



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:30 PM GMT

PDB ID : 1TVH
Title : Crystal structure of Modified Melanoma Antigen gp100(209-T2M) Bound to Human Class I MHC HLA-A2
Authors : Borbulevych, O.Y.; Baker, B.M.
Deposited on : 2004-06-29
Resolution : 1.80 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

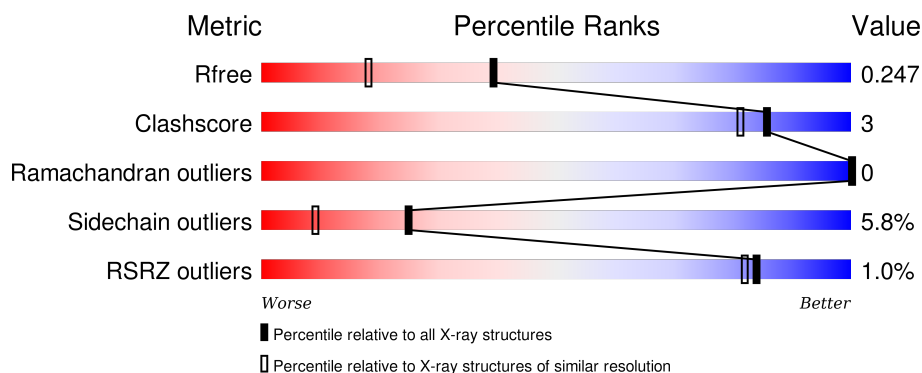
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	275	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
1	D	275	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
2	B	100	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
2	E	100	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
3	C	9	<div> <div></div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	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
4	GOL	A	1002	-	-	-	X
4	GOL	A	1004	-	-	-	X
4	GOL	A	1011	-	-	-	X
4	GOL	A	1018	-	-	-	X
4	GOL	A	1021	-	-	-	X
4	GOL	B	1003	-	-	-	X
4	GOL	B	1015	-	-	-	X
4	GOL	B	1023	-	-	-	X
4	GOL	C	1001	-	-	-	X
4	GOL	D	1005	-	-	-	X
4	GOL	D	1007	-	-	-	X
4	GOL	D	1008	-	-	-	X
4	GOL	D	1009	-	-	-	X
4	GOL	D	1013	-	-	-	X
4	GOL	D	1019	-	-	-	X
4	GOL	D	1020	-	-	-	X
4	GOL	D	1022	-	-	-	X
4	GOL	D	1024	-	-	-	X
4	GOL	D	1025	-	-	-	X
4	GOL	E	1016	-	-	-	X
4	GOL	E	1026	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7212 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2251	1406	409	426	10			
1	D	275	Total	C	N	O	S	0	1	0
			2249	1404	409	427	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769
E	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called epitope of Melanocyte protein Pmel 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			
3	F	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	MET	THR	ENGINEERED	UNP P40967
F	2	MET	THR	ENGINEERED	UNP P40967

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	233	Total 233	O 233	0	0
5	B	108	Total 108	O 108	0	0
5	C	10	Total 10	O 10	0	0
5	D	257	Total 257	O 257	0	0

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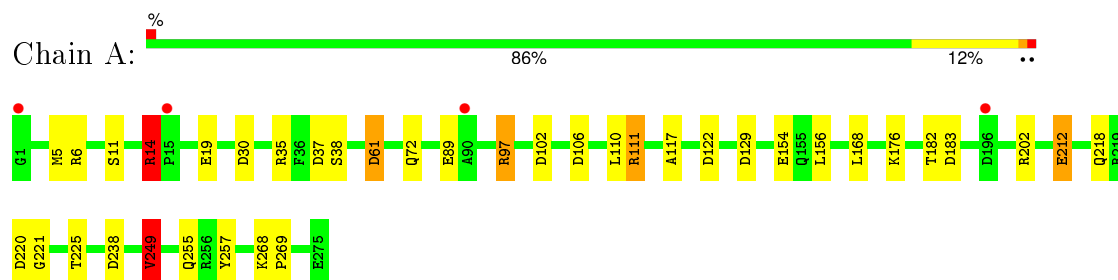
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	105	Total	O	0	0
			105	105		
5	F	13	Total	O	0	0
			13	13		

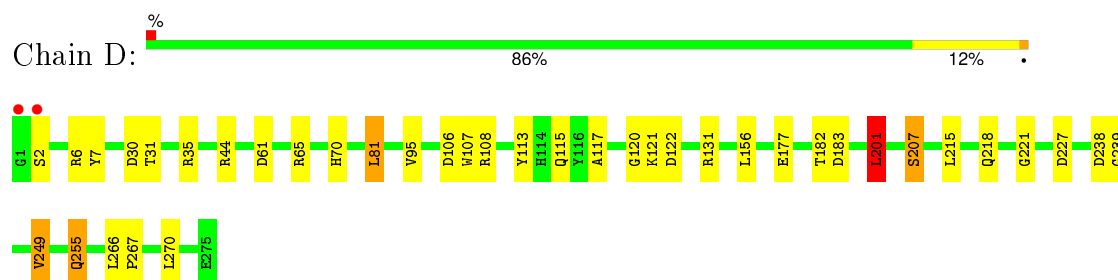
3 Residue-property plots [i](#)

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.

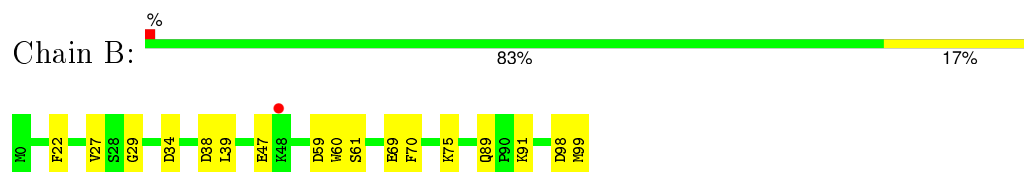
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



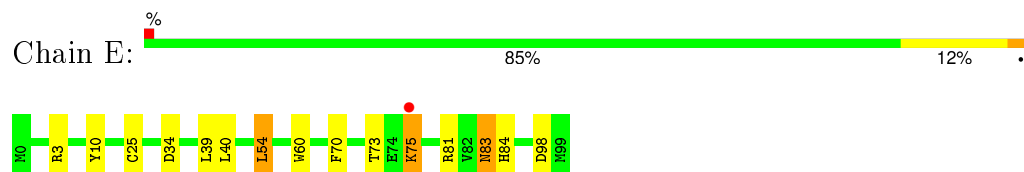
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: epitope of Melanocyte protein Pmel 17





- Molecule 3: epitope of Melanocyte protein Pmel 17

Chain F:  78% 22%

A horizontal bar chart representing the validation of Chain F. The bar is divided into two segments: a green segment on the left representing 78% and a yellow segment on the right representing 22%.



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.41Å 84.48Å 84.01Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 9.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (10.00-1.80) 98.3 (9.97-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.185 , 0.247 0.186 , 0.247	Depositor DCC
R_{free} test set	3703 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 37.8	EDS
Estimated twinning fraction	0.045 for -h,-l,-k 0.045 for -h,l,k 0.309 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 73767 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7212	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: GOL

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	1.03	0/2320	1.16	19/3147 (0.6%)
1	D	1.05	2/2318 (0.1%)	1.14	13/3145 (0.4%)
2	B	1.04	1/860 (0.1%)	1.06	4/1162 (0.3%)
2	E	1.04	1/860 (0.1%)	1.20	6/1162 (0.5%)
3	C	1.04	0/73	1.24	1/97 (1.0%)
3	F	1.15	0/73	1.21	1/97 (1.0%)
All	All	1.04	4/6504 (0.1%)	1.15	44/8810 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	27	VAL	CB-CG1	-5.67	1.41	1.52
1	D	95	VAL	CB-CG2	-5.38	1.41	1.52
2	E	10	TYR	CD2-CE2	5.03	1.46	1.39
1	D	7	TYR	CD2-CE2	5.01	1.46	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ARG	NE-CZ-NH1	-9.07	115.77	120.30
1	D	122	ASP	CB-CG-OD2	8.83	126.24	118.30
1	D	61	ASP	CB-CG-OD2	8.15	125.64	118.30
1	A	122	ASP	CB-CG-OD2	7.89	125.40	118.30
1	A	202	ARG	NE-CZ-NH1	-7.55	116.52	120.30
1	D	81	LEU	CB-CG-CD1	7.53	123.80	111.00
1	D	227	ASP	CB-CG-OD2	7.44	124.99	118.30
3	F	3	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	102	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	14	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	D	30	ASP	CB-CG-OD2	6.87	124.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ASP	CB-CG-OD2	6.55	124.19	118.30
2	B	98	ASP	CB-CG-OD2	6.54	124.19	118.30
1	D	270	LEU	CB-CG-CD1	-6.42	100.08	111.00
2	E	98	ASP	CB-CG-OD2	6.41	124.07	118.30
2	E	81	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	E	54	LEU	CB-CG-CD2	6.32	121.75	111.00
1	A	106	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	129	ASP	CB-CG-OD2	6.24	123.91	118.30
1	D	106	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	220	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	14	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	201	LEU	CB-CG-CD2	6.03	121.26	111.00
1	A	61	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	183	ASP	CB-CG-OD2	5.97	123.68	118.30
1	D	183	ASP	CB-CG-OD2	5.89	123.60	118.30
2	B	34	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	238	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	37	ASP	CB-CG-OD1	5.75	123.48	118.30
2	E	54	LEU	CA-CB-CG	5.73	128.48	115.30
3	C	3	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	97	ARG	NE-CZ-NH2	5.72	123.16	120.30
2	E	34	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	182	THR	OG1-CB-CG2	-5.54	97.27	110.00
2	E	40	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	D	238	ASP	CB-CG-OD2	5.42	123.18	118.30
2	B	38	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	6	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	249	VAL	CA-CB-CG1	5.35	118.92	110.90
1	A	249	VAL	N-CA-CB	-5.22	100.02	111.50
1	D	249	VAL	N-CA-CB	-5.03	100.44	111.50
1	D	182	THR	OG1-CB-CG2	-5.03	98.44	110.00
1	D	249	VAL	CA-CB-CG1	5.02	118.43	110.90
2	B	59	ASP	CB-CG-OD1	5.00	122.80	118.30

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	2251	0	2101	12	0
1	D	2249	0	2097	14	0
2	B	837	0	803	6	0
2	E	837	0	803	5	0
3	C	72	0	73	0	0
3	F	72	0	73	2	0
4	A	48	0	64	3	0
4	B	24	0	31	3	0
4	C	6	0	8	0	0
4	D	72	0	96	4	0
4	E	18	0	24	1	0
5	A	233	0	0	2	0
5	B	108	0	0	0	0
5	C	10	0	0	0	0
5	D	257	0	0	1	0
5	E	105	0	0	1	0
5	F	13	0	0	0	0
All	All	7212	0	6173	35	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 3.

All (35) 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:111:ARG:HH21	1:D:107:TRP:HB2	1.52	0.75
1:D:31:THR:HG23	4:D:1007:GOL:H2	1.68	0.72
1:D:70:HIS:CE1	3:F:2:MET:HE3	2.26	0.71
1:D:201:LEU:HD22	1:D:249:VAL:HG21	1.74	0.68
4:E:1016:GOL:H12	5:E:1127:HOH:O	1.96	0.65
2:E:73:THR:HG22	2:E:75:LYS:H	1.65	0.61
2:B:61:SER:OG	4:B:1015:GOL:C1	2.52	0.58
1:A:61:ASP:HB3	4:A:1012:GOL:H31	1.84	0.57
1:D:44:ARG:HH12	4:D:1022:GOL:H11	1.70	0.57
2:B:29:GLY:HA2	4:B:1015:GOL:H12	1.88	0.54
1:D:239:GLY:HA2	4:D:1007:GOL:H32	1.89	0.54
1:A:268:LYS:NZ	5:A:1258:HOH:O	2.41	0.53
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.73	0.53
2:B:61:SER:OG	4:B:1015:GOL:H11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.93	0.51
4:A:1004:GOL:H12	5:A:1156:HOH:O	2.10	0.50
1:A:14:ARG:HD2	1:A:19:GLU:O	2.11	0.49
1:A:255:GLN:CD	1:A:255:GLN:H	2.16	0.48
2:B:22:PHE:CZ	2:B:69:GLU:HG3	2.49	0.48
1:D:255:GLN:H	1:D:255:GLN:NE2	2.12	0.47
1:D:70:HIS:CE1	3:F:2:MET:CE	2.96	0.47
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.49	0.47
1:D:218:GLN:NE2	1:D:221:GLY:HA2	2.29	0.47
1:D:207:SER:O	1:D:207:SER:OG	2.31	0.46
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.99	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.44
1:D:266:LEU:HA	1:D:267:PRO:HD2	1.82	0.43
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.82	0.43
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.82	0.43
1:A:212:GLU:HB3	4:A:1011:GOL:H11	2.00	0.42
2:E:83:ASN:HD22	2:E:84:HIS:H	1.68	0.41
1:D:120:GLY:O	2:E:3:ARG:NH2	2.54	0.41
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.56	0.41
1:A:269:PRO:HG2	4:D:1020:GOL:H2	2.03	0.40
1:D:6:ARG:NH2	5:D:1281:HOH:O	2.44	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	274/275 (100%)	268 (98%)	6 (2%)	0	100	100
1	D	274/275 (100%)	269 (98%)	5 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	98/100 (98%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	758/768 (99%)	743 (98%)	15 (2%)	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	232/231 (100%)	218 (94%)	14 (6%)	24	8
1	D	232/231 (100%)	217 (94%)	15 (6%)	21	7
2	B	95/95 (100%)	89 (94%)	6 (6%)	22	8
2	E	95/95 (100%)	91 (96%)	4 (4%)	36	18
3	C	9/9 (100%)	9 (100%)	0	100	100
3	F	9/9 (100%)	9 (100%)	0	100	100
All	All	672/670 (100%)	633 (94%)	39 (6%)	25	9

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	14	ARG
1	A	35	ARG
1	A	38	SER
1	A	72	GLN
1	A	89	GLU
1	A	97	ARG
1	A	111	ARG
1	A	154	GLU
1	A	156	LEU
1	A	176	LYS
1	A	212	GLU

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Mol	Chain	Res	Type
1	A	225	THR
1	A	249	VAL
2	B	47	GLU
2	B	70	PHE
2	B	75	LYS
2	B	89	GLN
2	B	91	LYS
2	B	99	MET
1	D	2	SER
1	D	35	ARG
1	D	65	ARG
1	D	81	LEU
1	D	108	ARG
1	D	113	TYR
1	D	115	GLN
1	D	121	LYS
1	D	131	ARG
1	D	156	LEU
1	D	177	GLU
1	D	201	LEU
1	D	207	SER
1	D	215	LEU
1	D	255	GLN
2	E	54	LEU
2	E	70	PHE
2	E	75	LYS
2	E	83	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	218	GLN
2	B	83	ASN
3	C	4	GLN
1	D	86	ASN
1	D	115	GLN
1	D	218	GLN
1	D	255	GLN
2	E	17	ASN
2	E	83	ASN

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 ⓘ

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	1002	-	5,5,5	0.66	0	5,5,5	1.78	2 (40%)
4	GOL	A	1004	-	5,5,5	0.19	0	5,5,5	1.03	0
4	GOL	A	1011	-	5,5,5	0.63	0	5,5,5	1.82	1 (20%)
4	GOL	A	1012	-	5,5,5	0.24	0	5,5,5	0.92	0
4	GOL	A	1014	-	5,5,5	0.59	0	5,5,5	0.68	0
4	GOL	A	1018	-	5,5,5	0.50	0	5,5,5	0.94	0
4	GOL	A	1021	-	5,5,5	0.26	0	5,5,5	0.59	0
4	GOL	A	1027	-	5,5,5	0.33	0	5,5,5	1.08	0
4	GOL	B	1003	-	5,5,5	0.53	0	5,5,5	1.11	0
4	GOL	B	1010	-	5,5,5	0.46	0	5,5,5	0.54	0
4	GOL	B	1015	-	5,5,5	1.14	1 (20%)	5,5,5	1.88	2 (40%)
4	GOL	B	1023	-	5,5,5	0.37	0	5,5,5	0.13	0
4	GOL	C	1001	-	5,5,5	0.25	0	5,5,5	0.72	0
4	GOL	D	1005	-	5,5,5	0.35	0	5,5,5	0.80	0
4	GOL	D	1007	-	5,5,5	0.58	0	5,5,5	1.27	1 (20%)
4	GOL	D	1008	-	5,5,5	0.26	0	5,5,5	1.65	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	1009	-	5,5,5	0.30	0	5,5,5	0.89	0
4	GOL	D	1013	-	5,5,5	0.43	0	5,5,5	0.97	0
4	GOL	D	1017	-	5,5,5	0.30	0	5,5,5	0.79	0
4	GOL	D	1019	-	5,5,5	0.51	0	5,5,5	1.29	0
4	GOL	D	1020	-	5,5,5	0.56	0	5,5,5	1.29	1 (20%)
4	GOL	D	1022	-	5,5,5	0.56	0	5,5,5	1.20	1 (20%)
4	GOL	D	1024	-	5,5,5	0.87	0	5,5,5	1.22	1 (20%)
4	GOL	D	1025	-	5,5,5	0.17	0	5,5,5	1.40	1 (20%)
4	GOL	D	1028	-	5,5,5	0.38	0	5,5,5	0.71	0
4	GOL	E	1006	-	5,5,5	0.38	0	5,5,5	0.88	0
4	GOL	E	1016	-	5,5,5	0.84	0	5,5,5	1.14	0
4	GOL	E	1026	-	5,5,5	0.32	0	5,5,5	0.45	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
4	GOL	A	1002	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1004	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1011	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1012	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1014	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1018	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1021	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1027	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1003	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1010	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1015	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1023	-	-	0/4/4/4	0/0/0/0
4	GOL	C	1001	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1005	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1007	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1008	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1009	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1013	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1017	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1019	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1020	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1022	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1024	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	1025	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1028	-	-	0/4/4/4	0/0/0/0
4	GOL	E	1006	-	-	0/4/4/4	0/0/0/0
4	GOL	E	1016	-	-	0/4/4/4	0/0/0/0
4	GOL	E	1026	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1015	GOL	O2-C2	-2.32	1.36	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1015	GOL	O2-C2-C1	-3.01	94.84	108.65
4	D	1008	GOL	C3-C2-C1	-2.81	100.10	111.12
4	D	1025	GOL	C3-C2-C1	-2.48	101.41	111.12
4	A	1002	GOL	O1-C1-C2	-2.31	98.97	110.18
4	D	1024	GOL	C3-C2-C1	-2.02	103.22	111.12
4	D	1022	GOL	O3-C3-C2	2.05	120.14	110.18
4	D	1020	GOL	O1-C1-C2	2.08	120.28	110.18
4	D	1007	GOL	O2-C2-C1	2.35	119.44	108.65
4	D	1008	GOL	O3-C3-C2	2.37	121.66	110.18
4	A	1002	GOL	O3-C3-C2	2.50	122.30	110.18
4	A	1011	GOL	O1-C1-C2	2.66	123.10	110.18
4	B	1015	GOL	O1-C1-C2	2.71	123.34	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	GOL	1	0
4	A	1011	GOL	1	0
4	A	1012	GOL	1	0
4	B	1015	GOL	3	0
4	D	1007	GOL	2	0
4	D	1020	GOL	1	0
4	D	1022	GOL	1	0
4	E	1016	GOL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	275/275 (100%)	-0.32	4 (1%) 76 72	3, 11, 20, 29	0
1	D	275/275 (100%)	-0.38	2 (0%) 89 87	3, 11, 20, 25	0
2	B	100/100 (100%)	-0.44	1 (1%) 84 82	6, 11, 20, 25	0
2	E	100/100 (100%)	-0.39	1 (1%) 84 82	6, 11, 19, 23	0
3	C	9/9 (100%)	0.03	0 100 100	5, 6, 8, 10	0
3	F	9/9 (100%)	-0.04	0 100 100	2, 4, 10, 11	0
All	All	768/768 (100%)	-0.36	8 (1%) 84 82	2, 11, 20, 29	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	GLY	6.5
2	B	48	LYS	2.8
1	A	196	ASP	2.7
1	A	90	ALA	2.7
1	A	1	GLY	2.7
1	A	15	PRO	2.6
1	D	2	SER	2.1
2	E	75	LYS	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 ⓘ

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
4	GOL	D	1025	6/6	0.70	0.40	27.36	45,48,49,51	0
4	GOL	D	1007	6/6	0.84	0.38	21.57	28,36,37,38	0
4	GOL	A	1004	6/6	0.80	0.26	21.34	39,41,42,43	0
4	GOL	A	1002	6/6	0.77	0.27	11.78	26,38,39,43	0
4	GOL	E	1026	6/6	0.63	0.41	9.90	43,45,49,50	0
4	GOL	B	1015	6/6	0.83	0.26	8.92	22,37,38,40	0
4	GOL	D	1019	6/6	0.84	0.15	8.38	33,41,44,45	0
4	GOL	B	1023	6/6	0.36	0.41	8.19	54,58,59,60	0
4	GOL	D	1009	6/6	0.64	0.28	8.09	36,43,45,48	0
4	GOL	B	1003	6/6	0.85	0.22	8.06	25,38,43,47	0
4	GOL	D	1013	6/6	0.89	0.23	7.39	25,38,38,42	0
4	GOL	A	1021	6/6	0.86	0.23	5.76	22,40,42,46	0
4	GOL	D	1020	6/6	0.74	0.31	5.16	43,44,45,47	0
4	GOL	C	1001	6/6	0.88	0.19	5.07	31,38,39,43	0
4	GOL	D	1024	6/6	0.92	0.18	4.98	19,31,35,37	0
4	GOL	D	1022	6/6	0.87	0.34	4.64	31,44,45,46	0
4	GOL	E	1016	6/6	0.90	0.20	4.42	18,20,28,29	0
4	GOL	A	1011	6/6	0.90	0.23	3.11	21,34,37,41	0
4	GOL	A	1018	6/6	0.86	0.31	2.84	39,45,45,46	0
4	GOL	D	1005	6/6	0.94	0.12	2.60	25,30,32,33	0
4	GOL	D	1008	6/6	0.84	0.14	2.17	27,34,37,38	0
4	GOL	B	1010	6/6	0.90	0.18	1.32	39,42,45,46	0
4	GOL	A	1014	6/6	0.95	0.08	0.29	25,29,30,31	0
4	GOL	A	1027	6/6	0.95	0.09	0.27	30,33,35,42	0
4	GOL	D	1028	6/6	0.65	0.38	-	47,48,50,51	0
4	GOL	D	1017	6/6	0.77	0.32	-	37,42,45,46	0
4	GOL	A	1012	6/6	0.71	0.34	-	39,46,47,48	0
4	GOL	E	1006	6/6	0.82	0.31	-	24,40,45,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.