



Full wwPDB X-ray Structure Validation Report i

Mar 15, 2022 – 12:07 pm GMT

PDB ID : 7P0A

Title : CRYSTAL STRUCTURE OF THE MURINE CLASS I MAJOR HISTOCOMPATIBILITY COMPLEX H-2DB IN COMPLEX WITH LCMV-DERIVED GP33 PEPTIDE with D-AMINOACID (p3P6f)

Authors : Broggini, L.; Ricagno, S.

Deposited on : 2021-06-29

Resolution : 2.43 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the i symbol.

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

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.27

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.27

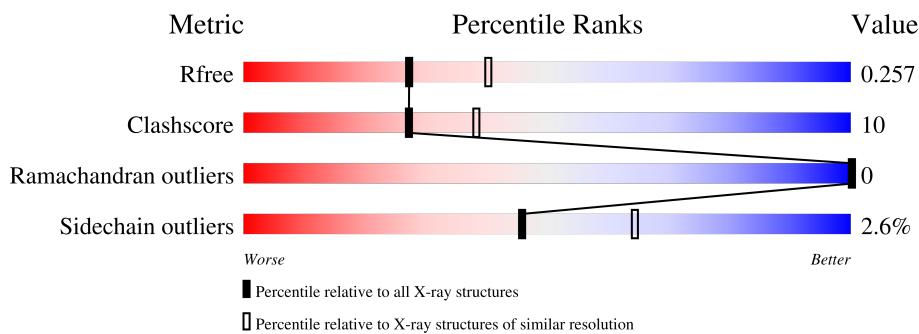
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5723 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C 1977	N 1254	O 352	S 363	8	0	0
1	D	255	Total	C 1900	N 1206	O 338	S 349	7	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C 764	N 491	O 127	S 140	6	0	0
2	E	99	Total	C 786	N 503	O 134	S 142	7	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP P01887
B	0	GLY	-	expression tag	UNP P01887
B	85	ASP	ALA	conflict	UNP P01887
E	-1	MET	-	initiating methionine	UNP P01887
E	0	GLY	-	expression tag	UNP P01887
E	85	ASP	ALA	conflict	UNP P01887

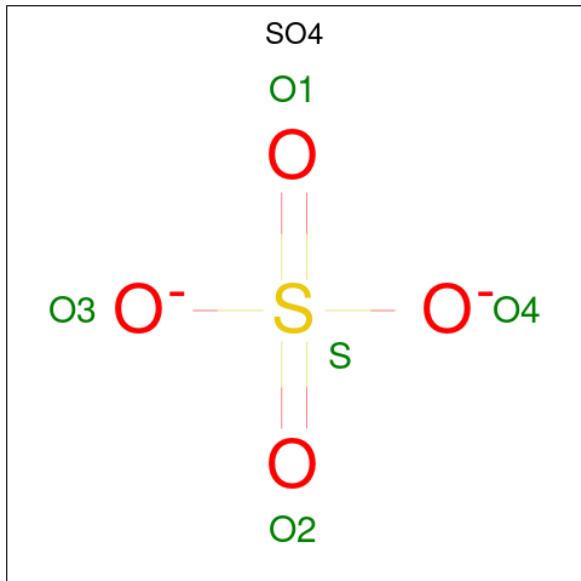
- Molecule 3 is a protein called Stable signal peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C 73	N 48	O 11	S 13	1	0	0
3	F	9	Total	C 73	N 48	O 11	S 13	1	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	PRO	VAL	conflict	UNP P09991
C	6	DPN	PHE	engineered mutation	UNP P09991
C	9	MET	CYS	conflict	UNP P09991
F	3	PRO	VAL	conflict	UNP P09991
F	6	DPN	PHE	engineered mutation	UNP P09991
F	9	MET	CYS	conflict	UNP P09991

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	2	Total Cl 2 2	0	0

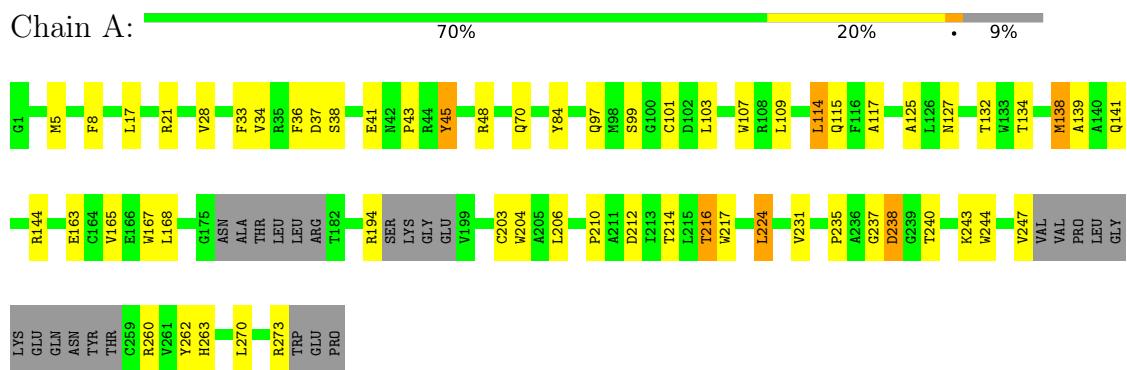
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	48	Total O 48 48	0	0
6	B	21	Total O 21 21	0	0
6	C	3	Total O 3 3	0	0
6	D	26	Total O 26 26	0	0
6	E	19	Total O 19 19	0	0
6	F	1	Total O 1 1	0	0

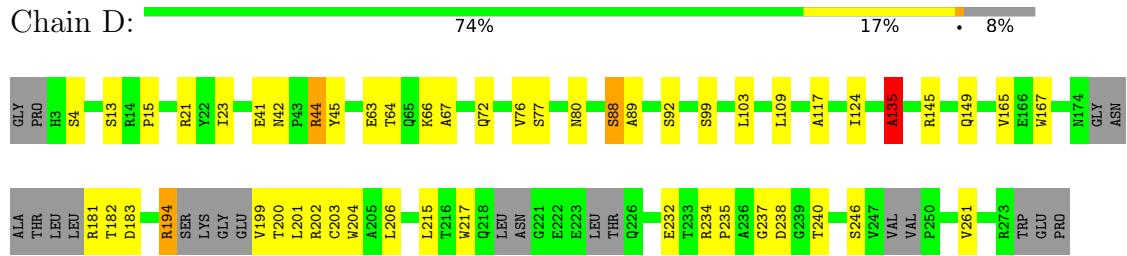
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

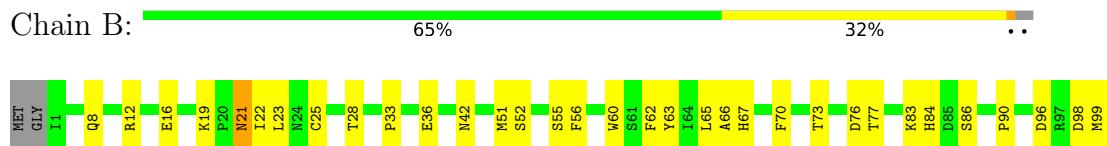
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



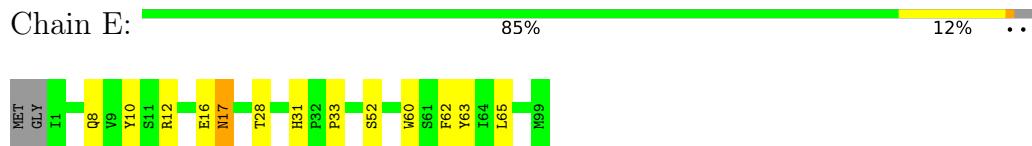
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



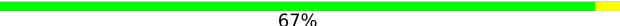
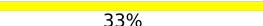
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

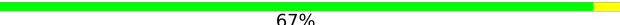
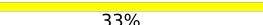


- Molecule 3: Stable signal peptide

Chain C:  67%  33%



- Molecule 3: Stable signal peptide

Chain F:  67%  33%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.65 Å 125.96 Å 92.93 Å 90.00° 126.63° 90.00°	Depositor
Resolution (Å)	48.41 – 2.43 48.41 – 2.43	Depositor EDS
% Data completeness (in resolution range)	72.1 (48.41-2.43) 72.1 (48.41-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.01 (at 2.42 Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ????)	Depositor
R , R_{free}	0.210 , 0.256 0.212 , 0.257	Depositor DCC
R_{free} test set	1989 reflections (6.57%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5723	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: DPN, SO4, 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	0.30	0/2035	0.59	4/2771 (0.1%)
1	D	0.25	0/1955	0.57	2/2672 (0.1%)
2	B	0.27	0/789	0.50	0/1081
2	E	0.26	0/812	0.57	3/1108 (0.3%)
3	C	0.25	0/62	0.49	0/80
3	F	0.29	0/62	0.59	0/80
All	All	0.27	0/5715	0.57	9/7792 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	ALA	N-CA-C	9.56	136.81	111.00
1	A	273	ARG	NE-CZ-NH2	8.90	124.75	120.30
1	A	238	ASP	CB-CA-C	-8.27	93.86	110.40
1	D	135	ALA	CB-CA-C	-7.00	99.59	110.10
2	E	17	ASN	CB-CA-C	6.88	124.17	110.40
1	A	224	LEU	CA-CB-CG	5.24	127.35	115.30
2	E	31	HIS	CB-CA-C	5.18	120.75	110.40
1	A	114	LEU	N-CA-C	-5.16	97.08	111.00
2	E	17	ASN	N-CA-C	-5.12	97.18	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	135	ALA	Peptide

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	1977	0	1791	42	0
1	D	1900	0	1620	37	0
2	B	764	0	687	23	0
2	E	786	0	734	13	0
3	C	73	0	71	5	0
3	F	73	0	71	5	0
4	A	15	0	0	0	0
4	D	10	0	0	0	0
4	E	5	0	0	0	0
5	E	2	0	0	1	0
6	A	48	0	0	2	0
6	B	21	0	0	0	0
6	C	3	0	0	0	0
6	D	26	0	0	0	0
6	E	19	0	0	2	0
6	F	1	0	0	0	0
All	All	5723	0	4974	107	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 10.

All (107) 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:D:41:GLU:HB3	1:D:44:ARG:HH12	1.37	0.89
1:A:97:GLN:HE22	3:C:5:ASN:HD21	1.28	0.80
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.65	0.78
1:A:204:TRP:HZ2	2:B:99:MET:HA	1.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASP:O	1:A:263:HIS:ND1	2.25	0.70
1:A:238:ASP:OD1	1:A:238:ASP:C	2.31	0.69
1:D:237:GLY:HA3	2:E:12:ARG:HE	1.59	0.67
5:E:103:CL:CL	6:E:216:HOH:O	2.51	0.65
2:B:36:GLU:HB2	2:B:83:LYS:HB2	1.79	0.64
1:A:70:GLN:HE22	3:C:5:ASN:H	1.45	0.64
2:B:16:GLU:HB2	2:B:19:LYS:HD3	1.80	0.63
1:A:238:ASP:OD1	1:A:238:ASP:O	2.18	0.62
1:D:80:ASN:ND2	3:F:9:MET:OXT	2.30	0.60
1:D:15:PRO:HD3	1:D:92:SER:HB2	1.83	0.60
1:D:194:ARG:HB2	1:D:200:THR:HG23	1.84	0.59
1:A:48:ARG:NH1	6:A:402:HOH:O	2.34	0.59
1:D:42:ASN:O	1:D:44:ARG:HD3	2.03	0.59
1:A:127:ASN:ND2	1:A:132:THR:OG1	2.30	0.58
1:A:235:PRO:HG2	2:B:65:LEU:HD13	1.86	0.57
1:D:194:ARG:H	1:D:199:VAL:HA	1.67	0.57
2:B:51:MET:HG3	2:B:66:ALA:HA	1.87	0.57
2:B:28:THR:HG22	2:B:63:TYR:HB2	1.87	0.56
1:D:72:GLN:O	1:D:76:VAL:HG22	2.06	0.56
1:A:216:THR:CG2	1:A:262:TYR:HE1	2.20	0.55
1:D:202:ARG:HA	1:D:246:SER:HB2	1.89	0.55
1:D:88:SER:OG	1:D:89:ALA:N	2.37	0.54
2:E:16:GLU:O	2:E:17:ASN:C	2.44	0.54
1:D:77:SER:HB3	3:F:9:MET:HB2	1.88	0.54
2:B:84:HIS:HD1	2:B:86:SER:HG	1.55	0.54
1:D:201:LEU:O	1:D:246:SER:OG	2.21	0.54
2:E:52:SER:HB2	2:E:65:LEU:HB3	1.90	0.53
2:B:96:ASP:HB2	2:B:98:ASP:OD2	2.08	0.53
1:A:216:THR:HG21	1:A:262:TYR:HE1	1.73	0.53
1:A:38:SER:HA	1:A:43:PRO:HB3	1.91	0.53
1:D:215:LEU:HD22	1:D:261:VAL:HG22	1.91	0.53
1:A:138:MET:HA	1:A:141:GLN:HG2	1.91	0.52
2:E:12:ARG:NH1	6:E:202:HOH:O	2.42	0.52
1:A:21:ARG:NH2	1:A:37:ASP:OD2	2.41	0.51
1:D:21:ARG:HH11	1:D:23:ILE:HD11	1.75	0.51
2:B:25:CYS:HB3	2:B:66:ALA:HB3	1.92	0.51
1:D:217:TRP:HE1	1:D:246:SER:HA	1.76	0.51
2:E:52:SER:HB3	2:E:65:LEU:H	1.75	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
1:D:217:TRP:NE1	1:D:246:SER:HA	2.26	0.50
1:A:216:THR:HG22	1:A:260:ARG:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:HG2	1:A:125:ALA:HB1	1.94	0.49
1:A:41:GLU:H	1:A:41:GLU:CD	2.16	0.49
1:D:204:TRP:HB3	1:D:206:LEU:HD11	1.93	0.48
1:D:99:SER:OG	3:F:3:PRO:HG3	2.14	0.48
1:A:231:VAL:O	1:A:243:LYS:NZ	2.35	0.48
1:A:84:TYR:HB3	1:A:139:ALA:HB1	1.96	0.48
1:A:34:VAL:HG22	1:A:45:TYR:HD1	1.78	0.48
1:A:8:PHE:HD2	2:B:56:PHE:CE1	2.32	0.47
1:D:13:SER:O	1:D:92:SER:OG	2.21	0.47
1:D:238:ASP:OD1	1:D:240:THR:HG22	2.13	0.47
1:A:260:ARG:HA	1:A:270:LEU:O	2.14	0.47
2:B:42:ASN:ND2	2:B:77:THR:H	2.13	0.47
2:B:33:PRO:HG3	2:B:62:PHE:CE1	2.50	0.47
2:B:33:PRO:HG3	2:B:62:PHE:CZ	2.50	0.46
1:D:103:LEU:HD21	1:D:165:VAL:HG12	1.96	0.46
1:D:167:TRP:CE3	3:F:1:LYS:HG2	2.50	0.46
2:E:33:PRO:HG3	2:E:62:PHE:CZ	2.50	0.46
1:D:232:GLU:HB2	2:E:8:GLN:NE2	2.30	0.46
2:B:8:GLN:HE21	2:B:8:GLN:HB3	1.61	0.46
1:D:232:GLU:HB2	2:E:8:GLN:HE22	1.80	0.45
1:A:109:LEU:HB2	1:A:165:VAL:HG11	1.98	0.45
1:A:127:ASN:OD1	1:A:134:THR:OG1	2.30	0.45
2:B:52:SER:HB3	2:B:65:LEU:H	1.81	0.45
2:B:83:LYS:HG2	2:B:90:PRO:HG3	1.98	0.45
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.52	0.45
2:B:55:SER:OG	2:B:56:PHE:N	2.49	0.45
1:D:124:ILE:HG13	1:D:135:ALA:HB2	1.98	0.45
1:D:42:ASN:H	1:D:44:ARG:NH1	2.15	0.44
1:D:181:ARG:HB3	1:D:182:THR:H	1.44	0.44
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.52	0.44
1:A:194:ARG:NH2	6:A:401:HOH:O	2.31	0.44
1:A:103:LEU:HD21	1:A:168:LEU:HD23	2.00	0.44
1:D:234:ARG:HD2	2:E:10:TYR:CE1	2.53	0.44
1:A:114:LEU:HD22	1:A:114:LEU:HA	1.88	0.44
1:A:36:PHE:CZ	1:A:43:PRO:HB2	2.53	0.43
1:A:204:TRP:HB3	1:A:206:LEU:CD1	2.48	0.43
1:A:141:GLN:OE1	1:A:144:ARG:NH2	2.50	0.43
1:A:99:SER:OG	3:C:3:PRO:HG3	2.18	0.43
2:B:73:THR:OG1	2:B:76:ASP:OD1	2.36	0.42
2:E:33:PRO:HG3	2:E:62:PHE:CE2	2.54	0.42
3:F:1:LYS:HD3	3:F:1:LYS:HA	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ARG:HA	1:D:64:THR:HG23	2.00	0.42
1:A:70:GLN:NE2	3:C:5:ASN:H	2.14	0.42
1:D:145:ARG:O	1:D:149:GLN:HB2	2.19	0.42
1:A:217:TRP:CE2	1:A:247:VAL:HG12	2.54	0.42
1:A:210:PRO:O	1:A:263:HIS:HE1	2.02	0.42
2:B:23:LEU:O	2:B:67:HIS:HA	2.20	0.42
1:A:237:GLY:HA3	2:B:22:ILE:HG21	2.02	0.41
2:B:42:ASN:HD21	2:B:77:THR:H	1.66	0.41
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.56	0.41
1:D:235:PRO:HG2	2:E:65:LEU:HD22	2.02	0.41
1:D:63:GLU:OE1	1:D:66:LYS:NZ	2.48	0.41
1:A:203:CYS:O	1:A:244:TRP:HA	2.21	0.41
3:C:5:ASN:O	3:C:6:DPN:HB2	2.19	0.41
1:D:103:LEU:HD23	1:D:109:LEU:HA	2.03	0.41
1:A:163:GLU:HG3	1:A:167:TRP:CD1	2.56	0.41
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.56	0.40
1:A:214:THR:HB	1:A:262:TYR:HB2	2.04	0.40
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.33	0.40
1:D:238:ASP:OD1	1:D:238:ASP:N	2.54	0.40
1:D:45:TYR:HE2	1:D:67:ALA:HB2	1.86	0.40
2:E:28:THR:HG22	2:E:63:TYR:HB2	2.04	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	244/276 (88%)	229 (94%)	15 (6%)	0	100 100
1	D	243/276 (88%)	227 (93%)	16 (7%)	0	100 100
2	B	97/101 (96%)	92 (95%)	5 (5%)	0	100 100
2	E	97/101 (96%)	95 (98%)	2 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	6/9 (67%)	4 (67%)	2 (33%)	0	100	100
3	F	6/9 (67%)	6 (100%)	0	0	100	100
All	All	693/772 (90%)	653 (94%)	40 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/234 (81%)	182 (96%)	7 (4%)	34	51
1	D	165/234 (70%)	160 (97%)	5 (3%)	41	59
2	B	79/95 (83%)	77 (98%)	2 (2%)	47	66
2	E	85/95 (90%)	85 (100%)	0	100	100
3	C	6/6 (100%)	6 (100%)	0	100	100
3	F	6/6 (100%)	6 (100%)	0	100	100
All	All	530/670 (79%)	516 (97%)	14 (3%)	46	64

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	45	TYR
1	A	101	CYS
1	A	107	TRP
1	A	138	MET
1	A	216	THR
1	A	224	LEU
2	B	12	ARG
2	B	21	ASN
1	D	4	SER
1	D	44	ARG
1	D	88	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	183	ASP
1	D	194	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
2	B	42	ASN
3	C	5	ASN
1	D	30	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
4	SO4	E	101	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	302	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.04	0
4	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.05	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 [\(i\)](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.