



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2025 – 01:34 PM EDT

PDB ID : 4L8S  
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](mailto: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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

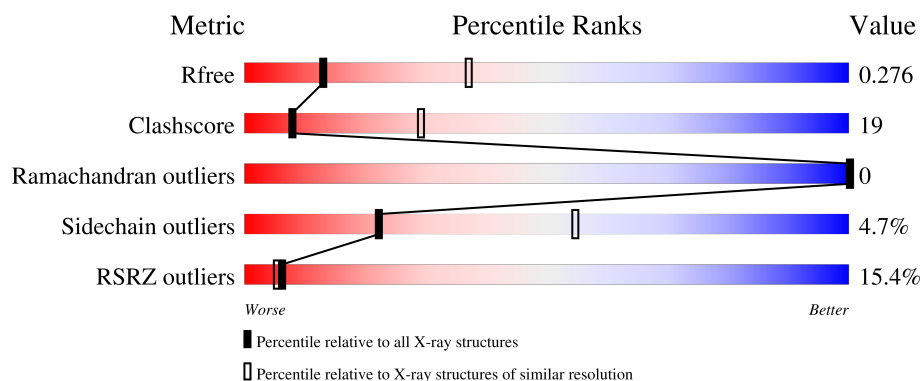
# 1 Overall quality at a glance

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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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  $\geq 3$ , 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	<div> <div>12%</div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div>
2	B	252	<div> <div>11%</div> <div>61%</div> <div>32%</div> <div>• •</div> </div>
3	C	392	<div> <div>18%</div> <div>61%</div> <div>31%</div> <div>• 5%</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
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

*Continued on next page...*

Continued from previous page...

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

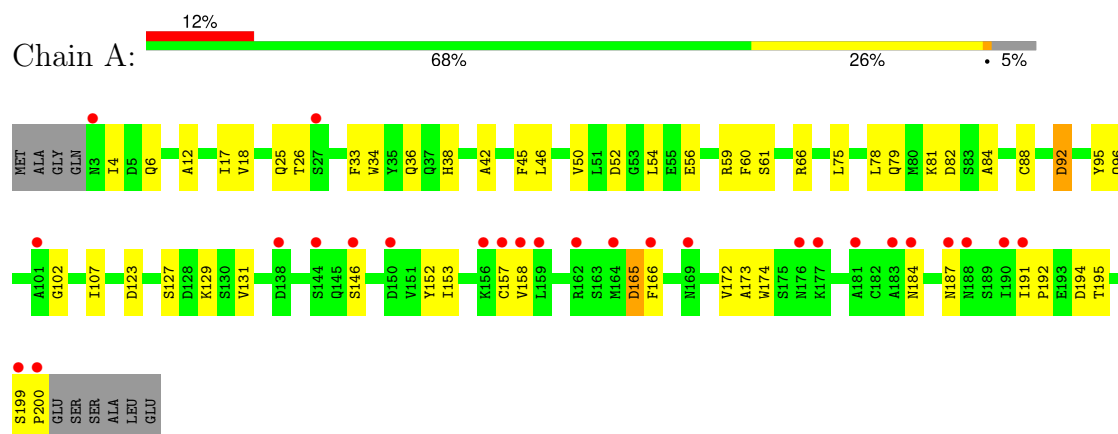
- Molecule 5 is water.

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		

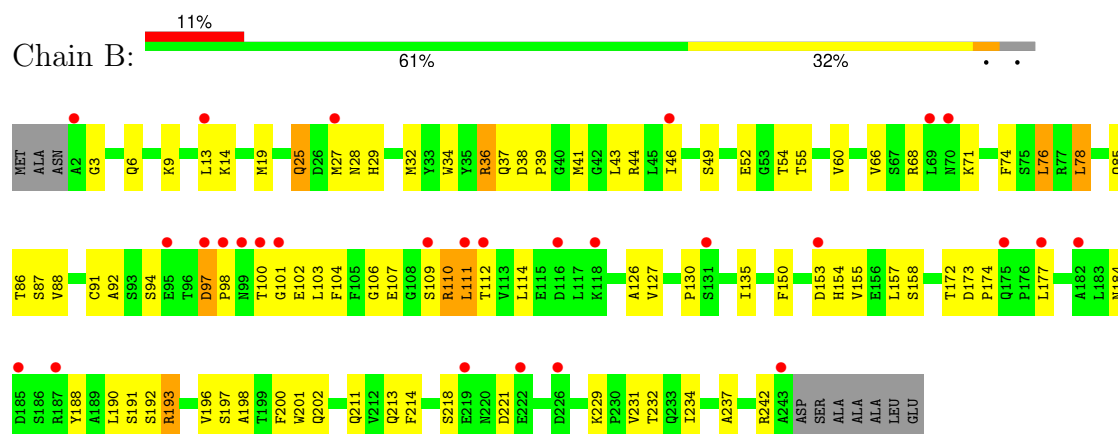
### 3 Residue-property plots [i](#)

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.

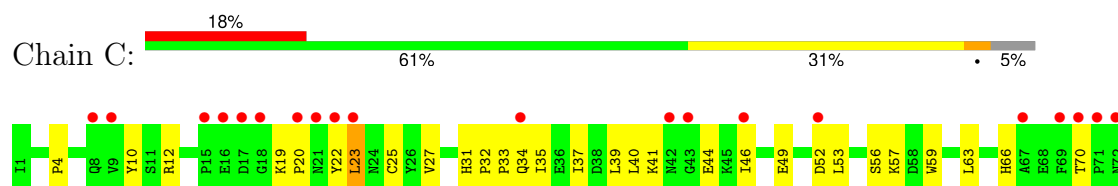
- Molecule 1: Muccosal Associated Invariant T Cell Receptor alpha chain

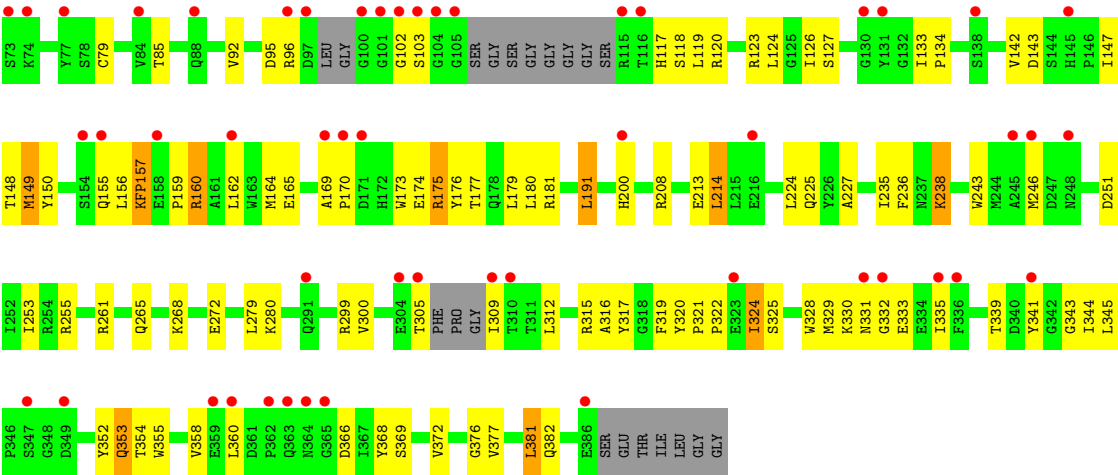


- Molecule 2: Muccosal Associated Invariant T Cell Receptor beta chain



- Molecule 3: Beta-2-microglobulin, MHC class I-related protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.24	0/1542	0.43	0/2101
2	B	0.24	0/1905	0.43	0/2603
3	C	0.23	0/3016	0.43	0/4106
All	All	0.24	0/6463	0.43	0/8810

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	1507	0	1371	45	0
2	B	1855	0	1710	87	0
3	C	2950	0	2678	112	0
4	A	10	0	0	0	0
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	234	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 19.

All (234) 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: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
2:B:32:MET:HE1	2:B:74:PHE:HB2	1.60	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
2:B:19:MET:HE1	2:B:111:LEU:HD21	1.63	0.81
3:C:322:PRO:HG3	3:C:352:TYR:CE2	2.16	0.81
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:6:GLN:HE21	2:B:109:SER:HB2	1.52	0.73
2:B:32:MET:CE	2:B:74:PHE:HB2	2.17	0.73
2:B:38:ASP:HB2	2:B:41:MET:HE3	1.70	0.72
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
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
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
3:C:59:TRP:CE2	3:C:227:ALA:HB2	2.40	0.56
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
2:B:3:GLY:HA2	2:B:27:MET:CE	2.37	0.54
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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: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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:41:MET:HE3	2:B:44:ARG:HH12	1.79	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
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:147:ILE:HG21	3:C:164:MET:HE2	1.97	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:3:GLY:HA2	2:B:27:MET:HE1	1.97	0.46
2:B:190:LEU:HD13	2:B:191:SER:N	2.31	0.46
3:C:34:GLN:CD	3:C:133:ILE:HD11	2.36	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:192:SER:C	2:B:193:ARG:HD3	2.38	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:147:ILE:CG2	3:C:164:MET:HE2	2.48	0.44
3:C:261:ARG:O	3:C:265:GLN:HG3	2.17	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:19:MET:CE	2:B:111:LEU:HD21	2.41	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:102:GLY:O	3:C:103:SER:HB2	2.17	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: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
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
2:B:173:ASP:HA	2:B:174:PRO:HD3	1.88	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:157:LEU:C	2:B:157:LEU:HD23	2.39	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:229:LYS:HG2	2:B:231:VAL:HG13	2.01	0.42
2:B:32:MET:HE2	2:B:68:ARG:NH1	2.35	0.42
2:B:157:LEU:HD23	2:B:158:SER:N	2.35	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
2:B:86:THR:HG23	2:B:111:LEU:O	2.19	0.42
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
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
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

### 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	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%)	157 (96%)	7 (4%)	25	57
2	B	195/216 (90%)	185 (95%)	10 (5%)	20	51
3	C	295/341 (86%)	281 (95%)	14 (5%)	22	55
All	All	654/740 (88%)	623 (95%)	31 (5%)	22	55

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	50	VAL
1	A	92	ASP
1	A	96	GLN
1	A	123	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	165	ASP
1	A	194	ASP
2	B	25	GLN
2	B	36	ARG
2	B	66	VAL
2	B	76	LEU
2	B	78	LEU
2	B	97	ASP
2	B	110	ARG
2	B	111	LEU
2	B	184	ASN
2	B	193	ARG
3	C	23	LEU
3	C	142	VAL
3	C	149	MET
3	C	160	ARG
3	C	162	LEU
3	C	175	ARG
3	C	191	LEU
3	C	200	HIS
3	C	214	LEU
3	C	238	LYS
3	C	246	MET
3	C	324	ILE
3	C	353	GLN
3	C	381	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

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	A	301	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	C	401	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	C	402	-	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

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	401	SO4	1	0
4	C	402	SO4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	198/208 (95%)	0.96	26 (13%) <b>8</b> <b>7</b>	42, 68, 110, 140	0
2	B	242/252 (96%)	0.85	28 (11%) <b>11</b> <b>9</b>	40, 70, 101, 128	0
3	C	371/392 (94%)	1.10	71 (19%) <b>4</b> <b>3</b>	43, 75, 125, 158	0
All	All	811/852 (95%)	0.99	125 (15%) <b>6</b> <b>5</b>	40, 72, 119, 158	0

All (125) 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	5.2
3	C	69	PHE	4.8
3	C	97	ASP	4.8
3	C	17	ASP	4.6
1	A	200	PRO	4.6
2	B	99	ASN	4.5
3	C	309	ILE	4.5
1	A	150	ASP	4.3
3	C	21	ASN	4.2
1	A	184	ASN	3.9
1	A	156	LYS	3.9
1	A	183	ALA	3.9
2	B	226	ASP	3.8
3	C	18	GLY	3.7
3	C	364	ASN	3.6
3	C	71	PRO	3.6
3	C	158	GLU	3.6
1	A	199	SER	3.6
3	C	72	ASN	3.6
1	A	190	ILE	3.6
2	B	118	LYS	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	100	GLY	3.5
3	C	20	PRO	3.5
1	A	144	SER	3.5
3	C	248	ASN	3.4
2	B	111	LEU	3.4
3	C	362	PRO	3.3
1	A	169	ASN	3.3
1	A	138	ASP	3.3
2	B	101	GLY	3.3
3	C	96	ARG	3.3
3	C	349	ASP	3.3
3	C	363	GLN	3.3
2	B	69	LEU	3.3
1	A	101	ALA	3.2
3	C	245	ALA	3.2
3	C	70	THR	3.2
3	C	155	GLN	3.2
2	B	95	GLU	3.2
1	A	162	ARG	3.1
1	A	3	ASN	3.1
2	B	98	PRO	3.1
2	B	46	ILE	3.1
3	C	115	ARG	3.0
3	C	15	PRO	3.0
2	B	2	ALA	3.0
1	A	188	ASN	3.0
3	C	360	LEU	3.0
2	B	219	GLU	3.0
3	C	23	LEU	2.9
3	C	145	HIS	2.9
1	A	157	CYS	2.9
3	C	67	ALA	2.9
2	B	222	GLU	2.9
2	B	153	ASP	2.8
3	C	43	GLY	2.8
3	C	169	ALA	2.7
2	B	116	ASP	2.7
3	C	101	GLY	2.7
1	A	164	MET	2.7
2	B	187	ARG	2.7
3	C	34	GLN	2.6
3	C	386	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	70	ASN	2.6
3	C	171	ASP	2.6
3	C	103	SER	2.6
1	A	158	VAL	2.5
1	A	159	LEU	2.5
1	A	166	PHE	2.5
2	B	182	ALA	2.5
2	B	243	ALA	2.5
3	C	84	VAL	2.5
3	C	365	GLY	2.5
3	C	22	TYR	2.5
3	C	347	SER	2.4
3	C	52	ASP	2.4
3	C	359	GLU	2.4
2	B	97	ASP	2.4
3	C	154	SER	2.4
3	C	323	GLU	2.4
3	C	310	THR	2.4
2	B	131	SER	2.4
1	A	177	LYS	2.4
1	A	191	ILE	2.4
3	C	46	ILE	2.4
3	C	170	PRO	2.3
3	C	104	GLY	2.3
3	C	130	GLY	2.3
3	C	335	ILE	2.3
3	C	138	SER	2.3
3	C	304	GLU	2.3
3	C	341	TYR	2.3
3	C	216	GLU	2.3
3	C	336	PHE	2.3
3	C	246	MET	2.3
3	C	42	ASN	2.3
3	C	331	ASN	2.3
3	C	8	GLN	2.3
2	B	13	LEU	2.3
3	C	73	SER	2.2
3	C	9	VAL	2.2
3	C	88	GLN	2.2
2	B	27	MET	2.2
2	B	112	THR	2.2
1	A	187	ASN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	131	TYR	2.2
3	C	102	GLY	2.2
3	C	291	GLN	2.2
1	A	176	ASN	2.2
3	C	16	GLU	2.2
1	A	27	SER	2.1
2	B	175	GLN	2.1
1	A	181	ALA	2.1
2	B	177	LEU	2.1
3	C	77	TYR	2.1
3	C	332	GLY	2.1
1	A	146	SER	2.1
3	C	162	LEU	2.1
3	C	74	LYS	2.1
3	C	200	HIS	2.1
3	C	116	THR	2.0
2	B	185	ASP	2.0
2	B	109	SER	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, 95<sup>th</sup> 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 <sup>2</sup> )	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 monosaccharides 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, 95<sup>th</sup> 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	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.