



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:20 PM GMT

PDB ID : 4LCC  
Title : Crystal structure of a human MAIT TCR in complex with a bacterial antigen bound to humanized bovine MR1  
Authors : Lopez-Sagaseta, J.; Adams, E.J  
Deposited on : 2013-06-21  
Resolution : 3.26 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

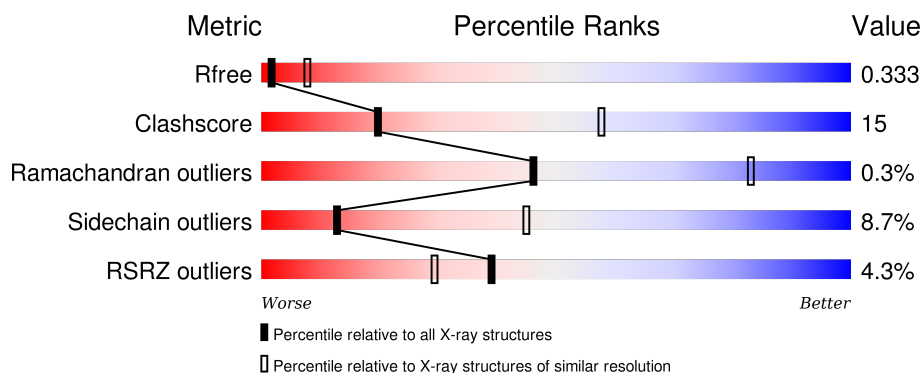
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.26 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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  $\geq 3$ , 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	C	392	<div> <div>4%</div> <div>60%</div> <div>22%</div> <div>•</div> <div>13%</div> </div>
2	A	208	<div> <div>5%</div> <div>55%</div> <div>19%</div> <div>•</div> <div>25%</div> </div>
3	B	253	<div> <div>2%</div> <div>59%</div> <div>30%</div> <div>•</div> <div>6%</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	1XL	C	401	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5827 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	341	Total	C	N	O	S	0	0	0
			2763	1778	470	501	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	MET	ALA	ENGINEERED MUTATION	UNP C1ITJ8
C	260	GLN	ARG	ENGINEERED MUTATION	UNP C1ITJ8
C	264	LEU	GLN	ENGINEERED MUTATION	UNP C1ITJ8
C	391	GLY	-	EXPRESSION TAG	UNP C1ITJ8
C	392	GLY	-	EXPRESSION TAG	UNP C1ITJ8
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

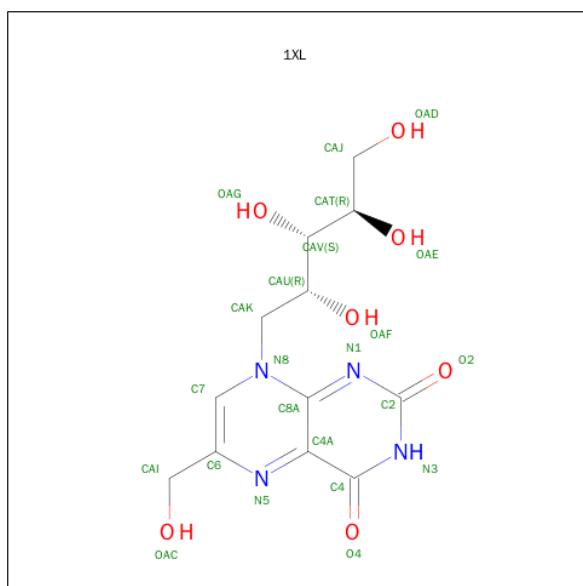
- Molecule 2 is a protein called Human MAIT TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	157	Total	C	N	O	S	0	0	0
			1196	759	192	240	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	238	Total	C	N	O	S	0	0	0
			1824	1154	307	354	9			

- Molecule 4 is 1-DEOXY-1-[6-(HYDROXYMETHYL)-2,4-DIOXO-3,4-DIHYDROPTERIDI N-8(2H)-YL]-D-ARABINITOL (three-letter code: 1XL) (formula: C<sub>12</sub>H<sub>16</sub>N<sub>4</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			23	12	4	7		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

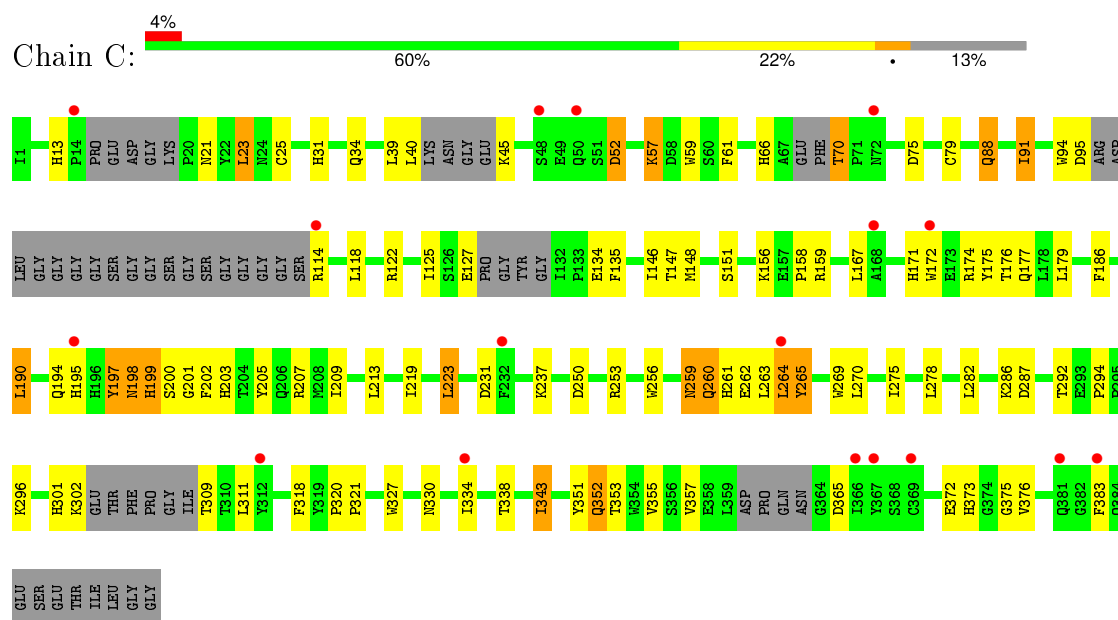
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

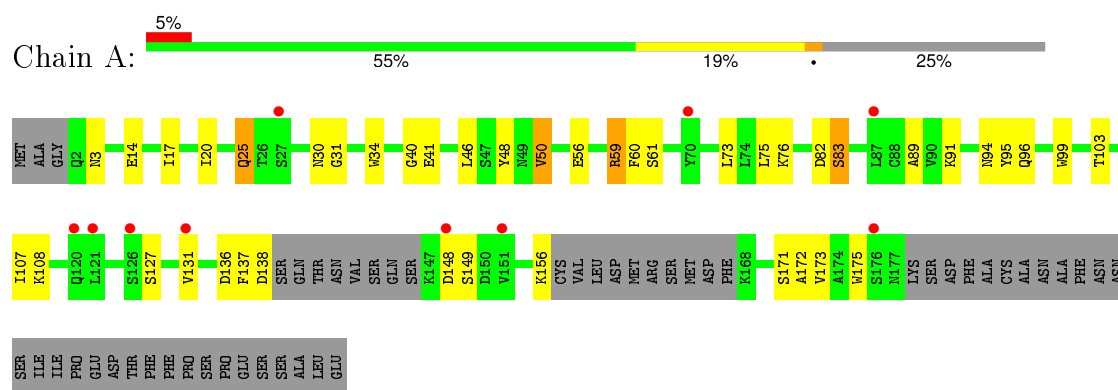
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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

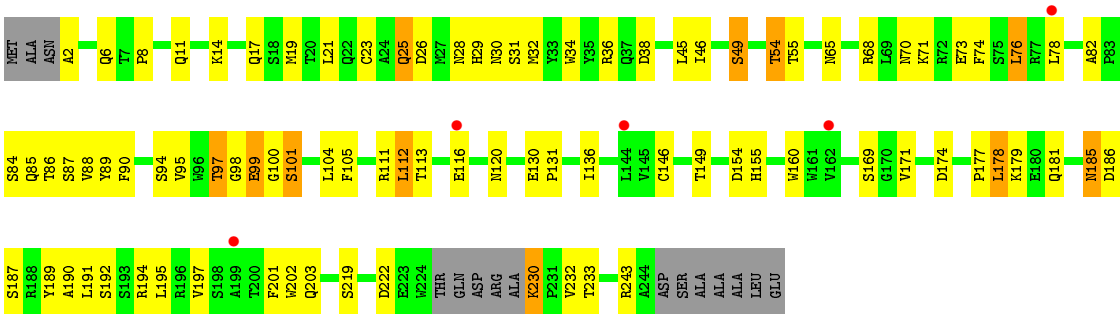


- Molecule 2: Human MAIT TCR alpha chain



- 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, $\alpha$ , $\beta$ , $\gamma$	85.90Å 88.58Å 155.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 3.26 48.32 – 3.26	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.32-3.26) 97.0 (48.32-3.26)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.257 , 0.312 0.289 , 0.333	Depositor DCC
$R_{free}$ test set	938 reflections (5.34%)	DCC
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> )	0.33 , 65.2	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 18508 reflections (0.011%)	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	5827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 1XL

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	0.30	0/2845	0.50	1/3865 (0.0%)
2	A	0.36	0/1221	0.53	0/1660
3	B	0.33	0/1874	0.52	0/2559
All	All	0.32	0/5940	0.52	1/8084 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	ASN	N-CA-C	5.75	126.53	111.00

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	C	2763	0	2551	78	0
2	A	1196	0	1098	32	0
3	B	1824	0	1676	64	0
4	C	23	0	16	4	0
5	A	5	0	0	1	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
All	All	5827	0	5341	166	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 15.

All (166) 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)
1:C:127:GLU:HG2	1:C:202:PHE:HE1	1.19	1.04
1:C:127:GLU:HG2	1:C:202:PHE:CE1	1.95	1.02
3:B:120:ASN:ND2	3:B:186:ASP:OD2	1.94	1.01
1:C:34:GLN:NE2	1:C:127:GLU:OE2	1.99	0.95
2:A:59:ARG:NH1	5:A:301:SO4:O1	2.04	0.89
2:A:59:ARG:NH2	2:A:82:ASP:OD2	2.06	0.88
1:C:177:GLN:NE2	3:B:54:THR:OG1	2.08	0.86
1:C:122:ARG:HE	4:C:401:1XL:H16	1.42	0.84
1:C:125:ILE:HG22	1:C:127:GLU:H	1.42	0.82
3:B:68:ARG:NH1	3:B:71:LYS:O	2.13	0.81
1:C:338:THR:HG22	1:C:357:VAL:HG22	1.63	0.79
3:B:30:ASN:O	3:B:68:ARG:NH2	2.17	0.77
1:C:263:LEU:HD12	1:C:263:LEU:H	1.49	0.76
2:A:60:PHE:HD1	2:A:75:LEU:HD22	1.52	0.75
2:A:148:ASP:OD2	2:A:149:SER:N	2.20	0.73
1:C:260:GLN:HA	1:C:263:LEU:HD13	1.72	0.72
2:A:131:VAL:HG12	2:A:175:TRP:HB3	1.73	0.70
3:B:86:THR:HG23	3:B:113:THR:HA	1.74	0.69
1:C:343:ILE:HA	1:C:353:THR:HG22	1.73	0.69
3:B:130:GLU:HG2	3:B:202:TRP:CH2	2.30	0.67
1:C:372:GLU:HG3	1:C:375:GLY:HA2	1.77	0.67
3:B:36:ARG:NH1	3:B:38:ASP:OD2	2.27	0.67
1:C:40:LEU:HA	1:C:45:LYS:HA	1.75	0.67
3:B:232:VAL:HG22	3:B:233:THR:H	1.60	0.66
1:C:127:GLU:CG	1:C:202:PHE:HE1	2.03	0.66
3:B:179:LYS:HE2	3:B:187:SER:OG	1.96	0.65
3:B:49:SER:OG	3:B:68:ARG:NE	2.23	0.64
1:C:262:GLU:OE2	3:B:101:SER:OG	2.15	0.64
4:C:401:1XL:OAF	2:A:95:TYR:OH	2.14	0.64
3:B:181:GLN:O	3:B:187:SER:HB3	1.98	0.63
1:C:59:TRP:NE1	1:C:231:ASP:OD1	2.25	0.63
3:B:36:ARG:NH2	3:B:84:SER:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:PHE:HB3	1:C:151:SER:HB3	1.82	0.60
1:C:122:ARG:HH12	4:C:401:1XL:H2	1.67	0.59
3:B:6:GLN:HE22	3:B:90:PHE:HA	1.67	0.59
3:B:177:PRO:HB2	3:B:189:TYR:HB3	1.84	0.59
3:B:174:ASP:OD2	3:B:192:SER:OG	2.17	0.59
3:B:11:GLN:HB2	3:B:112:LEU:HD22	1.85	0.58
1:C:269:TRP:HE3	1:C:270:LEU:HD23	1.68	0.57
2:A:59:ARG:HH22	2:A:82:ASP:CG	2.07	0.57
2:A:137:PHE:HD1	2:A:138:ASP:N	2.02	0.56
2:A:91:LYS:NZ	3:B:100:GLY:HA2	2.21	0.56
3:B:34:TRP:CE2	3:B:76:LEU:HB2	2.41	0.55
1:C:118:LEU:HB2	1:C:278:LEU:HD13	1.86	0.55
1:C:125:ILE:HB	1:C:134:GLU:HA	1.88	0.55
1:C:259:ASN:O	1:C:261:HIS:N	2.40	0.55
3:B:34:TRP:O	3:B:45:LEU:HD12	2.07	0.54
3:B:25:GLN:OE1	3:B:28:ASN:N	2.40	0.54
3:B:85:GLN:O	3:B:89:TYR:OH	2.18	0.54
2:A:156:LYS:HA	2:A:171:SER:O	2.07	0.54
3:B:8:PRO:HD2	3:B:21:LEU:HD23	1.90	0.54
2:A:30:ASN:O	2:A:91:LYS:HB2	2.08	0.54
3:B:203:GLN:HA	3:B:243:ARG:O	2.08	0.53
3:B:32:MET:SD	3:B:74:PHE:HB2	2.48	0.53
1:C:375:GLY:N	1:C:376:VAL:HB	2.23	0.53
1:C:25:CYS:HB2	1:C:39:LEU:HD21	1.90	0.53
3:B:25:GLN:OE1	3:B:29:HIS:N	2.30	0.53
1:C:194:GLN:HB3	1:C:199:HIS:O	2.08	0.53
1:C:311:LEU:HD22	1:C:383:PHE:CE2	2.44	0.53
1:C:94:TRP:O	1:C:95:ASP:HB3	2.09	0.52
1:C:265:TYR:HA	2:A:50:VAL:HG11	1.91	0.52
1:C:52:ASP:OD2	1:C:159:ARG:NH1	2.41	0.52
3:B:28:ASN:OD1	3:B:71:LYS:NZ	2.31	0.52
1:C:177:GLN:HE22	3:B:54:THR:HG1	1.57	0.52
2:A:172:ALA:HA	3:B:194:ARG:HH21	1.74	0.52
1:C:321:PRO:HG3	1:C:351:TYR:CE2	2.44	0.52
1:C:146:ILE:HG13	1:C:147:THR:H	1.75	0.51
1:C:158:PRO:HG3	1:C:172:TRP:CZ2	2.44	0.51
3:B:179:LYS:HB3	3:B:187:SER:OG	2.10	0.51
3:B:31:SER:OG	3:B:97:THR:N	2.43	0.51
1:C:194:GLN:O	1:C:197:TYR:N	2.44	0.51
1:C:122:ARG:HB2	1:C:207:ARG:HB3	1.92	0.51
2:A:83:SER:HB3	2:A:107:ILE:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TRP:O	1:C:176:THR:HG23	2.11	0.50
2:A:34:TRP:CD2	2:A:73:LEU:HD13	2.47	0.50
3:B:34:TRP:CE3	3:B:76:LEU:HD12	2.47	0.50
1:C:122:ARG:HD2	1:C:207:ARG:HD3	1.94	0.50
1:C:52:ASP:OD1	1:C:52:ASP:N	2.44	0.50
3:B:130:GLU:HG2	3:B:202:TRP:CZ2	2.47	0.49
2:A:89:ALA:HB2	2:A:99:TRP:CE3	2.47	0.49
3:B:14:LYS:N	3:B:17:GLN:OE1	2.36	0.49
1:C:79:CYS:O	1:C:91:ILE:HA	2.12	0.49
1:C:269:TRP:CE3	1:C:270:LEU:HD23	2.47	0.49
2:A:34:TRP:CG	2:A:73:LEU:HD13	2.47	0.49
3:B:197:VAL:HG21	3:B:201:PHE:CD1	2.48	0.48
3:B:98:GLY:HA2	3:B:99:GLU:C	2.32	0.48
3:B:154:ASP:O	3:B:155:HIS:ND1	2.45	0.48
3:B:181:GLN:H	3:B:187:SER:HB2	1.78	0.48
1:C:327:TRP:CD1	1:C:357:VAL:HG23	2.48	0.48
1:C:171:HIS:HA	1:C:174:ARG:HH11	1.78	0.48
2:A:137:PHE:CD1	2:A:138:ASP:N	2.81	0.48
1:C:190:LEU:HG	1:C:205:TYR:HB2	1.95	0.48
1:C:327:TRP:HD1	1:C:355:VAL:HG12	1.78	0.48
2:A:20:ILE:HD13	2:A:103:THR:HB	1.96	0.48
2:A:56:GLU:HG2	2:A:61:SER:OG	2.15	0.47
3:B:49:SER:HB2	3:B:55:THR:HG22	1.96	0.47
1:C:40:LEU:HD12	1:C:91:ILE:HD12	1.97	0.47
3:B:232:VAL:HG22	3:B:233:THR:N	2.27	0.46
3:B:178:LEU:H	3:B:178:LEU:HD23	1.80	0.46
1:C:318:PHE:CE2	1:C:352:GLN:HA	2.51	0.46
1:C:256:TRP:O	1:C:263:LEU:HD11	2.15	0.46
1:C:88:GLN:CD	1:C:88:GLN:H	2.19	0.46
2:A:17:ILE:HG13	2:A:76:LYS:HA	1.97	0.46
1:C:125:ILE:CG2	1:C:127:GLU:HG3	2.46	0.46
1:C:57:LYS:HD3	1:C:57:LYS:H	1.81	0.46
3:B:181:GLN:C	3:B:187:SER:HB3	2.36	0.45
3:B:120:ASN:ND2	3:B:186:ASP:CG	2.66	0.45
1:C:318:PHE:HZ	1:C:353:THR:HG23	1.81	0.45
3:B:174:ASP:OD1	3:B:194:ARG:NH1	2.34	0.45
1:C:31:HIS:ND1	1:C:61:PHE:HE1	2.14	0.45
2:A:173:VAL:HG12	2:A:175:TRP:CE3	2.52	0.45
3:B:146:CYS:HB2	3:B:160:TRP:CH2	2.52	0.44
1:C:175:TYR:O	1:C:179:LEU:HD23	2.17	0.44
3:B:25:GLN:CD	3:B:29:HIS:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LYS:N	1:C:176:THR:HG22	2.33	0.44
3:B:219:SER:O	3:B:230:LYS:HE2	2.16	0.44
1:C:209:ILE:HG13	1:C:223:LEU:HG	2.00	0.43
2:A:31:GLY:HA3	2:A:48:TYR:CE1	2.53	0.43
1:C:330:ASN:HD21	1:C:365:ASP:HA	1.83	0.43
1:C:278:LEU:O	1:C:282:LEU:HG	2.19	0.43
3:B:130:GLU:HG2	3:B:202:TRP:HH2	1.81	0.43
1:C:264:LEU:HB3	2:A:50:VAL:HG21	2.00	0.43
3:B:171:VAL:HG22	3:B:195:LEU:HD13	2.01	0.43
3:B:174:ASP:HB2	3:B:191:LEU:HD22	2.00	0.43
3:B:19:MET:HE1	3:B:112:LEU:HD21	2.00	0.43
1:C:327:TRP:CD1	1:C:355:VAL:HG12	2.53	0.43
1:C:292:THR:HG22	1:C:320:PRO:HD3	2.01	0.43
3:B:70:ASN:HB2	3:B:73:GLU:H	1.84	0.43
1:C:175:TYR:O	1:C:179:LEU:HB2	2.19	0.42
2:A:137:PHE:C	2:A:137:PHE:CD1	2.92	0.42
3:B:29:HIS:HE1	3:B:105:PHE:CD2	2.38	0.42
3:B:94:SER:HB2	3:B:104:LEU:HD23	2.01	0.42
1:C:302:LYS:O	1:C:309:THR:OG1	2.33	0.42
3:B:149:THR:HG22	3:B:190:ALA:HB1	2.01	0.42
3:B:82:ALA:HB3	3:B:85:GLN:HG3	2.00	0.42
3:B:87:SER:OG	3:B:88:VAL:N	2.52	0.42
2:A:40:GLY:O	2:A:41:GLU:HG3	2.20	0.42
2:A:34:TRP:O	2:A:46:LEU:HB2	2.19	0.42
2:A:3:ASN:OD1	2:A:25:GLN:NE2	2.52	0.42
1:C:167:LEU:HA	1:C:167:LEU:HD13	1.83	0.42
1:C:125:ILE:O	1:C:134:GLU:HG3	2.20	0.42
2:A:173:VAL:HG12	2:A:175:TRP:HE3	1.83	0.42
1:C:23:LEU:N	1:C:70:THR:HG21	2.35	0.42
2:A:14:GLU:N	2:A:108:LYS:O	2.42	0.42
1:C:263:LEU:H	1:C:263:LEU:CD1	2.22	0.41
3:B:23:CYS:HB3	3:B:74:PHE:O	2.18	0.41
1:C:250:ASP:O	1:C:253:ARG:HB3	2.19	0.41
1:C:327:TRP:HB3	1:C:334:ILE:HD12	2.02	0.41
3:B:131:PRO:HD2	3:B:202:TRP:CZ2	2.56	0.41
2:A:91:LYS:HZ2	3:B:100:GLY:HA2	1.85	0.41
3:B:185:ASN:OD1	3:B:185:ASN:N	2.52	0.41
2:A:60:PHE:CD1	2:A:75:LEU:HD22	2.43	0.41
1:C:219:ILE:HD13	1:C:275:ILE:HG13	2.03	0.41
1:C:294:PRO:HA	1:C:373:HIS:CD2	2.56	0.41
1:C:200:SER:OG	1:C:201:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:HIS:C	1:C:195:HIS:ND1	2.74	0.41
1:C:282:LEU:O	1:C:286:LYS:N	2.54	0.41
1:C:94:TRP:C	1:C:94:TRP:CD1	2.94	0.41
1:C:23:LEU:O	1:C:66:HIS:HA	2.21	0.40
1:C:213:LEU:HG	1:C:219:ILE:HG22	2.03	0.40
3:B:2:ALA:HA	3:B:26:ASP:OD2	2.20	0.40
1:C:127:GLU:HG2	1:C:202:PHE:CD1	2.48	0.40
3:B:68:ARG:HG2	3:B:74:PHE:CD1	2.57	0.40
1:C:122:ARG:NH1	4:C:401:1XL:H2	2.33	0.40
1:C:199:HIS:ND1	1:C:203:HIS:CE1	2.89	0.40
3:B:104:LEU:HD23	3:B:104:LEU:HA	1.90	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	C	325/392 (83%)	305 (94%)	18 (6%)	2 (1%)	30	72
2	A	151/208 (73%)	144 (95%)	7 (5%)	0	100	100
3	B	234/253 (92%)	230 (98%)	4 (2%)	0	100	100
All	All	710/853 (83%)	679 (96%)	29 (4%)	2 (0%)	46	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	ASN
1	C	260	GLN

### 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	288/343 (84%)	263 (91%)	25 (9%)	13	45
2	A	126/183 (69%)	118 (94%)	8 (6%)	22	62
3	B	192/215 (89%)	172 (90%)	20 (10%)	9	34
All	All	606/741 (82%)	553 (91%)	53 (9%)	13	45

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	13	HIS
1	C	21	ASN
1	C	23	LEU
1	C	52	ASP
1	C	57	LYS
1	C	70	THR
1	C	75	ASP
1	C	88	GLN
1	C	91	ILE
1	C	114	ARG
1	C	148	MET
1	C	186	PHE
1	C	190	LEU
1	C	197	TYR
1	C	199	HIS
1	C	223	LEU
1	C	237	LYS
1	C	259	ASN
1	C	264	LEU
1	C	265	TYR
1	C	287	ASP
1	C	296	LYS
1	C	301	HIS
1	C	343	ILE
1	C	352	GLN
2	A	25	GLN

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Mol	Chain	Res	Type
2	A	50	VAL
2	A	59	ARG
2	A	83	SER
2	A	94	ASN
2	A	96	GLN
2	A	127	SER
2	A	136	ASP
3	B	25	GLN
3	B	46	ILE
3	B	49	SER
3	B	54	THR
3	B	65	ASN
3	B	76	LEU
3	B	78	LEU
3	B	95	VAL
3	B	97	THR
3	B	99	GLU
3	B	101	SER
3	B	111	ARG
3	B	112	LEU
3	B	116	GLU
3	B	136	ILE
3	B	169	SER
3	B	178	LEU
3	B	185	ASN
3	B	222	ASP
3	B	230	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	177	GLN
3	B	120	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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$
5	SO4	A	301	-	4,4,4	0.29	0	6,6,6	0.28	0
5	SO4	B	301	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	B	302	-	4,4,4	0.28	0	6,6,6	0.14	0
4	1XL	C	401	-	20,24,24	2.46	4 (20%)	20,34,34	2.52	8 (40%)
5	SO4	C	402	-	4,4,4	0.21	0	6,6,6	0.15	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
5	SO4	A	301	-	-	0/0/0/0	0/0/0/0
5	SO4	B	301	-	-	0/0/0/0	0/0/0/0
5	SO4	B	302	-	-	0/0/0/0	0/0/0/0
4	1XL	C	401	-	-	0/16/16/16	0/2/2/2
5	SO4	C	402	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	1XL	CAI-C6	-8.53	1.37	1.51
4	C	401	1XL	C8A-N8	-4.15	1.34	1.39
4	C	401	1XL	C8A-N1	2.88	1.40	1.35
4	C	401	1XL	C4-N3	4.10	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	1XL	CAK-N8-C8A	-6.49	109.80	120.50
4	C	401	1XL	C4A-C4-N3	-2.75	119.83	123.59
4	C	401	1XL	OAE-CAT-CAJ	-2.68	102.96	109.22
4	C	401	1XL	OAG-CAV-CAT	-2.42	102.64	108.75
4	C	401	1XL	OAD-CAJ-CAT	-2.36	105.96	111.10
4	C	401	1XL	OAC-CAI-C6	-2.22	107.58	112.37
4	C	401	1XL	C7-C6-N5	2.05	122.59	120.98
4	C	401	1XL	C4-N3-C2	5.46	119.97	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	SO4	1	0
4	C	401	1XL	4	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, 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	C	341/392 (86%)	0.59	17 (4%) 32 24	55, 90, 130, 167	0
2	A	157/208 (75%)	0.58	10 (6%) 23 17	55, 81, 113, 154	0
3	B	238/253 (94%)	0.52	5 (2%) 67 57	44, 82, 121, 139	0
All	All	736/853 (86%)	0.57	32 (4%) 39 29	44, 86, 126, 167	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	383	PHE	3.9
2	A	121	LEU	3.0
1	C	334	ILE	3.0
2	A	151	VAL	2.9
2	A	27	SER	2.9
3	B	116	GLU	2.6
2	A	148	ASP	2.5
1	C	172	TRP	2.5
1	C	168	ALA	2.5
1	C	48	SER	2.5
1	C	114	ARG	2.5
1	C	232	PHE	2.4
1	C	366	ILE	2.4
1	C	72	ASN	2.4
1	C	369	CYS	2.4
1	C	367	TYR	2.4
1	C	264	LEU	2.3
3	B	199	ALA	2.3
2	A	131	VAL	2.3
2	A	70	TYR	2.3
1	C	381	GLN	2.3
2	A	176	SER	2.2
2	A	87	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	B	144	LEU	2.2
2	A	126	SER	2.2
3	B	162	VAL	2.2
1	C	14	PRO	2.2
1	C	195	HIS	2.2
1	C	50	GLN	2.2
3	B	78	LEU	2.1
1	C	312	TYR	2.0
2	A	120	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	1XL	C	401	23/23	0.78	0.42	3.41	92,98,106,110	0
5	SO4	C	402	5/5	0.77	0.35	0.66	129,129,133,134	0
5	SO4	B	301	5/5	0.94	0.16	-4.41	53,63,68,72	0
5	SO4	B	302	5/5	0.92	0.15	-	86,89,90,92	0
5	SO4	A	301	5/5	0.88	0.21	-	118,119,121,121	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.