



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:39 PM GMT

PDB ID : 4PJE
Title : Structure of human MR1-Ac-6-FP in complex with human MAIT B-B10 TCR
Authors : Birkinshaw, R.W.; Rossjohn, J.
Deposited on : 2014-05-12
Resolution : 1.95 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 ⓘ](#)) 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

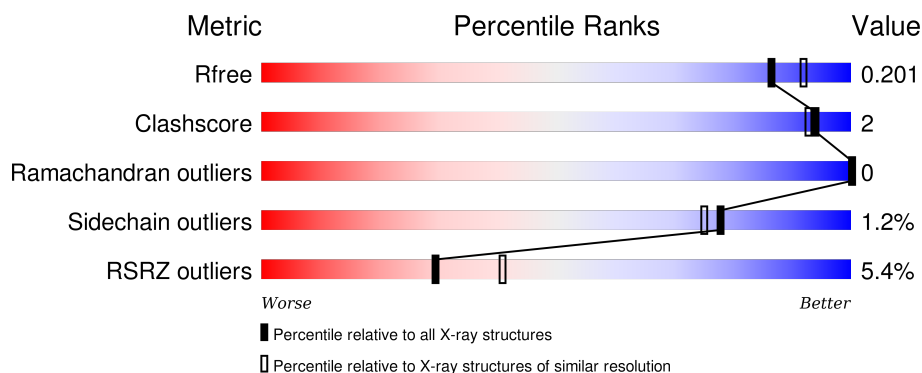
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



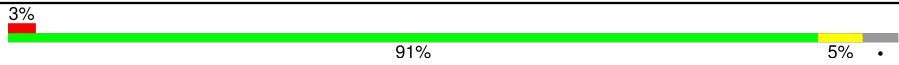
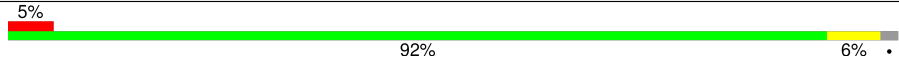
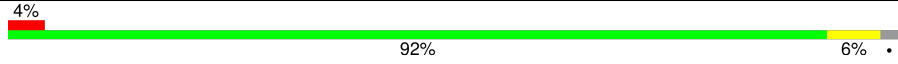
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 $\leq 5\%$. 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	271	<div> <div>4%</div> <div>92%</div> <div>5%</div> </div>
1	C	271	<div> <div>6%</div> <div>89%</div> <div>7%</div> </div>
2	B	100	<div> <div>96%</div> </div>
2	D	100	<div> <div>9%</div> <div>94%</div> </div>
3	E	205	<div> <div>11%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	205	
4	F	245	
4	H	245	

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	A	302	-	-	-	X
6	GOL	A	303	-	-	-	X
6	GOL	D	101	-	-	-	X
6	GOL	F	303	-	-	-	X
6	GOL	F	304	-	-	-	X
6	GOL	H	302	-	-	-	X
7	ACT	E	301	-	-	-	X
9	NA	F	302	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14211 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	261	Total	C	N	O	S	0	0	0
			2153	1381	370	392	10			
1	C	252	Total	C	N	O	S	0	0	0
			2065	1323	358	374	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	engineered mutation	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	engineered mutation	UNP Q95460

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			808	514	136	155	3			
2	D	97	Total	C	N	O	S	0	0	0
			781	499	129	150	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 TCR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	189	Total	C	N	O	S	0	1	0
			1471	934	235	292	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	197	Total	C	N	O	S	0	1	0
			1535	967	247	311	10			

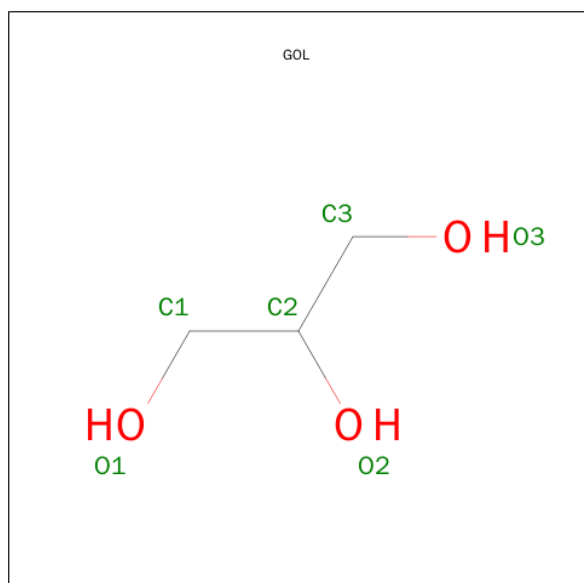
- Molecule 4 is a protein called TCR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	240	Total	C	N	O	S	0	9	0
			1950	1223	344	373	10			
4	H	240	Total	C	N	O	S	0	1	0
			1888	1183	335	361	9			

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

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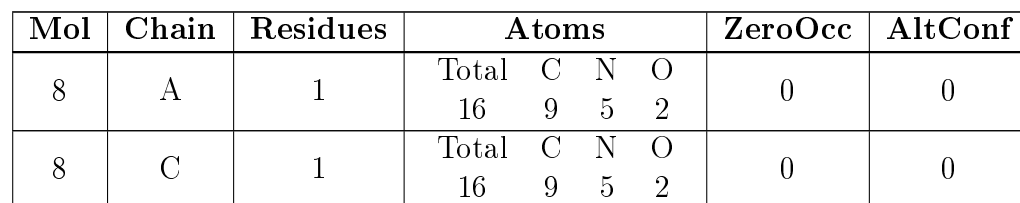
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 8 is N-(6-formyl-4-oxo-3,4-dihydropteridin-2-yl)acetamide (three-letter code: 30W) (formula: $C_9H_7N_5O_3$).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 9 | H | 1 | Total Na
1 1 | 0 | 0 |
| 9 | F | 1 | Total Na
1 1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 10 | A | 265 | Total O
265 265 | 0 | 0 |
| 10 | B | 106 | Total O
106 106 | 0 | 0 |
| 10 | C | 216 | Total O
216 216 | 0 | 0 |
| 10 | D | 70 | Total O
70 70 | 0 | 0 |
| 10 | E | 146 | Total O
146 146 | 0 | 0 |



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	222	Total 222	O 222	0	0
10	G	214	Total 214	O 214	0	0
10	H	224	Total 224	O 224	0	0

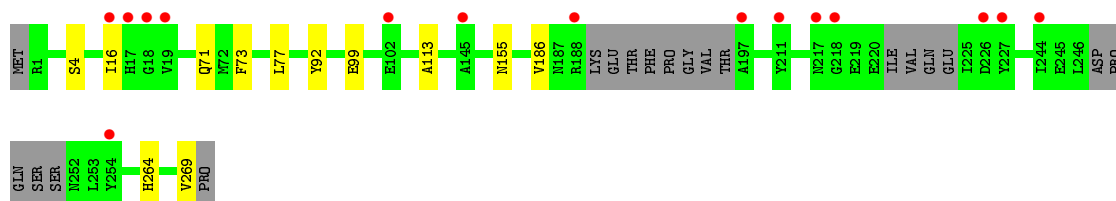
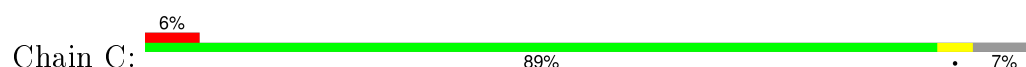
3 Residue-property plots [i](#)

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



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



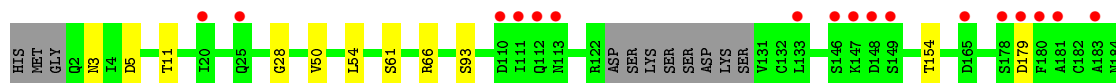
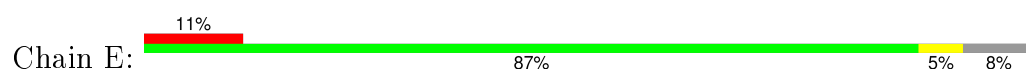
- Molecule 2: Beta-2-microglobulin

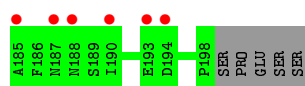


- Molecule 2: Beta-2-microglobulin

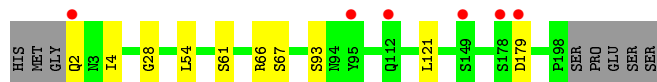
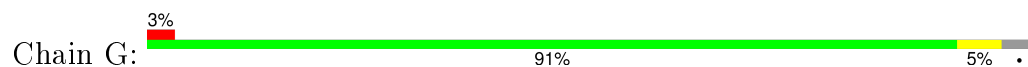


- Molecule 3: TCR-alpha

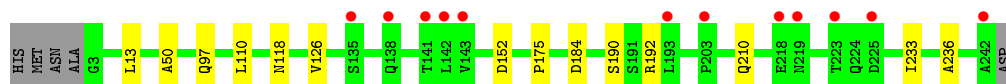
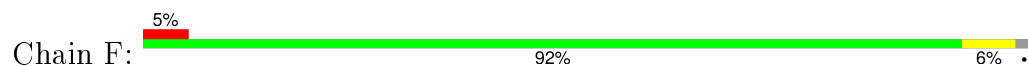




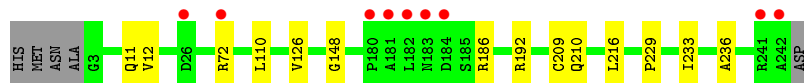
● Molecule 3: TCR-alpha



● Molecule 4: TCR-beta



● Molecule 4: TCR-beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.04Å 72.46Å 143.36Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	28.55 – 1.95 28.44 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.55-1.95) 97.7 (28.44-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.171 , 0.197 0.173 , 0.201	Depositor DCC
R_{free} test set	7803 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 155058 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14211	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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, 0.375 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: ACT, GOL, 3OW, NA, CL

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	0.55	0/2217	0.61	0/3012
1	C	0.52	0/2126	0.61	0/2888
2	B	0.49	0/831	0.62	0/1131
2	D	0.42	0/804	0.62	0/1097
3	E	0.50	0/1504	0.64	0/2042
3	G	0.53	0/1569	0.67	0/2129
4	F	0.50	0/2000	0.65	0/2723
4	H	0.51	0/1938	0.67	0/2640
All	All	0.51	0/12989	0.64	0/17662

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

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	2153	0	2046	9	0
1	C	2065	0	1942	7	0
2	B	808	0	746	1	0
2	D	781	0	712	1	0
3	E	1471	0	1366	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1535	0	1426	5	0
4	F	1950	0	1829	11	0
4	H	1888	0	1769	10	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	A	12	0	16	0	0
6	B	12	0	16	0	0
6	D	6	0	8	1	0
6	F	12	0	16	2	0
6	H	6	0	8	0	0
7	A	8	0	6	0	0
7	E	4	0	3	0	0
8	A	16	0	6	0	0
8	C	16	0	6	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
10	A	265	0	0	1	0
10	B	106	0	0	0	0
10	C	216	0	0	0	0
10	D	70	0	0	1	0
10	E	146	0	0	0	0
10	F	222	0	0	0	0
10	G	214	0	0	0	0
10	H	224	0	0	2	0
All	All	14211	0	11921	44	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 2.

All (44) 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:G:66[B]:ARG:HG2	3:G:66[B]:ARG:HH11	1.39	0.85
1:A:65:LEU:HA	4:F:97:GLN:HE22	1.50	0.76
4:H:148:GLY:O	4:H:186[A]:ARG:HD2	1.96	0.67
4:H:72:ARG:HG2	4:H:72:ARG:HH11	1.62	0.64
4:F:118:ASN:HB3	6:F:303:GOL:H2	1.80	0.64
4:H:11:GLN:HB3	4:H:110:LEU:HD22	1.79	0.63
4:F:50:ALA:HB1	4:F:97:GLN:NE2	2.20	0.57
1:A:155:ASN:HD21	3:E:66[B]:ARG:HH11	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HA	4:F:97:GLN:NE2	2.19	0.54
4:F:13:LEU:CD1	4:F:110[B]:LEU:HD11	2.37	0.54
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.89	0.54
1:A:4:SER:HB3	1:A:99:GLU:HG2	1.91	0.53
3:G:28:GLY:HA3	3:G:93:SER:OG	2.08	0.53
3:E:28:GLY:HA3	3:E:93:SER:OG	2.08	0.52
1:A:186:VAL:HG11	1:A:269:VAL:HG22	1.92	0.52
3:E:154:THR:HG21	4:F:190:SER:OG	2.11	0.51
4:F:210:GLN:HG3	4:F:233:ILE:HG23	1.93	0.50
3:E:54:LEU:HD11	3:E:61:SER:HB3	1.94	0.49
4:F:13:LEU:HD12	4:F:110[B]:LEU:HD11	1.93	0.49
3:E:50:VAL:O	3:E:66[A]:ARG:HD3	2.13	0.49
4:H:126:VAL:CG2	4:H:209:CYS:SG	3.01	0.49
4:H:12:VAL:HG23	10:H:482:HOH:O	2.13	0.49
4:H:210:GLN:HG3	4:H:233:ILE:HG23	1.94	0.48
3:E:3:ASN:ND2	3:E:5:ASP:OD2	2.46	0.48
3:G:54:LEU:HD11	3:G:61:SER:HB3	1.97	0.47
4:H:11:GLN:HB3	4:H:110:LEU:CD2	2.44	0.47
1:A:221:ILE:HD13	1:A:223:GLN:O	2.15	0.46
1:C:4:SER:HB3	1:C:99:GLU:HG2	1.98	0.46
3:G:66[B]:ARG:HG2	3:G:66[B]:ARG:NH1	2.17	0.46
1:C:71:GLN:HG3	10:H:604:HOH:O	2.16	0.46
6:D:101:GOL:H31	10:D:244:HOH:O	2.17	0.45
1:A:104:GLY:O	10:A:539:HOH:O	2.21	0.45
1:C:155:ASN:HD21	3:G:66[B]:ARG:HH21	1.65	0.44
1:C:264:HIS:HB2	3:E:11:THR:HB	2.00	0.44
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
1:C:113:ALA:HB2	2:D:60:TRP:CE2	2.54	0.43
4:H:72:ARG:HG2	4:H:72:ARG:NH1	2.32	0.42
4:F:126:VAL:HG23	4:F:236:ALA:HB3	2.02	0.42
4:H:216:LEU:HD13	4:H:229:PRO:HG2	2.02	0.42
4:H:126:VAL:HG23	4:H:236:ALA:HB3	2.02	0.42
4:F:152:ASP:CG	4:F:175:PRO:HG3	2.40	0.41
1:C:186:VAL:HG11	1:C:269:VAL:HG22	2.02	0.41
1:A:221:ILE:HD11	1:A:225:ILE:HG13	2.02	0.40
4:F:184:ASP:OD2	6:F:303:GOL:O3	2.31	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	255/271 (94%)	251 (98%)	4 (2%)	0	100	100
1	C	244/271 (90%)	240 (98%)	4 (2%)	0	100	100
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	D	95/100 (95%)	94 (99%)	1 (1%)	0	100	100
3	E	186/205 (91%)	182 (98%)	4 (2%)	0	100	100
3	G	196/205 (96%)	194 (99%)	2 (1%)	0	100	100
4	F	247/245 (101%)	244 (99%)	3 (1%)	0	100	100
4	H	239/245 (98%)	236 (99%)	3 (1%)	0	100	100
All	All	1559/1642 (95%)	1537 (99%)	22 (1%)	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	229/241 (95%)	227 (99%)	2 (1%)	84	83
1	C	216/241 (90%)	214 (99%)	2 (1%)	84	83
2	B	89/95 (94%)	87 (98%)	2 (2%)	60	51
2	D	85/95 (90%)	83 (98%)	2 (2%)	57	47
3	E	159/181 (88%)	158 (99%)	1 (1%)	90	89
3	G	169/181 (93%)	164 (97%)	5 (3%)	48	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	209/212 (99%)	208 (100%)	1 (0%)	92	91
4	H	202/212 (95%)	201 (100%)	1 (0%)	92	91
All	All	1358/1458 (93%)	1342 (99%)	16 (1%)	78	75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	PHE
1	A	246	LEU
2	B	70	PHE
2	B	73	THR
1	C	16	ILE
1	C	73	PHE
2	D	50	GLU
2	D	70	PHE
3	E	179	ASP
4	F	192	ARG
3	G	2	GLN
3	G	4	ILE
3	G	67	SER
3	G	121	LEU
3	G	179	ASP
4	H	192	ARG

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

Mol	Chain	Res	Type
1	A	111	GLN
4	F	97	GLN

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

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 for Mogul analysis.

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
6	GOL	A	302	-	5,5,5	0.23	0	5,5,5	0.50	0
6	GOL	A	303	-	5,5,5	0.23	0	5,5,5	0.64	0
7	ACT	A	304	-	1,3,3	4.05	1 (100%)	0,3,3	0.00	-
7	ACT	A	305	-	1,3,3	4.79	1 (100%)	0,3,3	0.00	-
8	30W	A	306	1	16,17,18	1.90	3 (18%)	19,24,25	3.08	8 (42%)
6	GOL	B	101	-	5,5,5	0.14	0	5,5,5	0.27	0
6	GOL	B	102	-	5,5,5	0.28	0	5,5,5	0.50	0
8	30W	C	302	1	16,17,18	1.77	3 (18%)	19,24,25	3.38	8 (42%)
6	GOL	D	101	-	5,5,5	0.13	0	5,5,5	0.45	0
7	ACT	E	301	-	1,3,3	5.11	1 (100%)	0,3,3	0.00	-
6	GOL	F	303	-	5,5,5	0.30	0	5,5,5	0.61	0
6	GOL	F	304	-	5,5,5	0.16	0	5,5,5	0.56	0
6	GOL	H	302	-	5,5,5	0.13	0	5,5,5	0.28	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
6	GOL	A	302	-	-	0/4/4/4	0/0/0/0
6	GOL	A	303	-	-	0/4/4/4	0/0/0/0
7	ACT	A	304	-	-	0/0/0/0	0/0/0/0
7	ACT	A	305	-	-	0/0/0/0	0/0/0/0
8	30W	A	306	1	-	0/4/4/6	0/2/2/2
6	GOL	B	101	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	102	-	-	0/4/4/4	0/0/0/0
8	30W	C	302	1	-	0/4/4/6	0/2/2/2
6	GOL	D	101	-	-	0/4/4/4	0/0/0/0
7	ACT	E	301	-	-	0/0/0/0	0/0/0/0
6	GOL	F	303	-	-	0/4/4/4	0/0/0/0
6	GOL	F	304	-	-	0/4/4/4	0/0/0/0
6	GOL	H	302	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	302	30W	C2-N2	-4.90	1.33	1.39
8	A	306	30W	C2-N2	-4.76	1.33	1.39
8	C	302	30W	C4-N3	2.79	1.38	1.33
8	A	306	30W	C4-N3	2.83	1.38	1.33
8	C	302	30W	C4-C4A	3.13	1.47	1.41
8	A	306	30W	C4-C4A	3.82	1.48	1.41
7	A	304	ACT	CH3-C	4.05	1.54	1.48
7	A	305	ACT	CH3-C	4.79	1.55	1.48
7	E	301	ACT	CH3-C	5.11	1.55	1.48

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	302	30W	C4A-C4-N3	-6.12	115.22	123.59
8	C	302	30W	N1-C2-N3	-5.40	117.92	126.22
8	A	306	30W	C4A-C4-N3	-4.95	116.82	123.59
8	A	306	30W	N1-C2-N3	-4.95	118.61	126.22
8	A	306	30W	C2-N2-C10	-4.44	123.26	130.17
8	C	302	30W	C2-N2-C10	-3.67	124.47	130.17
8	A	306	30W	C4-C4A-C8A	-2.81	118.14	119.94
8	A	306	30W	N2-C2-N1	-2.39	109.05	116.44
8	C	302	30W	N2-C2-N1	-2.21	109.62	116.44
8	C	302	30W	N8-C8A-N1	2.28	119.41	116.14
8	A	306	30W	C2-N1-C8A	4.95	121.05	115.09
8	A	306	30W	N2-C2-N3	5.10	132.21	116.44
8	C	302	30W	N2-C2-N3	5.18	132.45	116.44
8	A	306	30W	C4-N3-C2	6.35	124.55	115.31
8	C	302	30W	C2-N1-C8A	6.46	122.87	115.09
8	C	302	30W	C4-N3-C2	7.15	125.70	115.31

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
6	D	101	GOL	1	0
6	F	303	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	261/271 (96%)	-0.08	11 (4%) 40 51	18, 27, 51, 73	1 (0%)
1	C	252/271 (92%)	0.06	15 (5%) 25 35	20, 32, 58, 94	0
2	B	99/100 (99%)	-0.11	0 100 100	21, 33, 56, 65	0
2	D	97/100 (97%)	0.47	9 (9%) 11 17	26, 52, 82, 96	0
3	E	189/205 (92%)	0.47	23 (12%) 5 9	20, 39, 84, 109	0
3	G	197/205 (96%)	-0.04	6 (3%) 54 64	20, 30, 54, 71	6 (3%)
4	F	240/245 (97%)	-0.00	12 (5%) 32 44	19, 33, 65, 193	2 (0%)
4	H	240/245 (97%)	-0.11	9 (3%) 44 56	22, 31, 55, 78	4 (1%)
All	All	1575/1642 (95%)	0.05	85 (5%) 29 41	18, 32, 66, 193	13 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	VAL	7.8
3	E	179	ASP	6.2
3	E	149	SER	6.1
4	H	182	LEU	5.5
3	E	178	SER	5.2
4	H	181	ALA	5.0
4	H	183	ASN	4.7
3	E	112	GLN	4.6
1	C	18	GLY	4.6
4	F	242	ALA	4.2
1	C	218	GLY	4.1
1	A	221	ILE	4.1
4	F	135	SER	4.0
3	G	179	ASP	4.0
3	E	180	PHE	3.9
4	F	223	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	211	TYR	3.8
1	C	17	HIS	3.5
3	E	147	LYS	3.5
1	A	103	ASP	3.5
1	A	16	ILE	3.4
1	C	188	ARG	3.4
3	E	133	LEU	3.3
1	C	16	ILE	3.2
3	G	112	GLN	3.2
2	D	16	GLU	3.1
4	F	141	THR	3.1
2	D	74	GLU	3.1
3	E	194	ASP	3.0
3	E	193	GLU	3.0
2	D	88	SER	3.0
4	F	225	ASP	3.0
4	F	142	LEU	2.9
1	C	244	ILE	2.9
3	E	25	GLN	2.9
3	E	148	ASP	2.9
3	E	20	ILE	2.8
4	F	143	VAL	2.8
1	A	217	ASN	2.8
3	E	188	ASN	2.8
4	F	138	GLN	2.8
4	H	242	ALA	2.7
3	G	178	SER	2.7
1	A	224	GLU	2.7
3	E	190	ILE	2.7
3	G	149	SER	2.7
1	A	19	VAL	2.7
3	E	183	ALA	2.7
4	F	219	ASN	2.7
4	F	203	PRO	2.7
3	E	110	ASP	2.6
3	E	165	ASP	2.6
1	C	217	ASN	2.6
3	E	185	ALA	2.5
2	D	47	GLU	2.5
4	F	193	LEU	2.5
3	E	146	SER	2.5
1	C	19	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	73	THR	2.4
1	C	197	ALA	2.4
3	E	111	ILE	2.3
4	F	218	GLU	2.3
2	D	34	ASP	2.3
1	A	220	GLU	2.3
1	C	227	TYR	2.3
1	C	254	TYR	2.3
2	D	44	GLU	2.3
1	C	145	ALA	2.3
4	H	241	ARG	2.3
1	C	226	ASP	2.3
1	C	102	GLU	2.2
4	H	26	ASP	2.2
2	D	18	GLY	2.2
3	G	2	GLN	2.2
4	H	180	PRO	2.1
1	A	102	GLU	2.1
1	A	253	LEU	2.1
3	E	113	ASN	2.1
3	E	187	ASN	2.1
4	H	72	ARG	2.1
2	D	75	LYS	2.1
4	H	184	ASP	2.1
3	G	95	TYR	2.1
3	E	181	ALA	2.1
1	A	223	GLN	2.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	GOL	D	101	6/6	0.80	0.25	12.08	47,52,54,57	0
6	GOL	A	302	6/6	0.84	0.28	9.56	32,36,37,39	6
6	GOL	F	303	6/6	0.87	0.29	7.33	31,42,46,47	0
6	GOL	A	303	6/6	0.89	0.17	6.66	32,42,46,49	0
6	GOL	F	304	6/6	0.60	0.29	3.61	58,60,62,64	0
7	ACT	E	301	4/4	0.62	0.23	2.95	49,49,52,58	0
9	NA	F	302	1/1	0.99	0.15	2.42	27,27,27,27	0
6	GOL	H	302	6/6	0.92	0.10	2.28	35,36,38,39	6
8	30W	C	302	16/17	0.97	0.18	1.19	23,26,28,29	0
6	GOL	B	102	6/6	0.97	0.14	0.67	23,24,28,32	6
7	ACT	A	304	4/4	0.95	0.14	0.28	40,62,64,64	0
8	30W	A	306	16/17	0.98	0.13	-0.07	23,24,25,27	0
6	GOL	B	101	6/6	0.97	0.09	-0.75	23,25,28,29	0
5	CL	F	301	1/1	0.99	0.05	-0.80	41,41,41,41	0
9	NA	H	301	1/1	0.95	0.05	-3.06	32,32,32,32	0
5	CL	C	301	1/1	0.98	0.05	-3.17	34,34,34,34	0
7	ACT	A	305	4/4	0.26	0.23	-	97,97,97,99	0
5	CL	A	301	1/1	0.92	0.06	-	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.