



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:02 PM GMT

PDB ID : 1W72
Title : CRYSTAL STRUCTURE OF HLA-A1:MAGE-A1 IN COMPLEX WITH FAB-HYB3
Authors : Hulsmeyer, M.; Chames, P.; Hillig, R.C.; Stanfield, R.L.; Held, G.; Coulie, P.G.; Alings, C.; Wille, G.; Saenger, W.; Uchanska-Ziegler, B.; Hoogenboom, H.R.; Ziegler, A.
Deposited on : 2004-08-27
Resolution : 2.15 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

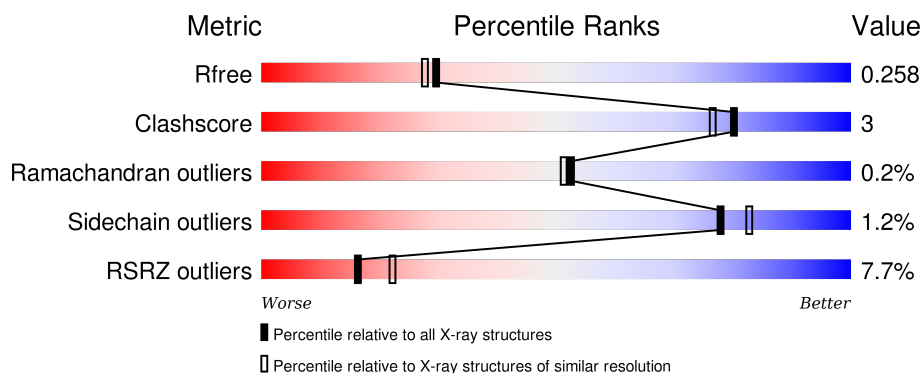
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	274	<div> <div>7%</div> <div>88%</div> <div>11%</div> </div>
1	D	274	<div> <div>10%</div> <div>92%</div> <div>7%</div> </div>
2	B	100	<div> <div>5%</div> <div>85%</div> <div>14%</div> </div>
2	E	100	<div> <div>31%</div> <div>91%</div> <div>9%</div> </div>
3	C	9	<div> <div>100%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	9	 100%
4	H	223	 8% 90% 9%
4	I	223	 8% 89% 9%
5	L	210	 2% 93% 7%
5	M	210	 2% 91% 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	A	1275	-	-	-	X
6	GOL	M	1212	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13471 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2228	1383	408	427	10			
1	D	274	Total	C	N	O	S	0	0	0
			2228	1383	408	427	10			

- 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	-	EXPRESSION TAG	UNP P61769
E	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called MELANOMA-ASSOCIATED ANTIGEN 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			69	41	11	17			
3	F	9	Total	C	N	O	0	0	0
			69	41	11	17			

- Molecule 4 is a protein called HYB3 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	223	Total	C	N	O	S	0	0	0
			1675	1056	285	327	7			

Continued on next page...

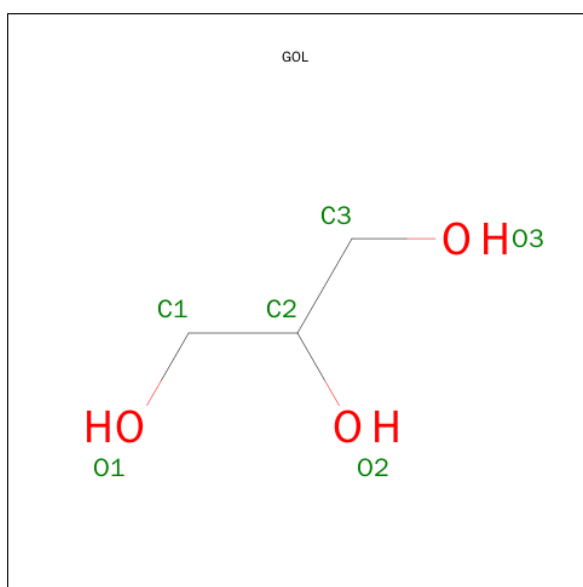
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	223	Total	C	N	O	S	0	0	0
			1679	1059	286	327	7			

- Molecule 5 is a protein called HYB3 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	210	Total	C	N	O	S	0	0	0
			1586	990	272	319	5			
5	M	210	Total	C	N	O	S	0	0	0
			1586	990	272	319	5			

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



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

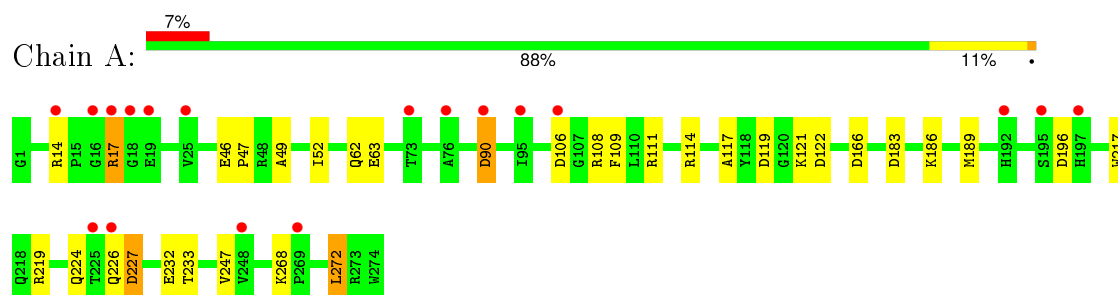
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	140	Total 140	O 140	0	0
7	B	30	Total 30	O 30	0	0
7	C	6	Total 6	O 6	0	0
7	D	67	Total 67	O 67	0	0
7	E	11	Total 11	O 11	0	0
7	F	4	Total 4	O 4	0	0
7	H	116	Total 116	O 116	0	0
7	I	93	Total 93	O 93	0	0
7	L	88	Total 88	O 88	0	0
7	M	98	Total 98	O 98	0	0

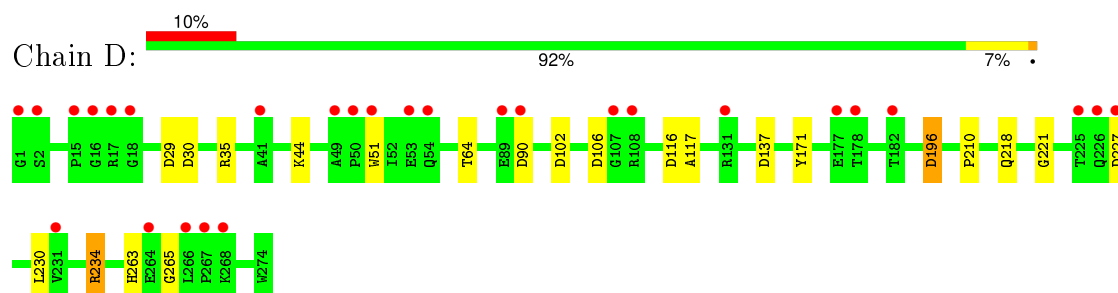
3 Residue-property plots [i](#)

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.

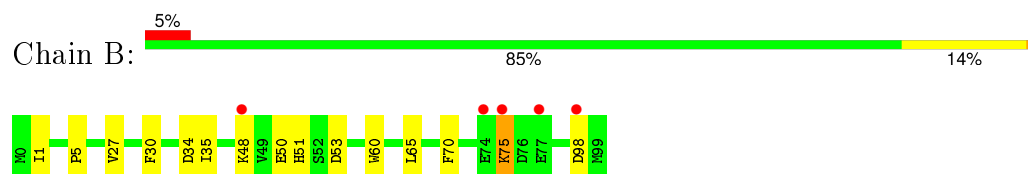
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN



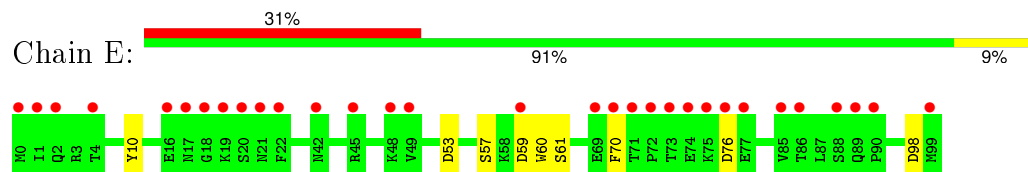
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN



- Molecule 2: BETA-2-MICROGLOBULIN



- Molecule 2: BETA-2-MICROGLOBULIN



- Molecule 3: MELANOMA-ASSOCIATED ANTIGEN 1




There are no outlier residues recorded for this chain.

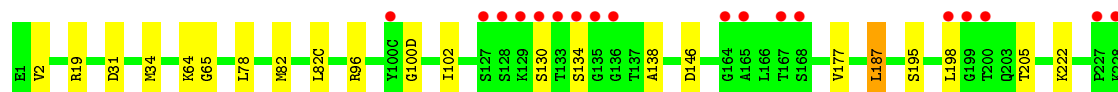
• Molecule 3: MELANOMA-ASSOCIATED ANTIGEN 1

Chain F:  100%


There are no outlier residues recorded for this chain.

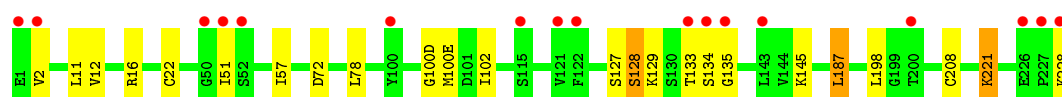
• Molecule 4: HYB3 HEAVY CHAIN

Chain H:  8% 90% 9%

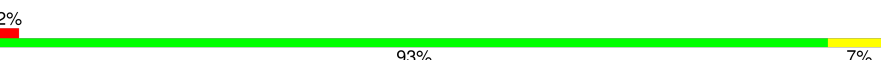


• Molecule 4: HYB3 HEAVY CHAIN

Chain I:  8% 89% 9%




• Molecule 5: HYB3 LIGHT CHAIN

Chain L:  2% 93% 7%



• Molecule 5: HYB3 LIGHT CHAIN

Chain M:  2% 91% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.36Å 50.05Å 136.71Å 90.00° 109.85° 90.00°	Depositor
Resolution (Å)	120.00 – 2.15 29.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	89.7 (120.00-2.15) 89.7 (29.02-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.182 , 0.248 0.192 , 0.258	Depositor DCC
R_{free} test set	3961 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78438 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13471	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.65	0/2288	0.91	10/3101 (0.3%)
1	D	0.53	0/2288	0.86	7/3101 (0.2%)
2	B	0.56	0/860	0.85	3/1162 (0.3%)
2	E	0.49	0/860	0.81	3/1162 (0.3%)
3	C	0.71	0/71	0.86	0/95
3	F	0.55	0/71	0.87	0/95
4	H	0.60	0/1718	0.83	3/2337 (0.1%)
4	I	0.59	0/1722	0.78	1/2341 (0.0%)
5	L	0.57	0/1628	0.83	2/2225 (0.1%)
5	M	0.59	0/1628	0.84	2/2225 (0.1%)
All	All	0.58	0/13134	0.84	31/17844 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	95(A)	ASP	CB-CG-OD2	7.24	124.81	118.30
2	B	53	ASP	CB-CG-OD2	7.13	124.72	118.30
1	D	137	ASP	CB-CG-OD2	7.00	124.59	118.30
1	A	90	ASP	CB-CG-OD2	6.78	124.40	118.30
5	L	94	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	119	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	106	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	196	ASP	CB-CG-OD2	6.17	123.85	118.30
2	E	98	ASP	CB-CG-OD2	6.10	123.79	118.30
5	L	53	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	106	ASP	CB-CG-OD2	6.08	123.77	118.30
1	D	102	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	29	ASP	CB-CG-OD2	5.71	123.44	118.30
2	B	98	ASP	CB-CG-OD2	5.67	123.40	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ASP	CB-CG-OD2	5.62	123.36	118.30
5	M	151	ASP	CB-CG-OD2	5.60	123.34	118.30
4	H	146	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	272	LEU	CA-CB-CG	5.47	127.89	115.30
1	D	196	ASP	CB-CG-OD2	5.46	123.21	118.30
4	I	72	ASP	CB-CG-OD2	5.37	123.13	118.30
2	E	76	ASP	CB-CG-OD2	5.26	123.04	118.30
2	E	59	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	90	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	122	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	114	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	166	ASP	CB-CG-OD2	5.13	122.92	118.30
4	H	31	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	30	ASP	CB-CG-OD2	5.04	122.84	118.30
4	H	19	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	227	ASP	CB-CG-OD2	5.02	122.82	118.30
2	B	34	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2228	0	2086	17	0
1	D	2228	0	2086	11	1
2	B	837	0	803	12	0
2	E	837	0	803	5	0
3	C	69	0	55	0	0
3	F	69	0	55	0	0
4	H	1675	0	1618	15	0
4	I	1679	0	1629	19	0
5	L	1586	0	1520	7	0
5	M	1586	0	1520	11	1
6	A	12	0	16	0	0
6	I	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	6	0	8	0	0
7	A	140	0	0	0	0
7	B	30	0	0	0	0
7	C	6	0	0	0	0
7	D	67	0	0	0	0
7	E	11	0	0	0	0
7	F	4	0	0	0	0
7	H	116	0	0	2	0
7	I	93	0	0	1	0
7	L	88	0	0	0	0
7	M	98	0	0	1	0
All	All	13471	0	12207	86	1

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 (86) 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)
4:H:2:VAL:HG11	4:H:102:ILE:HD13	1.60	0.82
4:I:2:VAL:HG11	4:I:102:ILE:HD13	1.60	0.82
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.23	0.74
5:M:104:LEU:HD23	5:M:104:LEU:C	2.10	0.72
1:A:219:ARG:HB2	1:A:224:GLN:HE21	1.55	0.72
1:A:108:ARG:HD2	1:A:109:PHE:O	1.95	0.67
4:I:11:LEU:HD23	4:I:12:VAL:N	2.10	0.66
4:H:96:ARG:NE	7:H:2073:HOH:O	2.29	0.62
1:A:219:ARG:CB	1:A:224:GLN:HE21	2.13	0.61
4:I:228:LYS:HE2	5:M:122:SER:OG	2.00	0.59
4:I:187:LEU:HD12	4:I:187:LEU:C	2.23	0.58
2:B:1:ILE:HD12	2:B:1:ILE:N	2.20	0.57
4:I:127:SER:C	4:I:129:LYS:H	2.06	0.57
5:L:17:GLN:O	5:L:78:VAL:HG23	2.05	0.55
1:D:263:HIS:CD2	1:D:265:GLY:H	2.25	0.54
4:I:127:SER:OG	4:I:128:SER:N	2.40	0.52
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.45	0.52
4:H:96:ARG:O	4:H:96:ARG:HG2	2.08	0.52
5:M:104:LEU:HD23	5:M:105:THR:N	2.26	0.51
1:A:46:GLU:HB2	1:A:47:PRO:HD2	1.92	0.50
1:A:121:LYS:HD3	2:B:1:ILE:HD13	1.93	0.50
5:M:104:LEU:CD2	5:M:104:LEU:C	2.78	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:VAL:HG11	2:B:35:ILE:HD13	1.94	0.50
2:B:75:LYS:H	2:B:75:LYS:HD3	1.77	0.49
2:B:27:VAL:HG11	2:B:35:ILE:CD1	2.42	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.49
1:D:44:LYS:HA	1:D:64:THR:HG23	1.94	0.49
2:B:27:VAL:HG12	2:B:30:PHE:CE2	2.48	0.48
4:H:82:MET:HE2	4:H:82(C):LEU:HD21	1.96	0.48
5:M:22:THR:HB	5:M:70:MET:SD	2.53	0.48
5:L:149:LYS:HE2	5:L:195:GLN:OE1	2.13	0.47
5:M:40:PRO:HD3	7:M:2040:HOH:O	2.15	0.47
4:H:205:THR:HG23	4:H:222:LYS:HE3	1.96	0.47
5:L:120:PRO:HD3	5:L:132:LEU:CD2	2.45	0.47
1:D:35:ARG:HG3	2:E:53:ASP:CG	2.35	0.47
5:M:170:ASN:O	5:M:171:ASN:HB2	2.14	0.47
1:A:227:ASP:OD1	1:A:227:ASP:O	2.33	0.46
4:H:2:VAL:HG11	4:H:102:ILE:CD1	2.40	0.45
4:I:2:VAL:HG11	4:I:102:ILE:CD1	2.38	0.45
4:I:127:SER:O	4:I:129:LYS:N	2.49	0.45
5:M:166:LYS:HG2	5:M:173:TYR:CE1	2.51	0.45
1:D:210:PRO:O	1:D:263:HIS:HE1	1.99	0.45
5:M:17:GLN:O	5:M:78:VAL:HG12	2.17	0.45
1:A:186:LYS:HD2	1:A:186:LYS:N	2.32	0.45
1:A:189:MET:SD	1:A:217:TRP:HH2	2.40	0.45
2:B:27:VAL:HG12	2:B:30:PHE:CD2	2.52	0.44
4:H:100(D):GLY:HA3	5:L:34:HIS:CD2	2.52	0.44
2:B:50:GLU:HG3	2:B:51:HIS:N	2.32	0.44
1:A:62:GLN:OE1	1:A:63:GLU:OE2	2.36	0.44
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.53	0.44
1:D:234:ARG:HD3	2:E:10:TYR:CE1	2.52	0.44
5:L:108:GLN:HB2	5:L:140:TYR:CZ	2.54	0.43
4:I:51:ILE:HG13	4:I:57:ILE:HG12	2.00	0.43
1:D:227:ASP:O	1:D:227:ASP:OD1	2.35	0.43
4:I:221:LYS:HB2	4:I:221:LYS:NZ	2.34	0.43
1:A:226:GLN:HA	1:A:226:GLN:HE21	1.82	0.43
4:I:100(E):MET:N	4:I:100(E):MET:SD	2.91	0.43
4:H:187:LEU:C	4:H:187:LEU:HD12	2.39	0.43
4:I:133:THR:C	4:I:135:GLY:H	2.22	0.43
4:H:82:MET:CE	4:H:82(C):LEU:HD21	2.49	0.43
1:A:217:TRP:CD1	1:A:247:VAL:HG13	2.53	0.43
4:I:2:VAL:CG1	4:I:102:ILE:HD13	2.41	0.42
4:H:130:SER:HB3	4:H:138:ALA:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:O	1:A:52:ILE:HG22	2.19	0.42
1:A:232:GLU:HG2	1:A:233:THR:O	2.19	0.42
4:I:187:LEU:CD1	4:I:187:LEU:C	2.88	0.42
4:I:208:CYS:SG	4:I:221:LYS:HB3	2.60	0.42
4:H:34:MET:HB3	4:H:78:LEU:HD22	2.01	0.42
4:H:96:ARG:CD	7:H:2073:HOH:O	2.68	0.42
4:I:127:SER:C	4:I:129:LYS:N	2.73	0.42
4:I:145:LYS:HE2	7:I:2071:HOH:O	2.20	0.41
2:B:5:PRO:HB2	2:B:27:VAL:HG13	2.03	0.41
1:A:109:PHE:CZ	1:A:111:ARG:HA	2.55	0.41
2:B:75:LYS:N	2:B:75:LYS:HD3	2.35	0.41
1:D:51:TRP:CZ3	1:D:171:TYR:HB3	2.56	0.41
5:L:37:GLN:HG3	5:L:86:TYR:CE1	2.56	0.41
4:H:177:VAL:HA	5:L:162:THR:HG22	2.01	0.41
1:A:14:ARG:HB3	1:A:17:ARG:HB3	2.03	0.41
4:H:64:LYS:HD2	4:H:65:GLY:N	2.35	0.41
1:D:218:GLN:HE21	1:D:221:GLY:HA2	1.86	0.41
1:A:268:LYS:HE2	1:A:268:LYS:HB3	1.89	0.41
4:I:22:CYS:HB3	4:I:78:LEU:HB3	2.02	0.41
4:I:100(D):GLY:HA3	5:M:34:HIS:CD2	2.56	0.41
2:B:51:HIS:HA	2:B:65:LEU:O	2.21	0.40
4:H:195:SER:O	4:H:198:LEU:HD13	2.21	0.40
5:M:55:PRO:HD2	5:M:58:ILE:HG13	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ASP:OD2	5:M:1:SER:N[2_656]	2.07	0.13

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	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
1	D	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	1 (1%)	1 (1%)	19	11
2	E	98/100 (98%)	92 (94%)	6 (6%)	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
4	H	221/223 (99%)	215 (97%)	5 (2%)	1 (0%)	34	26
4	I	221/223 (99%)	211 (96%)	8 (4%)	2 (1%)	21	13
5	L	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
5	M	208/210 (99%)	203 (98%)	5 (2%)	0	100	100
All	All	1612/1632 (99%)	1569 (97%)	39 (2%)	4 (0%)	52	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	128	SER
2	B	48	LYS
4	H	134	SER
4	I	134	SER

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	231/231 (100%)	228 (99%)	3 (1%)	76	82
1	D	231/231 (100%)	228 (99%)	3 (1%)	76	82
2	B	95/95 (100%)	93 (98%)	2 (2%)	61	65
2	E	95/95 (100%)	92 (97%)	3 (3%)	46	45
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
4	H	183/184 (100%)	182 (100%)	1 (0%)	92	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	184/184 (100%)	180 (98%)	4 (2%)	60	63
5	L	176/176 (100%)	176 (100%)	0	100	100
5	M	176/176 (100%)	175 (99%)	1 (1%)	90	94
All	All	1385/1386 (100%)	1368 (99%)	17 (1%)	78	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	90	ASP
1	A	272	LEU
2	B	70	PHE
2	B	75	LYS
1	D	116	ASP
1	D	230	LEU
1	D	234	ARG
2	E	57	SER
2	E	61	SER
2	E	70	PHE
4	H	187	LEU
4	I	16	ARG
4	I	187	LEU
4	I	198	LEU
4	I	221	LYS
5	M	132	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	62	GLN
1	A	87	GLN
1	A	224	GLN
1	A	226	GLN
2	B	51	HIS
1	D	62	GLN
1	D	218	GLN
1	D	262	GLN
1	D	263	HIS
4	H	179	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	216	ASN
4	I	211	ASN
5	L	171	ASN
5	M	17	GLN
5	M	126	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
6	GOL	A	1275	-	5,5,5	0.41	0	5,5,5	1.10	0
6	GOL	A	1276	-	5,5,5	0.33	0	5,5,5	0.51	0
6	GOL	I	1229	-	5,5,5	0.42	0	5,5,5	0.31	0
6	GOL	M	1212	-	5,5,5	0.54	0	5,5,5	0.15	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	1275	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1276	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1229	-	-	0/4/4/4	0/0/0/0
6	GOL	M	1212	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	274/274 (100%)	0.39	18 (6%)	22 30	16, 21, 34, 44	0
1	D	274/274 (100%)	0.68	28 (10%)	9 15	16, 23, 33, 46	0
2	B	100/100 (100%)	0.42	5 (5%)	32 43	17, 23, 35, 54	0
2	E	100/100 (100%)	1.57	31 (31%)	1 1	20, 25, 34, 62	0
3	C	9/9 (100%)	0.41	0	100 100	19, 20, 23, 28	0
3	F	9/9 (100%)	0.67	0	100 100	20, 24, 26, 28	0
4	H	223/223 (100%)	0.63	18 (8%)	15 21	17, 23, 30, 35	0
4	I	223/223 (100%)	0.60	17 (7%)	17 23	15, 23, 32, 42	0
5	L	210/210 (100%)	0.18	4 (1%)	70 78	19, 23, 28, 32	0
5	M	210/210 (100%)	0.26	4 (1%)	70 78	18, 22, 29, 32	0
All	All	1632/1632 (100%)	0.53	125 (7%)	16 22	15, 23, 31, 62	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	134	SER	15.0
4	H	134	SER	9.6
2	E	1	ILE	8.2
4	H	133	THR	6.7
1	D	17	ARG	6.5
4	H	135	GLY	6.3
1	D	16	GLY	5.8
1	D	18	GLY	5.7
2	E	75	LYS	5.7
1	D	41	ALA	5.5
2	E	0	MET	5.5
4	H	227	PRO	5.4
4	H	200	THR	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	17	ASN	5.0
4	H	199	GLY	4.9
2	E	19	LYS	4.9
1	D	226	GLN	4.7
2	E	73	THR	4.6
4	I	1	GLU	4.6
4	I	227	PRO	4.5
2	E	77	GLU	4.5
1	A	16	GLY	4.3
4	I	133	THR	4.2
2	E	70	PHE	4.1
4	H	128	SER	4.0
2	B	74	GLU	4.0
1	D	108	ARG	4.0
1	A	225	THR	3.9
5	M	56	SER	3.9
4	H	165	ALA	3.8
2	E	59	ASP	3.7
1	A	17	ARG	3.7
2	E	74	GLU	3.7
2	E	85	VAL	3.6
4	H	198	LEU	3.6
1	D	90	ASP	3.6
1	A	226	GLN	3.5
4	I	135	GLY	3.4
2	E	16	GLU	3.4
4	I	228	LYS	3.3
1	D	50	PRO	3.3
1	D	267	PRO	3.3
2	E	18	GLY	3.3
4	H	129	LYS	3.3
1	D	227	ASP	3.2
2	E	48	LYS	3.1
1	D	225	THR	3.1
4	H	130	SER	3.1
1	D	182	THR	3.1
2	E	20	SER	3.0
1	D	1	GLY	3.0
4	H	228	LYS	3.0
1	D	53	GLU	3.0
2	E	76	ASP	2.9
2	E	2	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	69	GLU	2.9
2	E	45	ARG	2.9
4	H	127	SER	2.8
2	E	72	PRO	2.8
4	I	122	PHE	2.8
2	E	99	MET	2.7
2	E	90	PRO	2.7
4	I	2	VAL	2.7
1	D	107	GLY	2.7
1	A	19	GLU	2.7
1	D	54	GLN	2.7
2	B	75	LYS	2.6
4	I	143	LEU	2.6
4	I	200	THR	2.6
1	A	197	HIS	2.6
2	E	86	THR	2.6
4	H	164	GLY	2.6
1	D	268	LYS	2.6
1	D	264	GLU	2.5
2	E	71	THR	2.5
1	D	49	ALA	2.5
4	I	51	ILE	2.5
4	I	50	GLY	2.5
2	E	89	GLN	2.5
2	E	49	VAL	2.5
5	M	126	GLN	2.5
2	E	4	THR	2.5
1	D	266	LEU	2.5
1	D	2	SER	2.5
1	D	131	ARG	2.5
5	M	111	ALA	2.4
1	A	269	PRO	2.4
1	D	177	GLU	2.4
4	H	136	GLY	2.4
5	L	184	GLU	2.4
2	B	48	LYS	2.4
2	B	98	ASP	2.3
4	I	115	SER	2.3
1	D	15	PRO	2.3
2	E	42	ASN	2.3
1	A	192	HIS	2.3
1	A	18	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	100(C)	TYR	2.2
1	D	89	GLU	2.2
4	I	100	TYR	2.2
1	A	25	VAL	2.2
1	D	231	VAL	2.2
4	I	52	SER	2.2
1	A	90	ASP	2.2
2	B	77	GLU	2.2
2	E	22	PHE	2.2
4	I	121	VAL	2.1
1	A	95	ILE	2.1
1	A	106	ASP	2.1
1	A	195	SER	2.1
2	E	88	SER	2.1
5	L	76	SER	2.1
1	A	76	ALA	2.1
1	A	248	VAL	2.1
1	A	14	ARG	2.1
1	A	73	THR	2.1
2	E	21	ASN	2.1
4	H	168	SER	2.1
1	D	178	THR	2.0
5	L	182	THR	2.0
4	I	226	GLU	2.0
5	M	128	ASN	2.0
1	D	51	TRP	2.0
4	H	167	THR	2.0
5	L	211	PRO	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, 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	A	1275	6/6	0.84	0.26	4.31	52,53,55,55	0
6	GOL	M	1212	6/6	0.88	0.16	2.31	61,62,63,63	0
6	GOL	I	1229	6/6	0.95	0.18	0.40	33,36,36,38	0
6	GOL	A	1276	6/6	0.83	0.29	-	53,54,56,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.