



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 12:41 PM EDT

PDB ID : 4G43
Title : Structure of the chicken MHC class I molecule BF2*0401 complexed to P5E
Authors : Zhang, J.; Chen, Y.; Qi, J.; Gao, F.; Liu, J.; Kaufman, J.; Xia, C.; Gao, G.F.
Deposited on : 2012-07-16
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

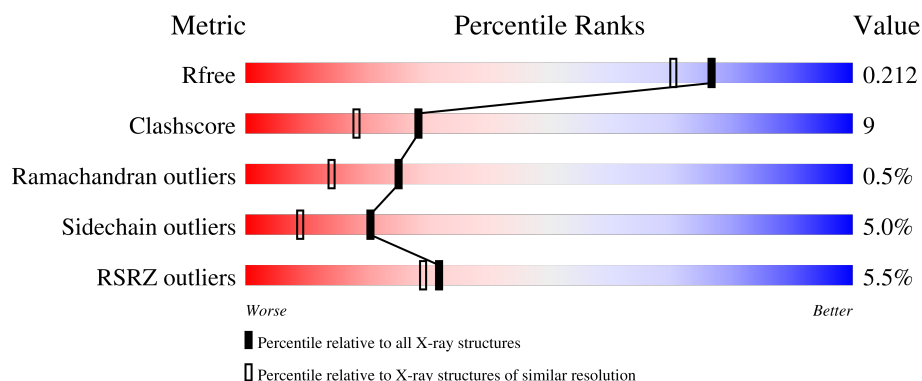
1 Overall quality at a glance

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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 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 $\leq 5\%$. 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>8%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	D	275	<div> <div>5%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
2	B	101	<div> <div>3%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
2	E	101	<div> <div>4%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
3	C	8	<div> <div>88%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	8	 75% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6721 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 MHC class I alpha chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2220	1397	402	414	7			
1	D	270	Total	C	N	O	S	0	0	0
			2207	1390	399	411	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP O46790
A	-1	GLU	-	expression tag	UNP O46790
A	0	PHE	-	expression tag	UNP O46790
A	244	GLU	ASP	engineered mutation	UNP O46790
A	271	LYS	-	expression tag	UNP O46790
A	272	LEU	-	expression tag	UNP O46790
D	-2	MET	-	expression tag	UNP O46790
D	-1	GLU	-	expression tag	UNP O46790
D	0	PHE	-	expression tag	UNP O46790
D	244	GLU	ASP	engineered mutation	UNP O46790
D	271	LYS	-	expression tag	UNP O46790
D	272	LEU	-	expression tag	UNP O46790

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			767	490	125	147	5			
2	E	97	Total	C	N	O	S	0	0	0
			767	490	125	147	5			

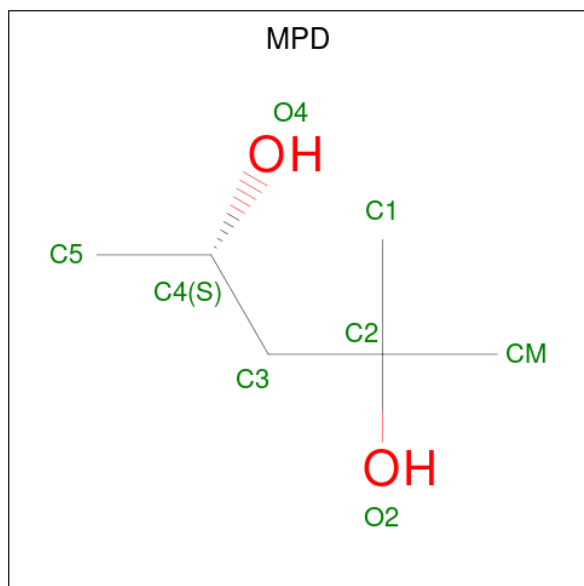
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P21611
B	-1	GLU	-	expression tag	UNP P21611
B	0	PHE	-	expression tag	UNP P21611
E	-2	MET	-	expression tag	UNP P21611
E	-1	GLU	-	expression tag	UNP P21611
E	0	PHE	-	expression tag	UNP P21611

- Molecule 3 is a protein called 8-MERIC PEPTIDE P5E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			73	48	10	15			
3	F	8	Total	C	N	O	0	0	0
			73	48	10	15			

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	244	Total	O	0	0
			244	244		

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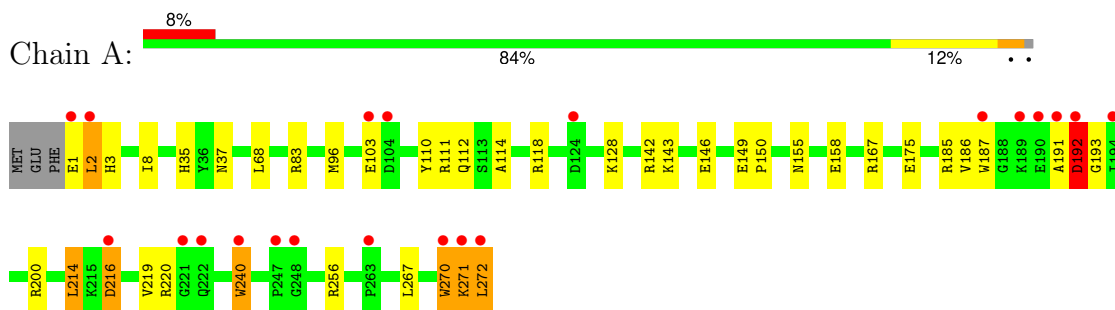
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	81	Total 81	O 81	0	0
5	C	5	Total 5	O 5	0	0
5	D	188	Total 188	O 188	0	0
5	E	82	Total 82	O 82	0	0
5	F	6	Total 6	O 6	0	0

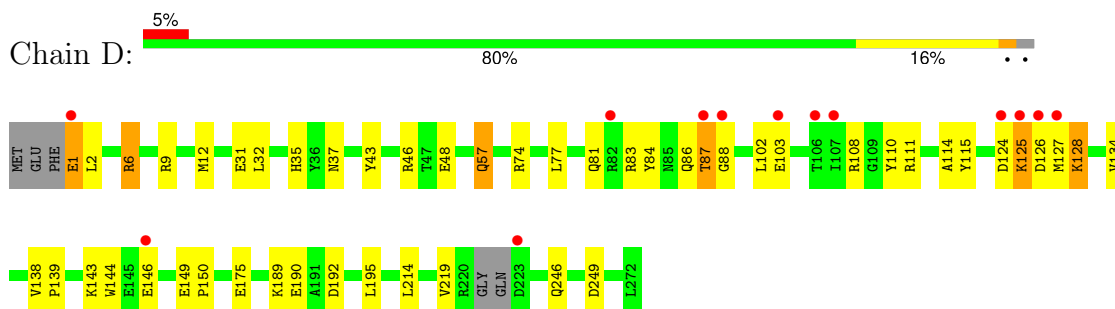
3 Residue-property plots

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 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.

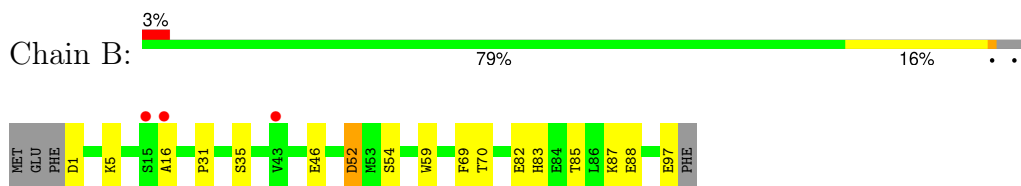
- Molecule 1: MHC class I alpha chain 2



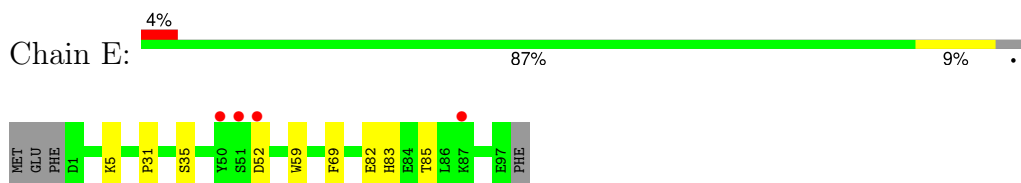
- Molecule 1: MHC class I alpha chain 2




- Molecule 2: Beta-2 microglobulin



- Molecule 2: Beta-2 microglobulin



- Molecule 3: 8-MERIC PEPTIDE P5E

Chain C:  88% 12%



● Molecule 3: 8-MERIC PEPTIDE P5E

Chain F:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.92Å 40.24Å 132.62Å 90.00° 120.35° 90.00°	Depositor
Resolution (Å)	41.31 – 1.80 41.31 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.31-1.80) 99.3 (41.31-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 1.81Å)	Xtriage
Refinement program	CNS, PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.183 , 0.218 0.179 , 0.212	Depositor DCC
R_{free} test set	3567 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6721	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: MPD

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	0.29	0/2283	0.51	0/3102
1	D	0.29	0/2269	0.47	0/3082
2	B	0.30	0/791	0.48	0/1076
2	E	0.31	0/791	0.48	0/1076
3	C	0.31	0/75	0.50	0/98
3	F	0.28	0/75	0.63	0/98
All	All	0.29	0/6284	0.49	0/8532

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2220	0	2106	51	0
1	D	2207	0	2094	35	0
2	B	767	0	728	16	0
2	E	767	0	728	5	0
3	C	73	0	64	1	0
3	F	73	0	64	0	0
4	D	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	244	0	0	12	0
5	B	81	0	0	4	1
5	C	5	0	0	0	0
5	D	188	0	0	1	1
5	E	82	0	0	0	0
5	F	6	0	0	0	0
All	All	6721	0	5798	104	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 9.

All (104) 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:96:MET:SD	1:A:110:TYR:CE1	2.56	0.99
1:A:96:MET:SD	1:A:110:TYR:HE1	1.87	0.95
1:A:272:LEU:C	1:A:272:LEU:HD22	1.96	0.87
2:B:16:ALA:HA	5:B:174:HOH:O	1.83	0.78
1:A:270:TRP:CZ2	1:A:272:LEU:HB3	2.21	0.76
1:A:192:ASP:HB3	5:A:352:HOH:O	1.88	0.74
2:B:70:THR:HG21	5:B:160:HOH:O	1.88	0.74
2:B:83:HIS:HD2	2:B:85:THR:OG1	1.74	0.71
1:A:83:ARG:NH1	5:A:345:HOH:O	2.25	0.70
4:D:301:MPD:O4	4:D:301:MPD:HM1	1.92	0.69
1:D:6:ARG:HD3	1:D:110:TYR:OH	1.93	0.68
1:A:270:TRP:CZ2	1:A:272:LEU:CB	2.79	0.65
1:A:35:HIS:NE2	2:B:52:ASP:CG	2.51	0.64
1:A:185:ARG:HD3	5:A:519:HOH:O	1.97	0.64
1:A:192:ASP:OD1	1:A:192:ASP:N	2.30	0.62
2:E:83:HIS:HD2	2:E:85:THR:OG1	1.82	0.62
1:A:272:LEU:C	1:A:272:LEU:HD13	2.22	0.60
1:A:128:LYS:HE3	5:A:522:HOH:O	2.01	0.60
1:D:1:GLU:CD	1:D:2:LEU:H	2.03	0.59
1:D:9:ARG:HG3	1:D:9:ARG:HH11	1.66	0.59
1:D:138:VAL:N	1:D:139:PRO:HD2	2.17	0.59
1:A:270:TRP:CG	1:A:271:LYS:N	2.67	0.59
1:A:1:GLU:HB3	1:A:103:GLU:HA	1.83	0.59
1:A:200:ARG:HG2	1:A:240:TRP:CB	2.35	0.57
1:A:1:GLU:O	1:A:2:LEU:C	2.43	0.57
1:A:200:ARG:HG2	1:A:240:TRP:HB2	1.86	0.57
1:A:270:TRP:O	1:A:271:LYS:CB	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:TRP:O	1:A:271:LYS:HG2	2.06	0.56
1:A:155:ASN:OD1	5:A:517:HOH:O	2.18	0.56
1:D:102:LEU:HD21	1:D:108:ARG:NH1	2.21	0.56
1:D:87:THR:HG22	1:D:88:GLY:N	2.19	0.56
1:D:103:GLU:HA	1:D:103:GLU:OE1	2.04	0.56
1:A:1:GLU:H3	1:A:103:GLU:HB2	1.71	0.56
1:A:35:HIS:HE1	1:A:37:ASN:ND2	2.03	0.55
1:D:35:HIS:HE1	1:D:37:ASN:ND2	2.05	0.55
1:A:1:GLU:HG3	1:A:3:HIS:CD2	2.43	0.54
1:A:270:TRP:CH2	1:A:272:LEU:HB3	2.43	0.54
1:D:35:HIS:HE1	1:D:37:ASN:HD22	1.56	0.54
2:E:31:PRO:O	2:E:83:HIS:HE1	1.91	0.53
1:A:270:TRP:C	1:A:271:LYS:HG2	2.29	0.53
2:B:31:PRO:O	2:B:83:HIS:HE1	1.91	0.52
1:A:270:TRP:O	1:A:271:LYS:HB2	2.10	0.52
1:D:57:GLN:NE2	1:D:57:GLN:H	2.06	0.52
1:D:57:GLN:H	1:D:57:GLN:HE21	1.56	0.52
1:A:35:HIS:CE1	1:A:37:ASN:HD22	2.27	0.52
1:D:127:MET:C	1:D:128:LYS:HG2	2.29	0.52
1:D:214:LEU:CD2	1:D:219:VAL:HG22	2.41	0.51
1:D:190:GLU:HG2	1:D:195:LEU:HD13	1.93	0.51
1:A:191:ALA:O	1:A:192:ASP:O	2.30	0.50
4:D:301:MPD:O4	4:D:301:MPD:CM	2.58	0.49
1:A:35:HIS:CE1	1:A:37:ASN:ND2	2.79	0.49
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.78	0.49
1:D:35:HIS:CE1	1:D:37:ASN:HD22	2.29	0.49
1:D:77:LEU:O	1:D:81:GLN:HG3	2.13	0.49
1:A:118:ARG:NH1	5:A:331:HOH:O	2.46	0.49
2:B:87:LYS:HG2	2:B:88:GLU:HG3	1.95	0.48
2:B:5:LYS:N	2:B:5:LYS:HD2	2.28	0.48
1:A:96:MET:HE3	1:A:112:GLN:HG2	1.95	0.48
1:D:74:ARG:NH2	5:D:512:HOH:O	2.45	0.48
1:D:114:ALA:HB2	2:E:59:TRP:CE2	2.49	0.48
1:A:192:ASP:HA	5:A:352:HOH:O	2.13	0.47
2:B:1:ASP:HA	5:B:136:HOH:O	2.15	0.47
1:D:84:TYR:OH	1:D:134:VAL:HG21	2.14	0.47
1:A:8:ILE:HG22	1:A:96:MET:HG2	1.96	0.47
1:A:256:ARG:HD2	5:A:462:HOH:O	2.14	0.47
1:A:272:LEU:C	1:A:272:LEU:CD2	2.68	0.47
1:A:8:ILE:HD11	2:B:54:SER:OG	2.15	0.46
1:D:143:LYS:O	1:D:146:GLU:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:GLU:HA	1:D:1:GLU:OE1	2.14	0.46
1:D:149:GLU:N	1:D:150:PRO:CD	2.78	0.46
1:D:126:ASP:HA	1:D:127:MET:SD	2.56	0.46
1:A:114:ALA:HB2	2:B:59:TRP:CE2	2.50	0.46
1:A:214:LEU:HD22	1:A:219:VAL:HG22	1.99	0.45
2:E:5:LYS:N	2:E:5:LYS:HD2	2.32	0.45
1:D:81:GLN:HG2	1:D:115:TYR:OH	2.16	0.44
1:D:102:LEU:HD12	1:D:102:LEU:N	2.33	0.44
1:A:111:ARG:NH2	3:C:5:GLU:OE1	2.44	0.44
1:A:158:GLU:HG2	5:A:392:HOH:O	2.18	0.43
2:B:1:ASP:CA	5:B:136:HOH:O	2.66	0.43
2:B:35:SER:HB3	2:B:82:GLU:HB2	2.00	0.43
1:A:270:TRP:CZ2	1:A:272:LEU:HB2	2.53	0.43
1:A:191:ALA:O	1:A:192:ASP:C	2.57	0.43
1:D:9:ARG:HG3	1:D:9:ARG:NH1	2.31	0.43
1:A:149:GLU:N	1:A:150:PRO:CD	2.82	0.42
1:D:103:GLU:OE1	1:D:103:GLU:CA	2.67	0.42
1:D:126:ASP:HA	1:D:127:MET:HA	1.62	0.42
2:B:83:HIS:CD2	2:B:85:THR:H	2.38	0.42
1:A:270:TRP:O	1:A:271:LYS:CG	2.67	0.42
1:D:144:TRP:HB3	1:D:149:GLU:HB2	2.01	0.42
1:D:190:GLU:CG	1:D:195:LEU:HD13	2.49	0.42
1:A:200:ARG:HG2	1:A:240:TRP:HB3	2.00	0.42
1:D:124:ASP:O	1:D:125:LYS:C	2.58	0.42
1:D:31:GLU:OE2	1:D:175:GLU:OE1	2.38	0.42
1:D:32:LEU:CD2	1:D:46:ARG:HG3	2.50	0.41
1:A:192:ASP:CA	5:A:352:HOH:O	2.68	0.41
1:A:216:ASP:HA	5:A:459:HOH:O	2.19	0.41
1:D:246:GLN:O	1:D:249:ASP:HB2	2.21	0.41
5:A:519:HOH:O	2:B:97:GLU:HG2	2.21	0.41
2:B:83:HIS:CD2	2:B:85:THR:OG1	2.64	0.41
1:A:187:TRP:CE2	2:B:97:GLU:HB3	2.57	0.40
2:E:35:SER:HB3	2:E:82:GLU:HB2	2.02	0.40
1:D:83:ARG:NH1	1:D:139:PRO:HG2	2.36	0.40
1:A:192:ASP:HB2	1:A:193:GLY:H	1.60	0.40
1:A:143:LYS:O	1:A:146:GLU:HG2	2.22	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)
5:B:160:HOH:O	5:D:480:HOH:O[2_555]	1.67	0.53

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	270/275 (98%)	262 (97%)	4 (2%)	4 (2%)	8	2
1	D	266/275 (97%)	262 (98%)	4 (2%)	0	100	100
2	B	95/101 (94%)	94 (99%)	1 (1%)	0	100	100
2	E	95/101 (94%)	94 (99%)	1 (1%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
All	All	738/768 (96%)	724 (98%)	10 (1%)	4 (0%)	25	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ASP
1	A	2	LEU
1	A	270	TRP
1	A	271	LYS

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	229/232 (99%)	217 (95%)	12 (5%)	19	8
1	D	228/232 (98%)	215 (94%)	13 (6%)	17	7
2	B	85/89 (96%)	82 (96%)	3 (4%)	31	19
2	E	85/89 (96%)	83 (98%)	2 (2%)	44	32
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	5 (71%)	2 (29%)	0	0
All	All	641/656 (98%)	609 (95%)	32 (5%)	20	9

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	142	ARG
1	A	167	ARG
1	A	175	GLU
1	A	186	VAL
1	A	192	ASP
1	A	214	LEU
1	A	216	ASP
1	A	220	ARG
1	A	240	TRP
1	A	267	LEU
1	A	272	LEU
2	B	46	GLU
2	B	52	ASP
2	B	69	PHE
1	D	1	GLU
1	D	6	ARG
1	D	12	MET
1	D	43	TYR
1	D	48	GLU
1	D	57	GLN
1	D	86	GLN
1	D	87	THR
1	D	111	ARG
1	D	125	LYS
1	D	128	LYS
1	D	189	LYS
1	D	192	ASP
2	E	52	ASP
2	E	69	PHE

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Mol	Chain	Res	Type
3	F	5	GLU
3	F	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	73	ASN
2	B	83	HIS
1	D	35	HIS
1	D	57	GLN
1	D	67	GLN
1	D	73	ASN
1	D	81	GLN
1	D	86	GLN
1	D	112	GLN
1	D	254	GLN
2	E	83	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	MPD	D	301	-	7,7,7	0.30	0	9,10,10	0.23	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	MPD	D	301	-	-	0/5/5/5	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	MPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/275 (98%)	0.10	21 (7%) 21 18	8, 19, 45, 100	0
1	D	270/275 (98%)	0.06	13 (4%) 36 34	8, 20, 45, 106	0
2	B	97/101 (96%)	-0.03	3 (3%) 51 49	10, 21, 36, 53	0
2	E	97/101 (96%)	-0.08	4 (4%) 42 39	9, 18, 40, 59	0
3	C	8/8 (100%)	-0.49	0 100 100	13, 17, 20, 24	0
3	F	8/8 (100%)	-0.42	0 100 100	13, 16, 23, 29	0
All	All	752/768 (97%)	0.03	41 (5%) 32 29	8, 19, 43, 106	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	MET	7.6
1	D	126	ASP	5.7
1	A	272	LEU	5.4
1	A	192	ASP	4.7
2	E	52	ASP	4.2
1	A	271	LYS	4.2
1	A	1	GLU	4.2
1	D	125	LYS	4.1
1	D	88	GLY	4.0
1	D	124	ASP	3.9
1	A	191	ALA	3.7
1	A	190	GLU	3.6
1	A	104	ASP	3.5
1	D	87	THR	3.3
1	A	248	GLY	3.3
1	D	103	GLU	3.3
1	D	1	GLU	3.2
1	A	247	PRO	3.1
1	A	194	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	263	PRO	2.9
1	D	106	THR	2.9
1	A	222	GLN	2.9
1	A	240	TRP	2.9
1	A	187	TRP	2.8
1	D	146	GLU	2.8
2	E	51	SER	2.7
1	A	103	GLU	2.7
1	D	107	ILE	2.7
1	A	221	GLY	2.6
2	B	16	ALA	2.6
1	D	82	ARG	2.5
1	A	270	TRP	2.4
1	D	223	ASP	2.3
2	E	50	TYR	2.2
1	A	124	ASP	2.2
2	B	15	SER	2.2
2	E	87	LYS	2.1
2	B	43	VAL	2.1
1	A	216	ASP	2.0
1	A	2	LEU	2.0
1	A	189	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 monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
4	MPD	D	301	8/8	0.89	0.10	6,15,20,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.