



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:19 AM UTC

PDB ID : 4LCC / pdb_00004lcc
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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

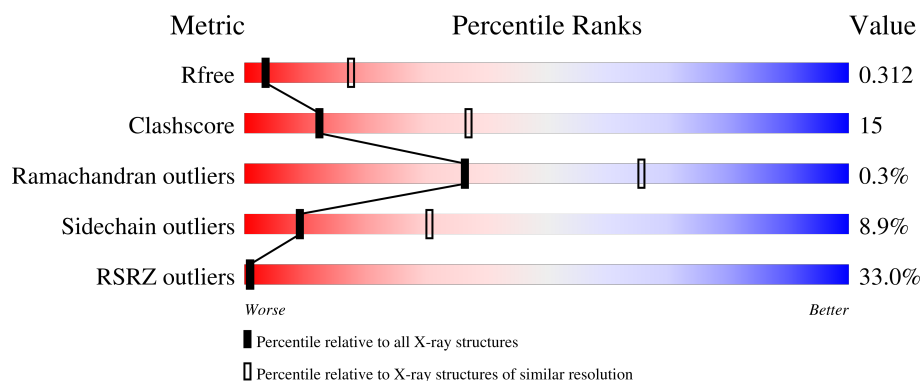
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	32% 59% 22% 5% 13%
2	A	208	19% 55% 19% • 25%
3	B	253	30% 58% 30% 6% 6%

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

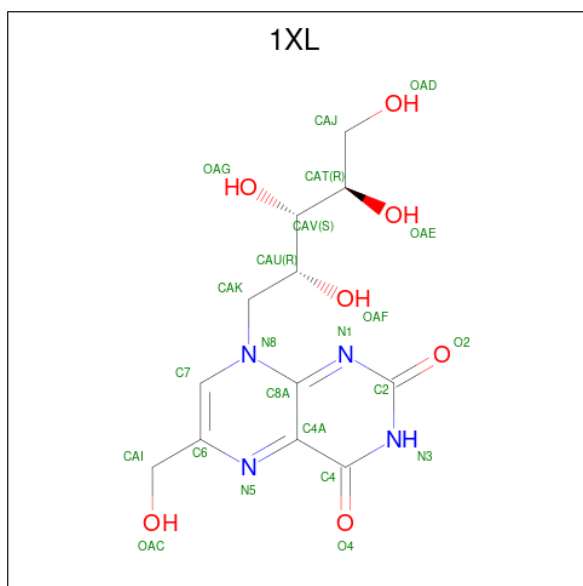
- Molecule 2 is a protein called Human MAIT TCR alpha chain.

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-dihydropteridin-8(2H)-yl]-D-arabinitol (CCD ID: 1XL) (formula: C₁₂H₁₆N₄O₇).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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		

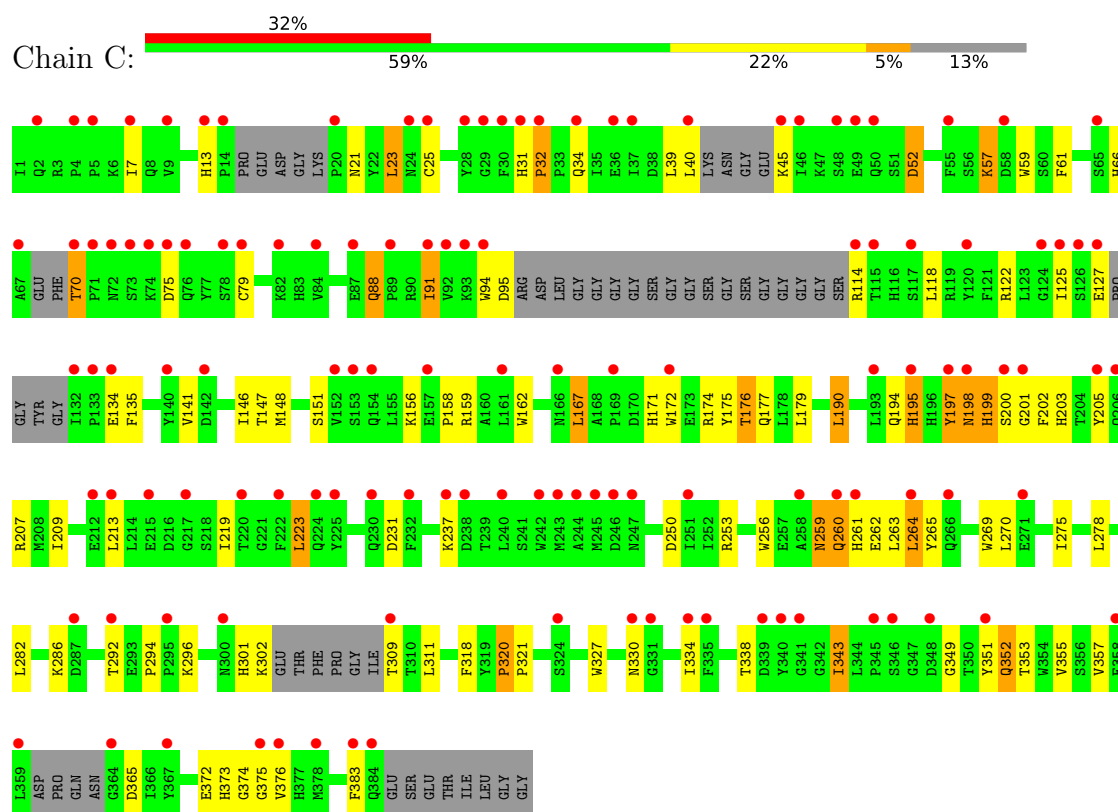
- Molecule 6 is water.

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

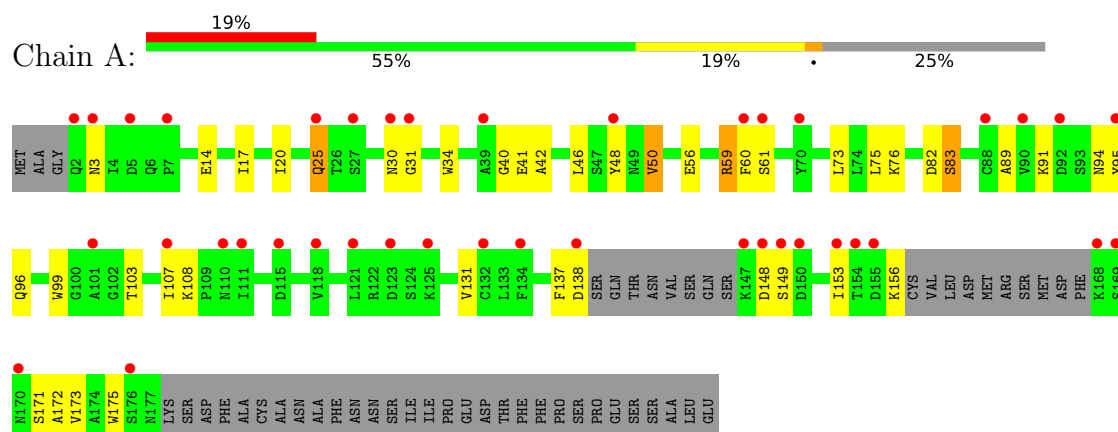
3 Residue-property plots

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



Chain B:

30% 58% 30% 6% 6%

MET
ALA
ASN
A2
G3
V4
F5
Q6
T7
P8
Q11
V12
L13
K14
Q17
S18
M19
T20
L21
Q22
C23
A24
Q25
D26
M27
N28
H29
N30
S31
M32
Y33
W34
Y35
R36
Q37
D38
G42
L45
L46
S49
A50
S51
T54
D56
K57
G58
S59
V60
M65
R68
L69

N70
K71
R72
E73
F74
S75
L76
R77
L78
E79
A82
P83
S84
Q85
T86
S87
R88
H89
F90
S94
V95
R96
T97
G98
E99
G100
S101
L104
F105
S110
R111
L112
T113
V114
L115
E116
D117
L118
M119
M120
P123
P124
V128
F129
E130
P131
I136
S137
H138
T139
C146
L147
A148
T149
P153
D154
H155
W160
M163
G164
K165
E166
S169
G170
V171
G172
T173
D174
P177
L178
K179
E180
Q181
P182
A183
L184
N185
D186
S187
R188
Y189
A190
L191
S192
S193
R194
L195
F196
V197
T200
F201
W202
Q203
G217
L218
S219
E220
N221
D222
E223
W224
THR
GLN
ASP
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.257 , 0.312 0.259 , 0.312	Depositor DCC
R_{free} test set	938 reflections (3.52%)	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)	0.34 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	5827	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1XL, SO4

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	0/2845	0.79	8/3865 (0.2%)
2	A	0.45	0/1221	0.84	2/1660 (0.1%)
3	B	0.41	0/1874	0.85	2/2559 (0.1%)
All	All	0.39	0/5940	0.82	12/8084 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	100	GLY	N-CA-C	7.57	122.80	114.40
1	C	198	ASN	N-CA-C	7.38	126.53	110.80
3	B	186	ASP	N-CA-C	7.33	121.93	112.92
1	C	176	THR	N-CA-C	-6.37	104.21	112.23
1	C	349	GLY	N-CA-C	-5.51	107.72	115.32
1	C	320	PRO	CA-C-N	5.49	125.84	119.47
1	C	320	PRO	C-N-CA	5.49	125.84	119.47
1	C	32	PRO	CA-C-N	5.35	125.06	119.82
1	C	32	PRO	C-N-CA	5.35	125.06	119.82
1	C	374	GLY	N-CA-C	-5.27	107.78	114.16
2	A	42	ALA	CA-C-N	-5.13	114.49	119.78
2	A	42	ALA	C-N-CA	-5.13	114.49	119.78

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	82	0
2	A	1196	0	1098	32	0
3	B	1824	0	1676	66	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
6	A	1	0	0	0	0
All	All	5827	0	5341	172	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 (172) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:C:401:1XL:OAF	2:A:95:TYR:OH	2.14	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
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
2:A:59:ARG:HH22	2:A:82:ASP:CG	2.07	0.62
1:C:135:PHE:HB3	1:C:151:SER:HB3	1.82	0.60
3:B:174:ASP:OD2	3:B:192:SER:OG	2.17	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: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: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:98:GLY:HA2	3:B:99:GLU:C	2.32	0.53
1:C:25:CYS:HB2	1:C:39:LEU:HD21	1.90	0.53
1:C:375:GLY:N	1:C:376:VAL:HB	2.23	0.53
3:B:32:MET:SD	3:B:74:PHE:HB2	2.48	0.53
3:B:25:GLN:OE1	3:B:29:HIS:N	2.30	0.53
1:C:162:TRP:H	1:C:162:TRP:CD1	2.26	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
3:B:120:ASN:ND2	3:B:186:ASP:CG	2.66	0.52
1:C:265:TYR:HA	2:A:50:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:321:PRO:HG3	1:C:351:TYR:CE2	2.44	0.52
2:A:172:ALA:HA	3:B:194:ARG:HH21	1.74	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:31:SER:OG	3:B:97:THR:N	2.43	0.51
3:B:179:LYS:HB3	3:B:187:SER:OG	2.10	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
1:C:88:GLN:H	1:C:88:GLN:CD	2.19	0.51
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:N	1:C:52:ASP:OD1	2.44	0.50
2:A:89:ALA:HB2	2:A:99:TRP:CE3	2.47	0.49
3:B:130:GLU:HG2	3:B:202:TRP:CZ2	2.47	0.49
3:B:181:GLN:C	3:B:187:SER:HB3	2.36	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
3:B:25:GLN:CD	3:B:29:HIS:H	2.19	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:154:ASP:O	3:B:155:HIS:ND1	2.45	0.48
3:B:197:VAL:HG21	3:B:201:PHE:CD1	2.48	0.48
3:B:181:GLN:H	3:B:187:SER:HB2	1.78	0.48
1:C:171:HIS:HA	1:C:174:ARG:HH11	1.78	0.48
1:C:327:TRP:CD1	1:C:357:VAL:HG23	2.48	0.48
1:C:190:LEU:HG	1:C:205:TYR:HB2	1.95	0.48
2:A:137:PHE:CD1	2:A:138:ASP:N	2.81	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
1:C:40:LEU:HD12	1:C:91:ILE:HD12	1.97	0.47
2:A:137:PHE:CD1	2:A:137:PHE:C	2.92	0.47
3:B:49:SER:HB2	3:B:55:THR:HG22	1.96	0.47
3:B:3:GLY:HA2	3:B:27:MET:HE3	1.97	0.46
3:B:178:LEU:HD23	3:B:178:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:232:VAL:HG22	3:B:233:THR:N	2.27	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
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
1:C:195:HIS:ND1	1:C:195:HIS:C	2.74	0.46
1:C:94:TRP:C	1:C:94:TRP:CD1	2.94	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
1:C:175:TYR:O	1:C:179:LEU:HD23	2.17	0.44
3:B:146:CYS:HB2	3:B:160:TRP:CH2	2.52	0.44
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
1:C:330:ASN:HD21	1:C:365:ASP:HA	1.83	0.43
2:A:31:GLY:HA3	2:A:48:TYR:CE1	2.53	0.43
1:C:278:LEU:O	1:C:282:LEU:HG	2.19	0.43
1:C:264:LEU:HB3	2:A:50:VAL:HG21	2.00	0.43
3:B:130:GLU:HG2	3:B:202:TRP:HH2	1.81	0.43
3:B:171:VAL:HG22	3:B:195:LEU:HD13	2.01	0.43
1:C:194:GLN:O	1:C:195:HIS:C	2.60	0.43
3:B:174:ASP:HB2	3:B:191:LEU:HD22	2.00	0.43
1:C:292:THR:HG22	1:C:320:PRO:HD3	2.01	0.43
1:C:327:TRP:CD1	1:C:355:VAL:HG12	2.53	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
1:C:302:LYS:O	1:C:309:THR:OG1	2.33	0.42
3:B:19:MET:HE3	3:B:19:MET:HB3	1.89	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
3:B:149:THR:HG22	3:B:190:ALA:HB1	2.01	0.42
2:A:40:GLY:O	2:A:41:GLU:HG3	2.20	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
1:C:167:LEU:HD13	1:C:167:LEU:HA	1.83	0.42
2:A:3:ASN:OD1	2:A:25:GLN:NE2	2.52	0.42
2:A:34:TRP:O	2:A:46:LEU:HB2	2.19	0.42
1:C:125:ILE:O	1:C:134:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:HIS:HA	1:C:32:PRO:C	2.45	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
2:A:91:LYS:HZ2	3:B:100:GLY:HA2	1.85	0.41
3:B:131:PRO:HD2	3:B:202:TRP:CZ2	2.56	0.41
3:B:185:ASN:OD1	3:B:185:ASN:N	2.52	0.41
1:C:219:ILE:HD13	1:C:275:ILE:HG13	2.03	0.41
2:A:60:PHE:CD1	2:A:75:LEU:HD22	2.43	0.41
1:C:294:PRO:HA	1:C:373:HIS:CD2	2.56	0.41
1:C:34:GLN:CD	1:C:127:GLU:OE2	2.61	0.41
1:C:200:SER:OG	1:C:201:GLY:N	2.53	0.41
1:C:282:LEU:O	1:C:286:LYS:N	2.54	0.41
3:B:186:ASP:O	3:B:187:SER:C	2.62	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

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	325/392 (83%)	305 (94%)	18 (6%)	2 (1%)	21	51
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%)	36	66

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%)	262 (91%)	26 (9%)	9	30
2	A	126/183 (69%)	119 (94%)	7 (6%)	19	46
3	B	192/215 (89%)	171 (89%)	21 (11%)	6	23
All	All	606/741 (82%)	552 (91%)	54 (9%)	9	30

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	7	ILE
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

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Mol	Chain	Res	Type
1	C	141	VAL
1	C	148	MET
1	C	167	LEU
1	C	190	LEU
1	C	195	HIS
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	296	LYS
1	C	301	HIS
1	C	343	ILE
1	C	352	GLN
2	A	25	GLN
2	A	50	VAL
2	A	59	ARG
2	A	83	SER
2	A	94	ASN
2	A	96	GLN
2	A	153	ILE
3	B	25	GLN
3	B	32	MET
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

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Mol	Chain	Res	Type
3	B	230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	150	ASN
1	C	177	GLN
1	C	206	GLN
1	C	224	GLN
2	A	3	ASN
2	A	25	GLN
2	A	30	ASN
2	A	113	ASN
3	B	120	ASN

5.3.3 RNA [i](#)

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 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
5	SO4	A	301	-	4,4,4	0.22	0	6,6,6	0.25	0
5	SO4	B	302	-	4,4,4	0.22	0	6,6,6	0.11	0
5	SO4	C	402	-	4,4,4	0.23	0	6,6,6	0.14	0
5	SO4	B	301	-	4,4,4	0.21	0	6,6,6	0.15	0
4	1XL	C	401	-	24,24,24	3.61	4 (16%)	28,34,34	3.46	12 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1XL	C	401	-	-	5/16/16/16	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	1XL	CAI-C6	-16.31	1.37	1.50
4	C	401	1XL	C8A-N1	3.55	1.40	1.33
4	C	401	1XL	C7-C6	2.69	1.40	1.36
4	C	401	1XL	C8A-N8	-2.31	1.34	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	1XL	CAK-N8-C7	14.32	130.55	120.04
4	C	401	1XL	C6-C7-N8	-4.83	116.11	122.09
4	C	401	1XL	C4A-C8A-N8	3.99	122.19	116.48
4	C	401	1XL	C4-N3-C2	-3.20	119.97	125.64
4	C	401	1XL	C8A-C4A-N5	-2.83	119.11	124.80
4	C	401	1XL	OAG-CAV-CAT	-2.77	102.64	108.93
4	C	401	1XL	OAE-CAT-CAJ	-2.67	102.96	109.03
4	C	401	1XL	C4A-C4-N3	2.58	119.83	113.25
4	C	401	1XL	OAD-CAJ-CAT	-2.47	105.96	111.16
4	C	401	1XL	O4-C4-C4A	-2.31	120.44	126.53
4	C	401	1XL	CAJ-CAT-CAV	2.26	116.77	112.17
4	C	401	1XL	OAC-CAI-C6	-2.02	107.58	111.79

There are no chirality outliers.

All (5) torsion outliers are listed below:

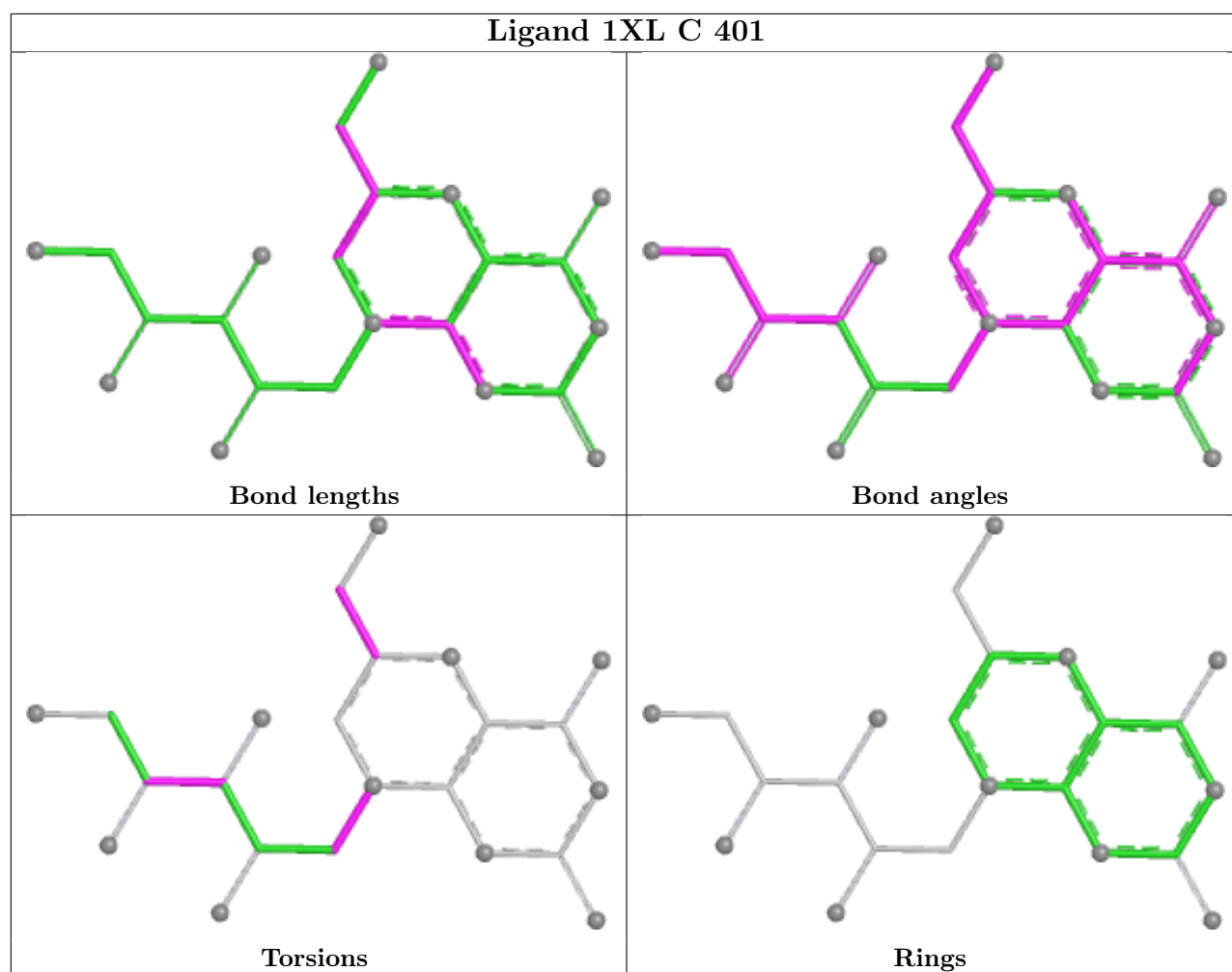
Mol	Chain	Res	Type	Atoms
4	C	401	1XL	CAU-CAK-N8-C7
4	C	401	1XL	CAU-CAK-N8-C8A
4	C	401	1XL	C7-C6-CAI-OAC
4	C	401	1XL	N5-C6-CAI-OAC
4	C	401	1XL	CAJ-CAT-CAV-OAG

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	341/392 (86%)	1.84	126 (36%)  	55, 90, 130, 167	0
2	A	157/208 (75%)	1.69	40 (25%)  	55, 81, 113, 154	0
3	B	238/253 (94%)	1.63	77 (32%)  	44, 82, 121, 139	0
All	All	736/853 (86%)	1.74	243 (33%)  	44, 86, 126, 167	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	PRO	5.6
3	B	117	ASP	5.3
1	C	132	ILE	5.2
2	A	155	ASP	4.6
1	C	50	GLN	4.6
1	C	247	ASN	4.5
3	B	244	ALA	4.4
1	C	92	VAL	4.3
1	C	309	THR	4.2
1	C	340	TYR	4.1
1	C	383	PHE	4.1
2	A	150	ASP	4.0
2	A	170	ASN	4.0
2	A	30	ASN	4.0
1	C	339	ASP	4.0
2	A	118	VAL	3.9
1	C	20	PRO	3.9
1	C	172	TRP	3.9
2	A	101	ALA	3.8
1	C	152	VAL	3.8
1	C	157	GLU	3.7
1	C	115	THR	3.6
1	C	193	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	B	116	GLU	3.6
3	B	97	THR	3.6
1	C	334	ILE	3.6
1	C	264	LEU	3.5
1	C	348	ASP	3.5
1	C	93	LYS	3.5
2	A	138	ASP	3.5
2	A	31	GLY	3.4
1	C	161	LEU	3.4
1	C	71	PRO	3.4
1	C	244	ALA	3.4
2	A	110	ASN	3.4
1	C	127	GLU	3.4
3	B	78	LEU	3.3
1	C	78	SER	3.3
1	C	153	SER	3.3
2	A	5	ASP	3.3
1	C	34	GLN	3.3
1	C	31	HIS	3.3
1	C	232	PHE	3.3
3	B	42	GLY	3.3
1	C	84	VAL	3.3
2	A	70	TYR	3.2
1	C	324	SER	3.2
2	A	25	GLN	3.2
1	C	76	GLN	3.2
3	B	101	SER	3.2
1	C	70	THR	3.2
3	B	50	ALA	3.2
1	C	230	GLN	3.1
3	B	139	THR	3.1
2	A	123	ASP	3.1
3	B	98	GLY	3.1
2	A	176	SER	3.1
1	C	91	ILE	3.0
1	C	67	ALA	3.0
2	A	147	LYS	3.0
3	B	79	GLU	3.0
2	A	95	TYR	3.0
2	A	134	PHE	2.9
1	C	237	LYS	2.9
1	C	45	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	169	SER	2.9
3	B	56	ASP	2.9
3	B	186	ASP	2.9
3	B	54	THR	2.9
1	C	169	PRO	2.9
3	B	224	TRP	2.8
1	C	73	SER	2.8
2	A	90	VAL	2.8
2	A	3	ASN	2.8
3	B	172	CYS	2.8
1	C	79	CYS	2.8
1	C	13	HIS	2.8
2	A	92	ASP	2.8
3	B	217	GLY	2.8
1	C	24	ASN	2.8
3	B	120	ASN	2.8
1	C	222	PHE	2.7
1	C	330	ASN	2.7
1	C	46	ILE	2.7
1	C	29	GLY	2.7
1	C	217	GLY	2.7
3	B	26	ASP	2.7
1	C	251	ILE	2.7
1	C	335	PHE	2.7
3	B	69	LEU	2.7
3	B	112	LEU	2.7
1	C	142	ASP	2.7
1	C	201	GLY	2.6
3	B	86	THR	2.6
2	A	27	SER	2.6
1	C	238	ASP	2.6
1	C	154	GLN	2.6
1	C	224	GLN	2.6
3	B	165	LYS	2.6
1	C	28	TYR	2.6
2	A	168	LYS	2.6
1	C	331	GLY	2.6
2	A	88	CYS	2.6
3	B	18	SER	2.6
3	B	104	LEU	2.6
3	B	83	PRO	2.6
1	C	266	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	72	ASN	2.6
2	A	148	ASP	2.6
3	B	239	GLU	2.6
3	B	60	VAL	2.6
2	A	154	THR	2.6
3	B	20	THR	2.6
3	B	123	PRO	2.5
1	C	364	GLY	2.5
2	A	115	ASP	2.5
2	A	48	TYR	2.5
3	B	177	PRO	2.5
2	A	2	GLN	2.5
1	C	358	GLU	2.5
3	B	180	GLU	2.5
1	C	195	HIS	2.5
3	B	124	PRO	2.5
1	C	375	GLY	2.5
1	C	2	GLN	2.5
3	B	153	PRO	2.5
3	B	137	SER	2.5
3	B	169	SER	2.5
1	C	287	ASP	2.5
3	B	96	TRP	2.5
1	C	120	TYR	2.5
1	C	341	GLY	2.5
1	C	55	PHE	2.4
3	B	200	THR	2.4
3	B	235	ILE	2.4
1	C	124	GLY	2.4
1	C	260	GLN	2.4
2	A	107	ILE	2.4
3	B	51	SER	2.4
1	C	4	PRO	2.4
3	B	128	VAL	2.4
1	C	206	GLN	2.4
1	C	376	VAL	2.4
3	B	231	PRO	2.4
1	C	246	ASP	2.4
1	C	351	TYR	2.4
3	B	115	LEU	2.4
3	B	166	GLU	2.4
1	C	126	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	B	84	SER	2.4
1	C	125	ILE	2.3
1	C	166	ASN	2.3
3	B	2	ALA	2.3
1	C	40	LEU	2.3
1	C	94	TRP	2.3
1	C	345	PRO	2.3
3	B	173	THR	2.3
1	C	367	TYR	2.3
3	B	154	ASP	2.3
1	C	359	LEU	2.3
1	C	220	THR	2.3
1	C	292	THR	2.3
1	C	243	MET	2.3
1	C	205	TYR	2.3
1	C	213	LEU	2.3
2	A	121	LEU	2.3
1	C	32	PRO	2.3
1	C	65	SER	2.3
3	B	70	ASN	2.3
1	C	87	GLU	2.3
3	B	57	LYS	2.3
1	C	9	VAL	2.3
1	C	58	ASP	2.3
1	C	117	SER	2.2
2	A	153	ILE	2.2
1	C	133	PRO	2.2
3	B	27	MET	2.2
3	B	100	GLY	2.2
1	C	261	HIS	2.2
3	B	188	ARG	2.2
3	B	87	SER	2.2
1	C	384	GLN	2.2
1	C	198	ASN	2.2
1	C	271	GLU	2.2
1	C	5	PRO	2.2
3	B	183	ALA	2.2
1	C	140	TYR	2.2
2	A	61	SER	2.2
3	B	65	ASN	2.2
1	C	240	LEU	2.2
3	B	220	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	245	MET	2.2
1	C	378	MET	2.2
3	B	222	ASP	2.2
3	B	201	PHE	2.2
3	B	234	GLN	2.2
3	B	147	LEU	2.2
1	C	49	GLU	2.2
3	B	163	ASN	2.2
1	C	89	PRO	2.2
1	C	225	TYR	2.1
3	B	19	MET	2.1
3	B	187	SER	2.1
1	C	212	GLU	2.1
1	C	74	LYS	2.1
3	B	230	LYS	2.1
1	C	258	ALA	2.1
1	C	215	GLU	2.1
2	A	7	PRO	2.1
3	B	164	GLY	2.1
2	A	60	PHE	2.1
1	C	242	TRP	2.1
2	A	132	CYS	2.1
2	A	111	ILE	2.1
1	C	197	TYR	2.1
1	C	134	GLU	2.1
2	A	149	SER	2.1
1	C	300	ASN	2.1
3	B	12	VAL	2.1
3	B	119	LYS	2.1
3	B	138	HIS	2.1
1	C	114	ARG	2.1
2	A	39	ALA	2.1
3	B	6	GLN	2.1
1	C	30	PHE	2.1
1	C	200	SER	2.1
1	C	346	SER	2.1
3	B	31	SER	2.1
3	B	110	SER	2.1
1	C	82	LYS	2.1
1	C	36	GLU	2.1
3	B	59	GLU	2.1
3	B	88	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	48	SER	2.0
3	B	189	TYR	2.0
3	B	184	LEU	2.0
1	C	7	ILE	2.0
1	C	75	ASP	2.0
1	C	25	CYS	2.0
1	C	295	PRO	2.0
2	A	125	LYS	2.0
3	B	4	VAL	2.0
1	C	37	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

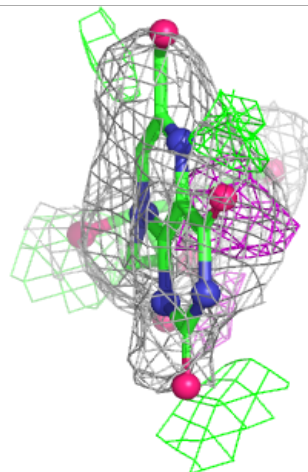
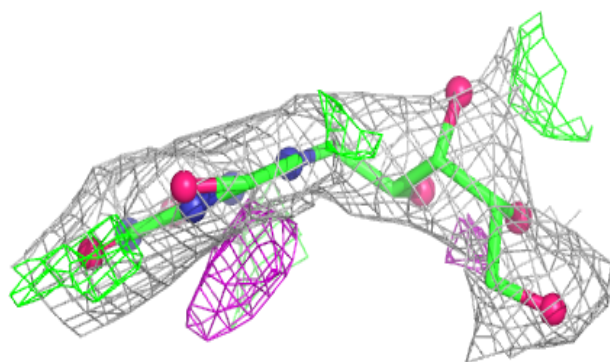
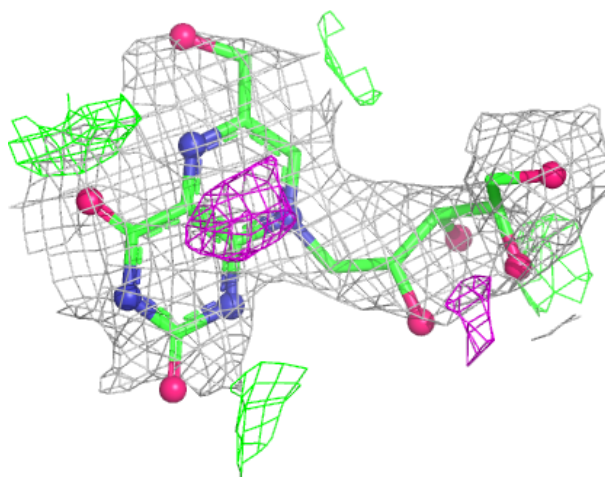
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	C	402	5/5	0.64	0.27	129,129,133,134	0
5	SO4	A	301	5/5	0.79	0.18	118,119,121,121	0
5	SO4	B	302	5/5	0.79	0.17	86,89,90,92	0
4	1XL	C	401	23/23	0.81	0.27	92,98,106,110	0
5	SO4	B	301	5/5	0.88	0.14	53,63,68,72	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1XL C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.