



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:35 AM GMT

PDB ID : 2AV1
Title : Crystal structure of HTLV-1 TAX peptide Bound to Human Class I MHC HLA-A2 with the E63Q and K66A mutations in the heavy chain.
Authors : Borbulevych, O.Y.; Baker, B.M.
Deposited on : 2005-08-29
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

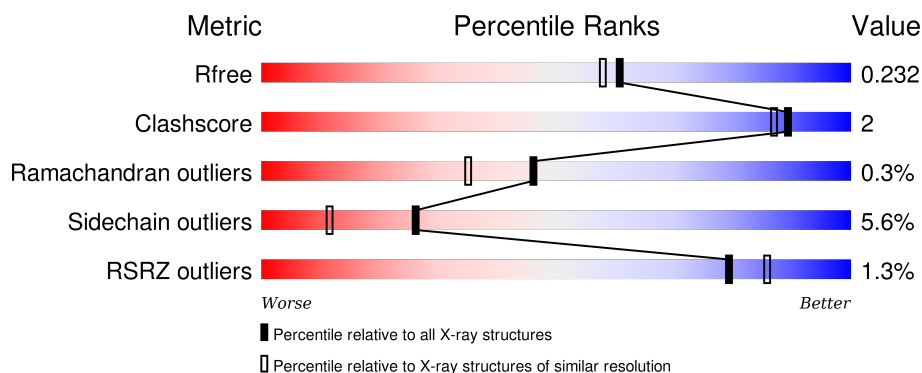
1 Overall quality at a glance ⓘ

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.



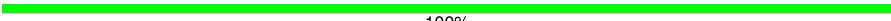
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	275	<div> <div></div> <div>92% 7% .</div> </div>
1	D	275	<div> <div>2%</div> <div>84% 14% .</div> </div>
2	B	100	<div> <div>2%</div> <div>80% 15% . .</div> </div>
2	E	100	<div> <div></div> <div>92% 7% .</div> </div>
3	C	9	<div> <div></div> <div>89% 11%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	9	 100%

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	SCN	B	801	-	-	-	X
5	GOL	A	907	-	-	-	X
5	GOL	A	910	-	-	-	X
5	GOL	A	912	-	-	-	X
5	GOL	A	913	-	-	-	X
5	GOL	A	920	-	-	-	X
5	GOL	B	903	-	-	-	X
5	GOL	B	906	-	-	-	X
5	GOL	B	919	-	-	-	X
5	GOL	B	921	-	-	-	X
5	GOL	B	923	-	-	-	X
5	GOL	C	908	-	-	-	X
5	GOL	D	905	-	-	-	X
5	GOL	D	915	-	-	-	X
5	GOL	D	917	-	-	-	X
5	GOL	D	918	-	-	-	X
5	GOL	D	922	-	-	-	X
5	GOL	E	901	-	-	-	X
5	GOL	E	911	-	-	-	X
5	GOL	E	916	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7206 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	0	0
			2243	1400	409	425	9			
1	D	275	Total	C	N	O	S	0	0	0
			2243	1400	409	425	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLN	GLU	ENGINEERED	UNP P01892
A	66	ALA	LYS	ENGINEERED	UNP P01892
D	63	GLN	GLU	ENGINEERED	UNP P01892
D	66	ALA	LYS	ENGINEERED	UNP P01892

- 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 P61770
E	0	MET	-	INITIATING METHIONINE	UNP P61770

- Molecule 3 is a protein called Trans-activating transcriptional regulatory peptide.

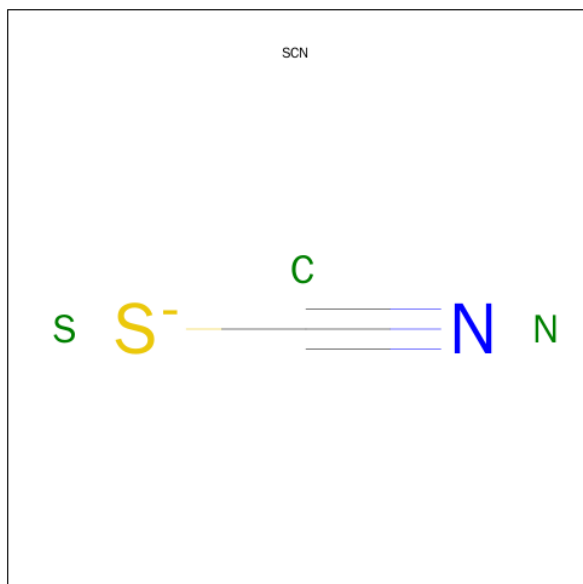
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			77	56	9	12			

Continued on next page...

Continued from previous page...

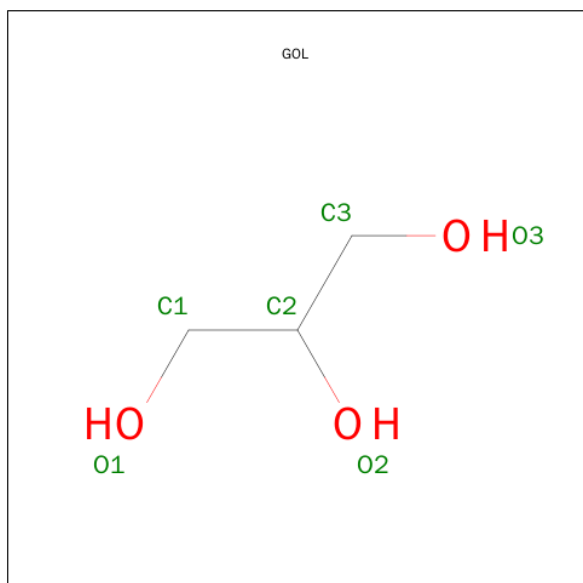
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	9	Total	C	N	O	0	0	0
			77	56	9	12			

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	250	Total	O	0	0
			250	250		
6	B	114	Total	O	0	0
			114	114		
6	C	7	Total	O	0	0
			7	7		
6	D	246	Total	O	0	0
			246	246		
6	E	123	Total	O	0	0
			123	123		
6	F	11	Total	O	0	0
			11	11		

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.

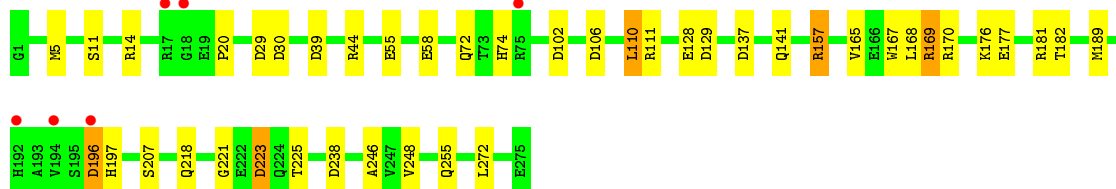
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A: 




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

Chain D: 



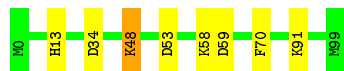
- Molecule 2: Beta-2-microglobulin

Chain B: 




- Molecule 2: Beta-2-microglobulin

Chain E: 



- Molecule 3: Trans-activating transcriptional regulatory peptide

Chain C: 



- Molecule 3: Trans-activating transcriptional regulatory peptide

Chain F:

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.33Å 62.54Å 74.75Å 82.10° 76.39° 78.10°	Depositor
Resolution (Å)	10.00 – 1.95 10.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.6 (10.00-1.95) 94.0 (10.00-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.174 , 0.231 0.175 , 0.232	Depositor DCC
R_{free} test set	3050 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 60276 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7206	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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, SCN

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	0.95	0/2308	1.06	8/3133 (0.3%)
1	D	0.96	2/2308 (0.1%)	1.15	20/3133 (0.6%)
2	B	1.01	0/860	1.10	8/1162 (0.7%)
2	E	1.00	0/860	1.10	4/1162 (0.3%)
3	C	0.82	0/80	0.94	0/108
3	F	1.01	0/80	0.83	0/108
All	All	0.97	2/6496 (0.0%)	1.10	40/8806 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	ALA	CA-CB	6.11	1.65	1.52
1	D	189	MET	SD-CE	-5.23	1.48	1.77

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	34	ASP	CB-CG-OD2	10.39	127.65	118.30
1	D	169	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	D	169	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	D	29	ASP	CB-CG-OD2	9.34	126.71	118.30
1	A	183	ASP	CB-CG-OD2	8.30	125.77	118.30
1	A	29	ASP	CB-CG-OD2	7.87	125.38	118.30
1	A	39	ASP	CB-CG-OD2	7.34	124.91	118.30
2	E	59	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	111	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	B	96	ASP	CB-CG-OD1	6.35	124.02	118.30
1	D	238	ASP	CB-CG-OD1	6.34	124.00	118.30
1	D	223	ASP	CB-CG-OD2	6.32	123.99	118.30
1	D	110	LEU	CA-CB-CG	6.24	129.65	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	ASP	CB-CG-OD2	6.24	123.91	118.30
1	D	157	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	D	30	ASP	CB-CG-OD1	-6.13	112.78	118.30
2	E	34	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	D	30	ASP	CB-CG-OD2	5.93	123.64	118.30
2	B	38	ASP	CB-CG-OD2	5.92	123.62	118.30
2	B	85	VAL	CG1-CB-CG2	5.79	120.17	110.90
1	D	44	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	D	102	ASP	CB-CG-OD1	5.77	123.49	118.30
1	D	137	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	122	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	106	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	30	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	85	VAL	CB-CA-C	-5.57	100.82	111.40
2	B	59	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	39	ASP	CB-CG-OD2	5.45	123.20	118.30
2	B	97	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	D	129	ASP	CB-CG-OD1	5.43	123.19	118.30
1	D	238	ASP	OD1-CG-OD2	-5.35	113.14	123.30
1	A	215	LEU	CA-CB-CG	5.30	127.49	115.30
2	E	53	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	181	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	119	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	238	ASP	CB-CG-OD2	5.06	122.85	118.30
2	B	53	ASP	CB-CG-OD2	5.03	122.83	118.30
2	B	97	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	247	VAL	CB-CA-C	-5.03	101.84	111.40

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	2243	0	2090	9	0
1	D	2243	0	2090	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	837	0	803	7	0
2	E	837	0	803	2	0
3	C	77	0	79	1	0
3	F	77	0	79	0	0
4	B	3	0	0	0	0
5	A	36	0	47	3	0
5	B	36	0	48	2	0
5	C	6	0	8	2	0
5	D	42	0	56	7	0
5	E	18	0	24	0	0
6	A	250	0	0	0	0
6	B	114	0	0	1	0
6	C	7	0	0	0	0
6	D	246	0	0	2	0
6	E	123	0	0	0	0
6	F	11	0	0	0	0
All	All	7206	0	6127	30	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 (30) 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)
2:B:96:ASP:O	2:B:98:ASP:N	2.25	0.69
1:D:223:ASP:OD1	1:D:225:THR:HG23	1.92	0.69
1:D:248:VAL:H	5:D:917:GOL:H11	1.61	0.63
1:A:159:TYR:HB2	5:C:908:GOL:H2	1.82	0.61
1:D:218:GLN:HE21	1:D:221:GLY:HA2	1.67	0.59
1:A:30:ASP:OD1	5:A:920:GOL:H31	2.06	0.56
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.40	0.56
2:B:79:ALA:HB2	5:B:903:GOL:H2	1.89	0.55
2:B:83:ASN:HD22	2:B:84:HIS:H	1.55	0.54
1:D:20:PRO:HD3	5:D:922:GOL:H12	1.90	0.53
1:A:196:ASP:N	1:A:196:ASP:OD1	2.43	0.48
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.95	0.48
1:D:128:GLU:HB2	5:D:904:GOL:H2	1.97	0.47
1:D:248:VAL:H	5:D:917:GOL:C1	2.26	0.46
1:D:165:VAL:O	1:D:169:ARG:HG3	2.16	0.46
1:D:248:VAL:N	5:D:917:GOL:H11	2.29	0.46
2:E:48:LYS:HA	2:E:48:LYS:HD3	1.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:TYR:CE2	5:C:908:GOL:H31	2.52	0.45
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.98	0.45
1:A:235:PRO:HG3	5:B:921:GOL:H32	1.97	0.44
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.98	0.44
1:A:110:LEU:HD13	5:A:910:GOL:H31	1.99	0.44
1:A:133:TRP:HB2	1:A:144:LYS:HG3	2.01	0.43
5:D:915:GOL:H2	2:E:13:HIS:CE1	2.53	0.42
1:A:240:THR:HG21	5:A:913:GOL:H11	2.01	0.42
2:B:98:ASP:N	6:B:977:HOH:O	2.52	0.42
1:D:167:TRP:CH2	5:D:918:GOL:H32	2.55	0.41
1:A:268:LYS:HE3	1:A:268:LYS:HB3	1.60	0.41
1:D:170:ARG:HD2	6:D:1092:HOH:O	2.21	0.41
1:D:72:GLN:NE2	6:D:1015:HOH:O	2.41	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	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
1	D	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
2	B	98/100 (98%)	95 (97%)	1 (1%)	2 (2%)	9	2
2	E	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	756/768 (98%)	737 (98%)	17 (2%)	2 (0%)	46	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ARG
2	B	98	ASP

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	230/230 (100%)	221 (96%)	9 (4%)	39	24
1	D	230/230 (100%)	214 (93%)	16 (7%)	19	6
2	B	95/95 (100%)	87 (92%)	8 (8%)	14	4
2	E	95/95 (100%)	91 (96%)	4 (4%)	36	21
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
All	All	666/666 (100%)	629 (94%)	37 (6%)	26	11

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	67	VAL
1	A	121	LYS
1	A	128	GLU
1	A	196	ASP
1	A	207	SER
1	A	226	GLN
1	A	247	VAL
1	A	268	LYS
2	B	48	LYS
2	B	69	GLU
2	B	70	PHE
2	B	83	ASN
2	B	85	VAL
2	B	88	SER
2	B	98	ASP
2	B	99	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	11	SER
1	D	14	ARG
1	D	55	GLU
1	D	58	GLU
1	D	74	HIS
1	D	110	LEU
1	D	141	GLN
1	D	157	ARG
1	D	176	LYS
1	D	177	GLU
1	D	182	THR
1	D	196	ASP
1	D	197	HIS
1	D	207	SER
1	D	255	GLN
1	D	272	LEU
2	E	48	LYS
2	E	58	LYS
2	E	70	PHE
2	E	91	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
2	B	2	GLN
2	B	83	ASN
1	D	218	GLN
1	D	255	GLN
2	E	2	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

24 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	GOL	A	902	-	5,5,5	0.69	0	5,5,5	2.20	3 (60%)
5	GOL	A	907	-	5,5,5	0.46	0	5,5,5	0.95	0
5	GOL	A	910	-	5,5,5	1.11	1 (20%)	5,5,5	0.64	0
5	GOL	A	912	-	5,5,5	0.67	0	5,5,5	0.93	0
5	GOL	A	913	-	5,5,5	0.36	0	5,5,5	0.44	0
5	GOL	A	920	-	5,5,5	0.25	0	5,5,5	0.56	0
4	SCN	B	801	-	2,2,2	2.05	1 (50%)	1,1,1	1.10	0
5	GOL	B	903	-	5,5,5	0.43	0	5,5,5	1.14	0
5	GOL	B	906	-	5,5,5	0.27	0	5,5,5	0.31	0
5	GOL	B	909	-	5,5,5	0.43	0	5,5,5	0.96	0
5	GOL	B	919	-	5,5,5	0.41	0	5,5,5	1.78	2 (40%)
5	GOL	B	921	-	5,5,5	0.51	0	5,5,5	1.52	1 (20%)
5	GOL	B	923	-	5,5,5	0.53	0	5,5,5	1.01	0
5	GOL	C	908	-	5,5,5	0.33	0	5,5,5	0.94	0
5	GOL	D	904	-	5,5,5	0.65	0	5,5,5	0.65	0
5	GOL	D	905	-	5,5,5	0.37	0	5,5,5	0.86	0
5	GOL	D	914	-	5,5,5	0.59	0	5,5,5	0.26	0
5	GOL	D	915	-	5,5,5	0.55	0	5,5,5	1.10	0
5	GOL	D	917	-	5,5,5	0.78	0	5,5,5	2.22	1 (20%)
5	GOL	D	918	-	5,5,5	0.32	0	5,5,5	0.82	0
5	GOL	D	922	-	5,5,5	0.57	0	5,5,5	1.36	1 (20%)
5	GOL	E	901	-	5,5,5	0.32	0	5,5,5	1.36	0
5	GOL	E	911	-	5,5,5	0.46	0	5,5,5	0.80	0
5	GOL	E	916	-	5,5,5	0.34	0	5,5,5	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	902	-	-	0/4/4/4	0/0/0/0
5	GOL	A	907	-	-	0/4/4/4	0/0/0/0
5	GOL	A	910	-	-	0/4/4/4	0/0/0/0
5	GOL	A	912	-	-	0/4/4/4	0/0/0/0
5	GOL	A	913	-	-	0/4/4/4	0/0/0/0
5	GOL	A	920	-	-	0/4/4/4	0/0/0/0
4	SCN	B	801	-	-	0/0/0/0	0/0/0/0
5	GOL	B	903	-	-	0/4/4/4	0/0/0/0
5	GOL	B	906	-	-	0/4/4/4	0/0/0/0
5	GOL	B	909	-	-	0/4/4/4	0/0/0/0
5	GOL	B	919	-	-	0/4/4/4	0/0/0/0
5	GOL	B	921	-	-	0/4/4/4	0/0/0/0
5	GOL	B	923	-	-	0/4/4/4	0/0/0/0
5	GOL	C	908	-	-	0/4/4/4	0/0/0/0
5	GOL	D	904	-	-	0/4/4/4	0/0/0/0
5	GOL	D	905	-	-	0/4/4/4	0/0/0/0
5	GOL	D	914	-	-	0/4/4/4	0/0/0/0
5	GOL	D	915	-	-	0/4/4/4	0/0/0/0
5	GOL	D	917	-	-	0/4/4/4	0/0/0/0
5	GOL	D	918	-	-	0/4/4/4	0/0/0/0
5	GOL	D	922	-	-	0/4/4/4	0/0/0/0
5	GOL	E	901	-	-	0/4/4/4	0/0/0/0
5	GOL	E	911	-	-	0/4/4/4	0/0/0/0
5	GOL	E	916	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	910	GOL	O2-C2	-2.26	1.36	1.43
4	B	801	SCN	C-S	2.79	1.81	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	902	GOL	O2-C2-C3	-2.12	98.92	108.65
5	B	919	GOL	O2-C2-C3	2.15	118.50	108.65
5	B	921	GOL	O1-C1-C2	2.46	122.13	110.18
5	D	922	GOL	O1-C1-C2	2.59	122.76	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	919	GOL	O2-C2-C1	2.91	122.00	108.65
5	A	902	GOL	O3-C3-C2	3.02	124.84	110.18
5	A	902	GOL	O1-C1-C2	3.05	124.96	110.18
5	D	917	GOL	O2-C2-C3	3.62	125.27	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	910	GOL	1	0
5	A	913	GOL	1	0
5	A	920	GOL	1	0
5	B	903	GOL	1	0
5	B	921	GOL	1	0
5	C	908	GOL	2	0
5	D	904	GOL	1	0
5	D	915	GOL	1	0
5	D	917	GOL	3	0
5	D	918	GOL	1	0
5	D	922	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 ⓘ

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	275/275 (100%)	-0.28	2 (0%) 89 93	2, 9, 19, 25	0
1	D	275/275 (100%)	-0.26	6 (2%) 65 74	4, 9, 18, 28	0
2	B	100/100 (100%)	-0.30	2 (2%) 68 77	5, 8, 18, 30	0
2	E	100/100 (100%)	-0.45	0 100 100	4, 9, 17, 23	0
3	C	9/9 (100%)	0.01	0 100 100	2, 4, 5, 9	0
3	F	9/9 (100%)	0.36	0 100 100	2, 5, 7, 9	0
All	All	768/768 (100%)	-0.28	10 (1%) 79 86	2, 9, 18, 30	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	99	MET	3.1
1	D	196	ASP	2.9
1	A	196	ASP	2.6
2	B	98	ASP	2.6
1	D	75	ARG	2.5
1	A	194	VAL	2.5
1	D	17	ARG	2.4
1	D	192	HIS	2.4
1	D	194	VAL	2.2
1	D	18	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
5	GOL	A	910	6/6	0.87	0.21	15.69	30,37,38,40	0
5	GOL	D	915	6/6	0.86	0.25	15.22	28,38,43,45	0
5	GOL	D	917	6/6	0.74	0.25	10.47	24,35,37,40	0
5	GOL	B	923	6/6	0.65	0.36	8.83	45,49,51,52	0
4	SCN	B	801	3/3	0.44	0.28	6.96	49,49,51,54	0
5	GOL	A	912	6/6	0.85	0.20	6.17	33,44,44,46	0
5	GOL	B	921	6/6	0.90	0.15	6.06	34,41,44,44	0
5	GOL	E	916	6/6	0.88	0.11	5.75	45,45,48,50	0
5	GOL	A	913	6/6	0.88	0.20	3.87	53,58,58,58	0
5	GOL	B	906	6/6	0.82	0.27	3.84	48,56,57,61	0
5	GOL	B	919	6/6	0.87	0.25	3.83	25,38,39,46	0
5	GOL	A	920	6/6	0.92	0.11	3.70	34,37,40,41	0
5	GOL	B	903	6/6	0.79	0.25	3.68	23,38,42,42	0
5	GOL	D	922	6/6	0.81	0.28	3.47	30,44,46,48	0
5	GOL	A	907	6/6	0.82	0.17	3.38	37,41,44,46	0
5	GOL	E	911	6/6	0.64	0.21	3.21	37,44,47,49	0
5	GOL	C	908	6/6	0.76	0.21	3.04	36,45,47,48	0
5	GOL	D	918	6/6	0.75	0.21	2.53	49,54,55,55	0
5	GOL	D	905	6/6	0.84	0.15	2.51	33,37,40,40	0
5	GOL	E	901	6/6	0.89	0.15	2.02	19,38,44,48	0
5	GOL	B	909	6/6	0.86	0.18	1.75	27,35,39,41	0
5	GOL	D	904	6/6	0.88	0.20	1.73	31,41,46,47	0
5	GOL	D	914	6/6	0.68	0.23	1.56	51,54,54,55	0
5	GOL	A	902	6/6	0.89	0.19	1.21	20,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.