Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:29 PM GMT

PDB ID	:	5D5M
Title	:	Structure of human MR1-5-OP-RU in complex with human MAIT M33.64 TCR
Authors	:	Keller, A.N.; Birkinshaw, R.W.; Rossjohn, J.
Deposited on	:	2015-08-11
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

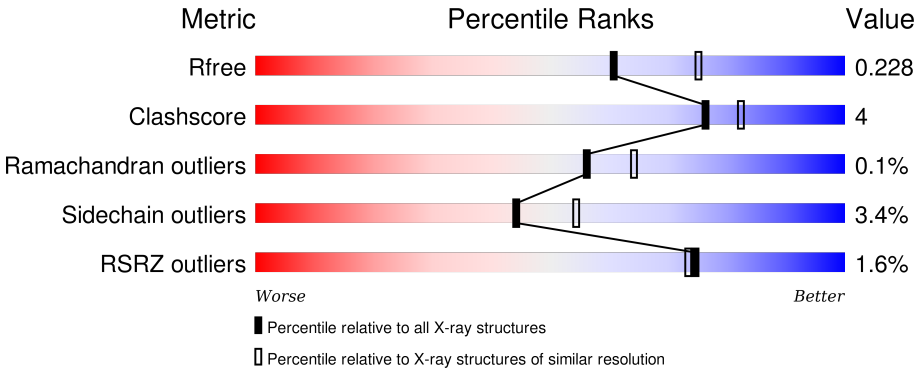
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 >=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 <=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	271	86% 12%
1	C	271	4% 87% 11%
2	B	100	88% 8%
2	D	100	90% 8%
3	E	204	89% 8%

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Mol	Chain	Length	Quality of chain
3	G	204	4% 83% 13%
4	F	245	84% 14%
4	H	245	% 89% 9%

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
6	GOL	C	302	-	-	-	X
6	GOL	F	301	-	-	-	X
7	ACT	C	303	-	-	-	X
7	ACT	H	302	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13782 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	3	0
			2206	1413	382	401	10			
1	C	269	Total	C	N	O	S	0	1	0
			2229	1425	384	410	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			
2	D	98	Total	C	N	O	S	0	0	0
			816	521	138	154	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called M33.64 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	200	Total	C	N	O	S	0	1	0
			1570	989	253	318	10			

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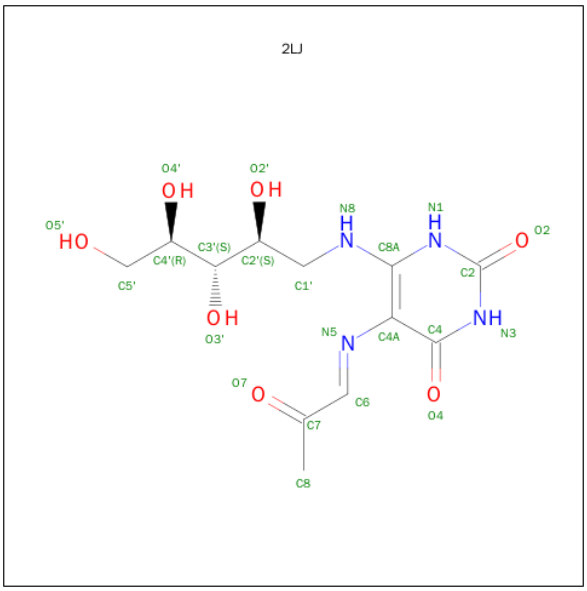
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	198	Total	C	N	O	S	0	0	0
			1555	980	251	314	10			

- Molecule 4 is a protein called M33.64 TCR Beta Chain.

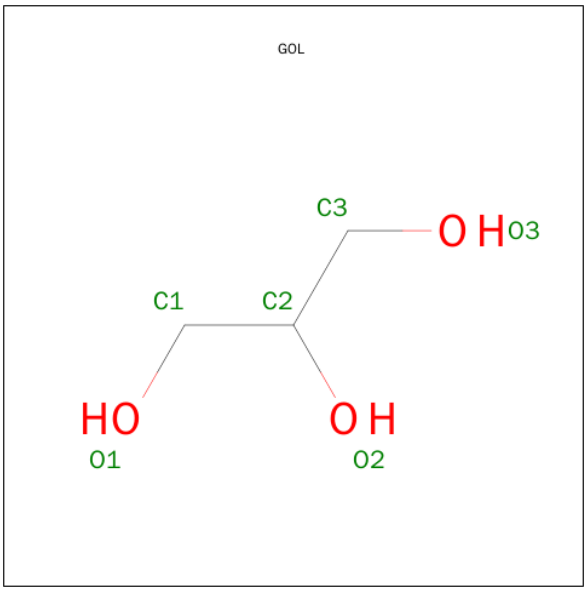
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	240	Total	C	N	O	S	0	0	0
			1872	1173	329	362	8			
4	H	241	Total	C	N	O	S	0	0	0
			1883	1179	333	363	8			

- Molecule 5 is 1-deoxy-1-({2,6-dioxo-5-[(E)-(2-oxopropylidene)amino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-ribitol (three-letter code: 2LJ) (formula: $C_{12}H_{18}N_4O_7$).



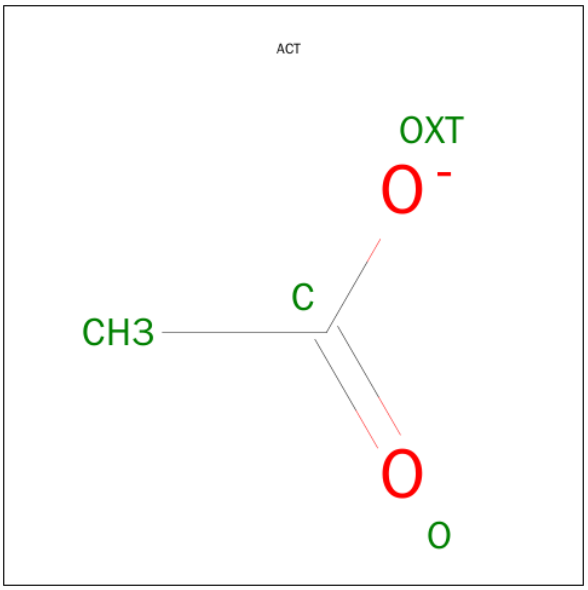
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	12	4	6		
5	C	1	Total	C	N	O	0	0
			22	12	4	6		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 6 3 3	0	0
6	F	1	Total C O 6 3 3	0	0
6	G	1	Total C O 6 3 3	0	0
6	H	1	Total C O 6 3 3	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

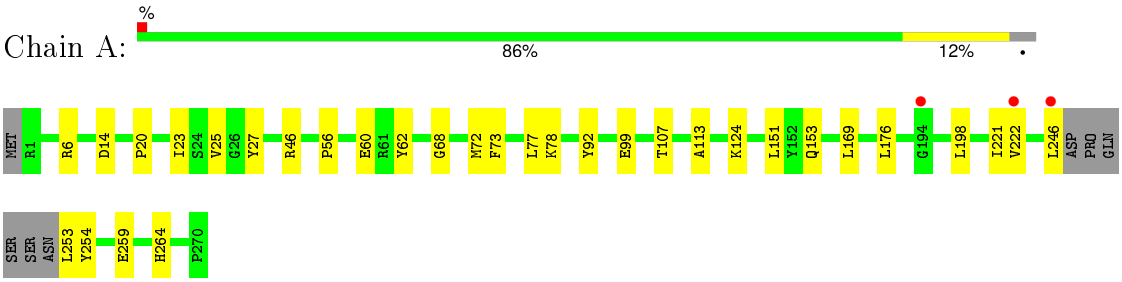
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	152	Total O 152 152	0	0
8	B	39	Total O 39 39	0	0
8	C	113	Total O 113 113	0	0
8	D	18	Total O 18 18	0	0
8	E	121	Total O 121 121	0	0
8	F	115	Total O 115 115	0	0
8	G	80	Total O 80 80	0	0
8	H	117	Total O 117 117	0	0

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.

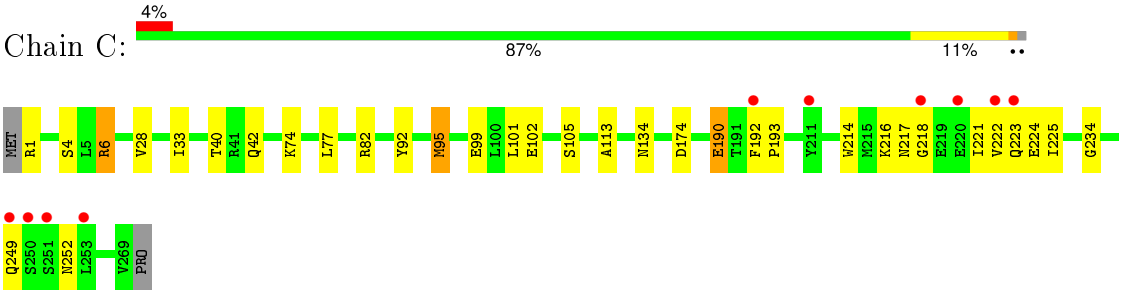
- Molecule 1: Major histocompatibility complex class I-related gene protein

Chain A:



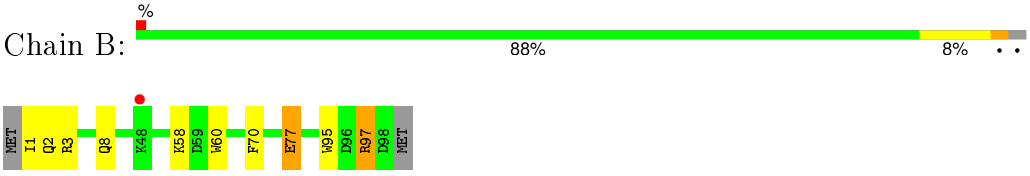
- Molecule 1: Major histocompatibility complex class I-related gene protein

Chain C:



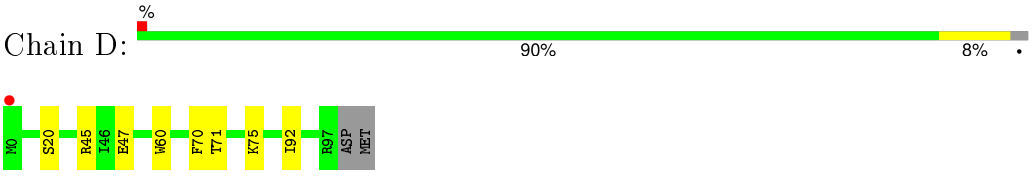
- Molecule 2: Beta-2-microglobulin

Chain B:



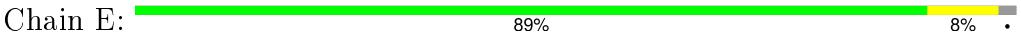
- Molecule 2: Beta-2-microglobulin

Chain D:

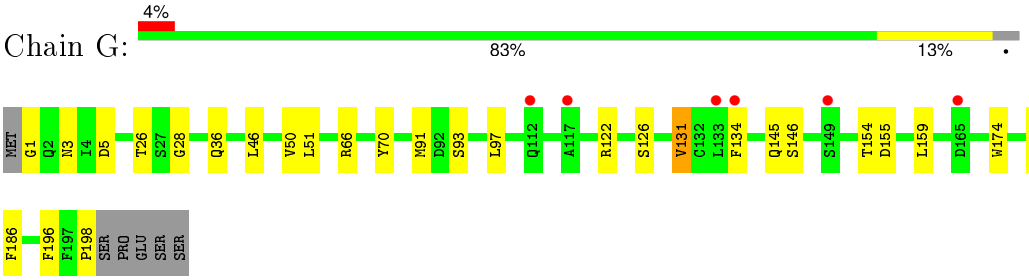


- Molecule 3: M33.64 TCR Alpha Chain

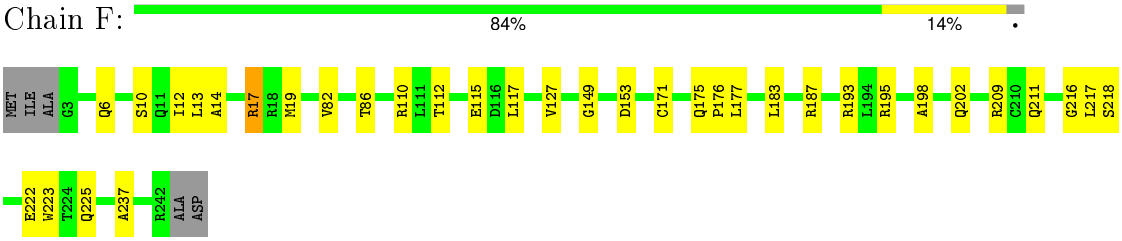
Chain E:



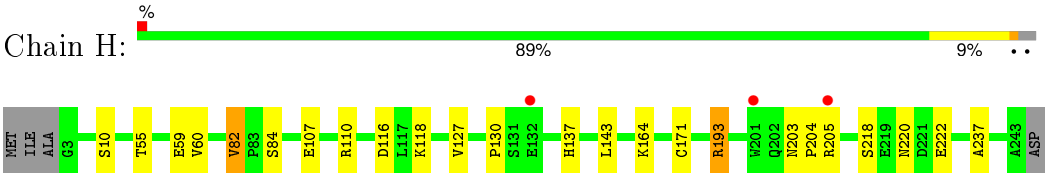
• Molecule 3: M33.64 TCR Alpha Chain



• Molecule 4: M33.64 TCR Beta Chain



• Molecule 4: M33.64 TCR Beta Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	216.20Å 70.26Å 142.38Å 90.00° 104.15° 90.00°	Depositor
Resolution (Å)	47.74 – 2.20 75.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.74-2.20) 99.9 (75.11-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.171 , 0.222 0.184 , 0.228	Depositor DCC
R_{free} test set	5253 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 105453 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13782	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 2LJ, ACT

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	0.45	0/2280	0.57	0/3098
1	C	0.42	0/2301	0.57	0/3129
2	B	0.43	0/843	0.56	1/1142 (0.1%)
2	D	0.32	0/839	0.49	0/1137
3	E	0.43	0/1609	0.55	0/2180
3	G	0.42	0/1589	0.57	0/2152
4	F	0.42	0/1920	0.55	0/2616
4	H	0.41	0/1931	0.55	0/2630
All	All	0.42	0/13312	0.56	1/18084 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	ARG	NE-CZ-NH2	-5.41	117.59	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	107	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2206	0	2099	20	0
1	C	2229	0	2117	22	0
2	B	820	0	785	8	0
2	D	816	0	779	3	0
3	E	1570	0	1489	12	0
3	G	1555	0	1476	12	0
4	F	1872	0	1776	21	0
4	H	1883	0	1792	9	0
5	A	22	0	18	2	0
5	C	22	0	18	1	0
6	C	6	0	8	0	0
6	F	6	0	8	0	0
6	G	6	0	8	0	0
6	H	6	0	8	0	0
7	C	4	0	3	0	0
7	H	4	0	3	0	0
8	A	152	0	0	5	0
8	B	39	0	0	1	0
8	C	113	0	0	4	0
8	D	18	0	0	1	0
8	E	121	0	0	1	0
8	F	115	0	0	2	0
8	G	80	0	0	0	0
8	H	117	0	0	1	0
All	All	13782	0	12387	97	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 4.

All (97) 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:A:6[B]:ARG:HH12	2:B:58:LYS:HE2	1.49	0.77
1:C:1:ARG:N	8:C:403:HOH:O	2.17	0.77
1:A:253:LEU:N	8:A:701:HOH:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:ARG:HH12	2:D:47:GLU:HG3	1.51	0.74
1:C:223:GLN:N	1:C:224:GLU:HA	2.04	0.73
1:C:174:ASP:OD1	8:C:401:HOH:O	2.07	0.73
3:G:154:THR:HG21	4:H:193:ARG:HH12	1.53	0.72
4:F:12:ILE:HD12	4:F:216:GLY:HA2	1.70	0.72
1:C:40:THR:HG23	1:C:42:GLN:H	1.54	0.71
1:C:102:GLU:OE2	8:C:402:HOH:O	2.12	0.67
4:F:198:ALA:O	4:F:202:GLN:HG2	1.96	0.65
1:C:217:ASN:N	1:C:218:GLY:HA2	2.13	0.64
3:G:1:GLY:HA3	3:G:26:THR:HA	1.79	0.63
3:E:70:TYR:HH	3:E:72:TYR:HD2	1.44	0.63
3:E:161:MET:HE1	4:F:195:ARG:HD3	1.81	0.62
1:A:124:LYS:NZ	8:A:705:HOH:O	2.33	0.61
3:G:3:ASN:ND2	3:G:5:ASP:OD2	2.36	0.58
3:G:28:GLY:HA3	3:G:93:SER:HB3	1.84	0.58
1:C:216:LYS:C	1:C:218:GLY:HA2	2.24	0.58
2:B:95:TRP:CE2	2:B:97:ARG:HA	2.40	0.57
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.40	0.57
3:E:156:LYS:HE3	8:E:372:HOH:O	2.06	0.56
1:A:6[B]:ARG:NH1	2:B:58:LYS:HE2	2.19	0.56
1:A:151:LEU:HD22	3:G:51:LEU:HD12	1.88	0.56
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.87	0.55
1:C:113:ALA:HB2	2:D:60:TRP:CE2	2.43	0.54
3:E:1:GLY:HA3	3:E:26:THR:HA	1.90	0.54
1:C:216:LYS:HD2	1:C:252:ASN:OD1	2.08	0.53
4:F:110:ARG:NH2	4:F:153:ASP:OD1	2.42	0.53
3:G:154:THR:HG22	3:G:155:ASP:O	2.09	0.53
4:F:149:GLY:O	4:F:187:ARG:HD2	2.08	0.53
1:C:216:LYS:HB3	1:C:221:ILE:HD11	1.91	0.53
4:H:59:GLU:HG2	4:H:60:VAL:HG13	1.92	0.52
1:C:222:VAL:C	1:C:224:GLU:HA	2.30	0.52
4:F:110:ARG:NH1	8:F:402:HOH:O	2.36	0.52
2:B:2:GLN:NE2	8:B:102:HOH:O	2.42	0.52
3:E:28:GLY:HA3	3:E:93:SER:HB3	1.92	0.52
1:A:153:GLN:NE2	8:A:708:HOH:O	2.39	0.51
1:C:28:VAL:HG23	1:C:33:ILE:HD13	1.90	0.51
4:F:127:VAL:HG23	4:F:237:ALA:HB3	1.93	0.51
3:E:91:MET:HG2	3:E:95:TYR:HA	1.93	0.51
1:C:190:GLU:H	1:C:190:GLU:CD	2.15	0.49
2:B:77:GLU:HG2	2:B:97:ARG:NH2	2.28	0.49
4:H:110:ARG:NH2	8:H:406:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:134:PHE:HB2	3:G:186:PHE:CZ	2.48	0.49
2:B:95:TRP:CZ2	2:B:97:ARG:HA	2.49	0.48
1:A:259:GLU:HG3	1:A:264[B]:HIS:ND1	2.29	0.48
4:F:209:ARG:NH1	4:F:211:GLN:HB2	2.29	0.47
1:A:246:LEU:HD11	8:A:851:HOH:O	2.15	0.47
4:F:209:ARG:NH1	4:F:211:GLN:OE1	2.39	0.46
4:F:177:LEU:H	4:F:177:LEU:HD23	1.80	0.46
3:E:161:MET:CE	4:F:195:ARG:HD3	2.44	0.46
1:A:68:GLY:O	1:A:72:MET:HG3	2.16	0.46
4:F:86:THR:HG23	4:F:112:THR:HA	1.98	0.45
4:F:13:LEU:HD21	4:F:19:MET:HB2	1.98	0.45
2:D:20:SER:HA	2:D:71:THR:HG22	1.98	0.45
3:G:131:VAL:HG22	3:G:174:TRP:HB3	1.99	0.45
3:G:196:PHE:CE2	3:G:198:PRO:HG3	2.52	0.45
3:E:150:ASP:HB2	3:E:177:LYS:HD3	1.99	0.45
4:H:203:ASN:OD1	4:H:205:ARG:HD2	2.17	0.45
1:C:6:ARG:HH11	1:C:95:MET:CE	2.30	0.45
1:A:46:ARG:HD3	1:A:46:ARG:HA	1.79	0.45
3:E:161:MET:HE3	3:E:166:PHE:CD1	2.52	0.44
5:A:600:2LJ:H1	5:A:600:2LJ:O4	2.17	0.44
1:C:221:ILE:HG22	1:C:223:GLN:H	1.82	0.44
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.99	0.44
4:F:222:GLU:HG3	8:F:512:HOH:O	2.16	0.44
2:B:8:GLN:HG2	1:C:134:ASN:OD1	2.18	0.44
3:G:159:LEU:HB3	4:H:171:CYS:HB2	2.00	0.43
4:H:127:VAL:HG23	4:H:237:ALA:HB3	1.98	0.43
3:G:36:GLN:HB2	3:G:46:LEU:HD11	1.99	0.43
1:C:101:LEU:HD12	1:C:105:SER:OG	2.18	0.43
1:A:20:PRO:HG2	1:A:23:ILE:HD11	2.00	0.43
4:F:14:ALA:O	4:F:17:ARG:HG3	2.19	0.43
4:H:204:PRO:HD2	4:H:205:ARG:NH1	2.34	0.42
1:C:214:TRP:H	1:C:225:ILE:HD13	1.85	0.42
1:A:99:GLU:HB2	1:A:107:THR:HB	2.00	0.42
3:E:161:MET:HE1	4:F:195:ARG:CD	2.49	0.42
1:C:4:SER:HB3	1:C:99:GLU:HG2	2.01	0.42
3:G:50:VAL:O	3:G:66:ARG:HD3	2.20	0.42
4:F:223:TRP:CZ2	4:F:225:GLN:HB2	2.55	0.42
1:A:56:PRO:O	1:A:60:GLU:HG3	2.20	0.42
5:C:301:2LJ:O4	5:C:301:2LJ:H1	2.19	0.42
1:A:246:LEU:HD13	1:A:254:TYR:CE1	2.54	0.42
4:F:183:LEU:HA	4:F:183:LEU:HD23	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:130:PRO:HD3	4:H:143:LEU:HG	2.02	0.41
3:E:125:LYS:HE2	3:E:125:LYS:HB3	1.85	0.41
3:E:159:LEU:HB2	4:F:171:CYS:HB2	2.01	0.41
4:F:175:GLN:HA	4:F:176:PRO:HD3	1.88	0.41
4:F:117:LEU:HD13	4:F:217:LEU:HD22	2.02	0.41
4:H:82:VAL:HG12	4:H:84:SER:H	1.85	0.41
1:A:62:TYR:CE2	5:A:600:2LJ:H3	2.56	0.41
1:A:78:LYS:NZ	8:A:713:HOH:O	2.54	0.41
1:A:25:VAL:HG23	1:A:27:TYR:CE2	2.56	0.41
1:A:169:LEU:HD23	1:A:176:LEU:HD13	2.03	0.40
1:C:74:LYS:NZ	8:C:408:HOH:O	2.44	0.40
1:C:234:GLY:HA3	8:D:108:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/271 (97%)	254 (97%)	9 (3%)	0	100	100
1	C	268/271 (99%)	259 (97%)	7 (3%)	2 (1%)	26	25
2	B	96/100 (96%)	96 (100%)	0	0	100	100
2	D	96/100 (96%)	93 (97%)	3 (3%)	0	100	100
3	E	199/204 (98%)	194 (98%)	5 (2%)	0	100	100
3	G	196/204 (96%)	186 (95%)	10 (5%)	0	100	100
4	F	238/245 (97%)	231 (97%)	7 (3%)	0	100	100
4	H	239/245 (98%)	232 (97%)	7 (3%)	0	100	100
All	All	1595/1640 (97%)	1545 (97%)	48 (3%)	2 (0%)	56	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	192	PHE
1	C	193	PRO

5.3.2 Protein sidechains (i)

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	236/241 (98%)	231 (98%)	5 (2%)	61	74
1	C	240/241 (100%)	235 (98%)	5 (2%)	61	74
2	B	93/95 (98%)	89 (96%)	4 (4%)	35	43
2	D	92/95 (97%)	89 (97%)	3 (3%)	45	56
3	E	178/181 (98%)	174 (98%)	4 (2%)	60	72
3	G	175/181 (97%)	166 (95%)	9 (5%)	29	34
4	F	201/205 (98%)	194 (96%)	7 (4%)	43	53
4	H	202/205 (98%)	191 (95%)	11 (5%)	27	31
All	All	1417/1444 (98%)	1369 (97%)	48 (3%)	44	54

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	73	PHE
1	A	198	LEU
1	A	221	ILE
1	A	222	VAL
2	B	1	ILE
2	B	70	PHE
2	B	77	GLU
2	B	97	ARG
1	C	6	ARG
1	C	82	ARG
1	C	95	MET
1	C	190	GLU
1	C	249	GLN

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Mol	Chain	Res	Type
2	D	70	PHE
2	D	75	LYS
2	D	92	ILE
3	E	145	GLN
3	E	147	LYS
3	E	159	LEU
3	E	188	ASN
4	F	6	GLN
4	F	10	SER
4	F	17	ARG
4	F	82	VAL
4	F	115	GLU
4	F	193	ARG
4	F	218	SER
3	G	70	TYR
3	G	91	MET
3	G	97	LEU
3	G	122	ARG
3	G	126	SER
3	G	131	VAL
3	G	145	GLN
3	G	146	SER
3	G	178	SER
4	H	10	SER
4	H	55	THR
4	H	82	VAL
4	H	116	ASP
4	H	118	LYS
4	H	137	HIS
4	H	164	LYS
4	H	193	ARG
4	H	218	SER
4	H	220	ASN
4	H	222	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	252	ASN
2	D	17	ASN
4	F	47	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	2LJ	A	600	1	19,22,23	1.03	1 (5%)	19,29,31	4.56	6 (31%)
5	2LJ	C	301	1	19,22,23	1.05	2 (10%)	19,29,31	4.46	5 (26%)
6	GOL	C	302	-	5,5,5	0.30	0	5,5,5	0.78	0
7	ACT	C	303	-	0,3,3	0.00	-	0,3,3	0.00	-
6	GOL	F	301	-	5,5,5	0.42	0	5,5,5	0.29	0
6	GOL	G	301	-	5,5,5	0.36	0	5,5,5	0.27	0
6	GOL	H	301	-	5,5,5	0.37	0	5,5,5	0.37	0
7	ACT	H	302	-	0,3,3	0.00	-	0,3,3	0.00	-

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	2LJ	A	600	1	-	0/18/19/20	0/1/1/1
5	2LJ	C	301	1	-	0/18/19/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	302	-	-	0/4/4/4	0/0/0/0
7	ACT	C	303	-	-	0/0/0/0	0/0/0/0
6	GOL	F	301	-	-	0/4/4/4	0/0/0/0
6	GOL	G	301	-	-	0/4/4/4	0/0/0/0
6	GOL	H	301	-	-	0/4/4/4	0/0/0/0
7	ACT	H	302	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	2LJ	C7-C6	-2.08	1.46	1.49
5	C	301	2LJ	C4-N3	3.04	1.38	1.33
5	A	600	2LJ	C4-N3	3.34	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	600	2LJ	C4A-C4-N3	-7.10	114.24	123.52
5	C	301	2LJ	C4A-C4-N3	-6.97	114.41	123.52
5	C	301	2LJ	N3-C2-N1	-6.55	116.67	127.69
5	A	600	2LJ	N3-C2-N1	-6.45	116.83	127.69
5	C	301	2LJ	C8A-C4A-N5	-3.44	113.22	126.67
5	A	600	2LJ	C8A-C4A-N5	-3.38	113.44	126.67
5	A	600	2LJ	C1'-N8-C8A	4.37	127.78	123.36
5	A	600	2LJ	C4-C4A-C8A	8.03	119.42	114.57
5	C	301	2LJ	C4-C4A-C8A	8.05	119.43	114.57
5	A	600	2LJ	C4-N3-C2	14.18	126.99	115.16
5	C	301	2LJ	C4-N3-C2	14.20	127.00	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	2LJ	2	0
5	C	301	2LJ	1	0

5.7 Other polymers

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	264/271 (97%)	-0.15	3 (1%) 82 82	23, 34, 74, 114	0
1	C	269/271 (99%)	-0.01	10 (3%) 45 44	29, 44, 93, 135	0
2	B	98/100 (98%)	-0.09	1 (1%) 84 83	28, 46, 80, 90	0
2	D	98/100 (98%)	0.09	1 (1%) 84 83	37, 70, 106, 122	0
3	E	200/204 (98%)	-0.21	0 100 100	24, 38, 75, 92	0
3	G	198/204 (97%)	0.21	8 (4%) 42 41	21, 48, 101, 121	0
4	F	240/245 (97%)	-0.14	0 100 100	30, 44, 70, 105	0
4	H	241/245 (98%)	-0.10	3 (1%) 81 80	23, 42, 81, 125	0
All	All	1608/1640 (98%)	-0.06	26 (1%) 74 73	21, 43, 88, 135	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	205	ARG	3.1
2	D	0	MET	3.1
4	H	132	GLU	3.1
1	C	253	LEU	3.0
1	C	223	GLN	3.0
3	G	149	SER	2.9
1	A	246	LEU	2.7
1	C	249	GLN	2.7
1	C	222	VAL	2.7
1	A	222	VAL	2.6
3	G	112	GLN	2.4
3	G	133	LEU	2.4
2	B	48	LYS	2.3
3	G	165	ASP	2.3
3	G	134	PHE	2.2
1	C	218	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	117	ALA	2.2
1	C	251	SER	2.1
4	H	201	TRP	2.1
1	C	211	TYR	2.1
1	C	250	SER	2.1
1	C	220	GLU	2.1
3	G	179	ASP	2.1
1	A	194	GLY	2.0
1	C	192	PHE	2.0
3	G	181	ALA	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^{th} 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^2)	Q<0.9
7	ACT	H	302	4/4	0.91	0.19	5.89	35,38,42,45	0
7	ACT	C	303	4/4	0.81	0.20	3.71	55,64,64,67	0
6	GOL	C	302	6/6	0.87	0.22	2.21	41,50,62,70	0
6	GOL	F	301	6/6	0.98	0.16	2.06	28,35,41,42	0
6	GOL	G	301	6/6	0.84	0.20	1.46	56,62,65,65	0
6	GOL	H	301	6/6	0.97	0.13	0.74	31,34,40,40	0
5	2LJ	C	301	22/23	0.98	0.12	-0.10	21,29,32,34	0
5	2LJ	A	600	22/23	0.98	0.12	-0.46	19,25,27,30	0

6.5 Other polymers (i)

There are no such residues in this entry.