C	156	22/23	0.86	0.21	82,100,107,112	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
4	SO4	B	301	5/5	0.79	0.16	86,87,92,92	0
4	SO4	A	301	5/5	0.86	0.17	115,116,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.