



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:12 am BST

PDB ID : 6CL2
Title : Caspase-7 in complex with Ac-ATS009-KE
Authors : Solania, A.T.; Gonzalez-Paez, G.E.; Wolan, D.W.
Deposited on : 2018-03-01
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

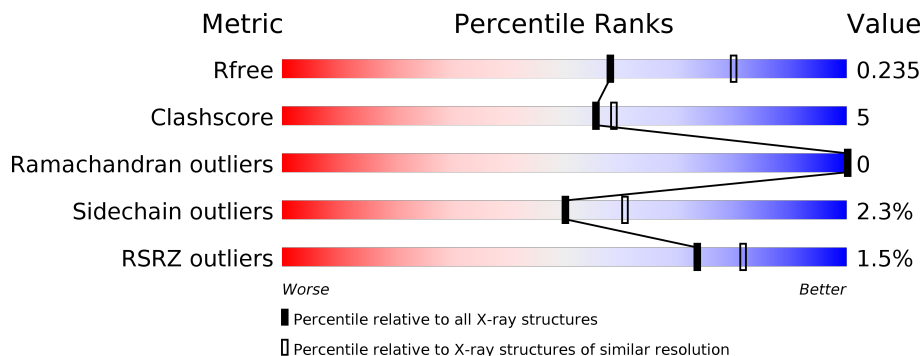
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	198	 1% 62% 9% 29%
1	C	198	 63% 7% 29%
2	B	113	 3% 66% 14% 19%
2	D	113	 2% 69% 12% 19%
3	E	6	 17% 67% 33%
3	F	6	 67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3829 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 Caspase-7 subunit p20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	140	1081	678	184	208	11	0	0	0
1	C	140	1093	686	186	209	12	0	1	0

- Molecule 2 is a protein called Caspase-7 subunit p11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	91	737	476	124	133	4	0	0	0
2	D	91	727	472	122	129	4	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	304	LEU	-	expression tag	UNP P55210
B	305	GLU	-	expression tag	UNP P55210
B	306	HIS	-	expression tag	UNP P55210
B	307	HIS	-	expression tag	UNP P55210
B	308	HIS	-	expression tag	UNP P55210
B	309	HIS	-	expression tag	UNP P55210
B	310	HIS	-	expression tag	UNP P55210
B	311	HIS	-	expression tag	UNP P55210
D	304	LEU	-	expression tag	UNP P55210
D	305	GLU	-	expression tag	UNP P55210
D	306	HIS	-	expression tag	UNP P55210
D	307	HIS	-	expression tag	UNP P55210
D	308	HIS	-	expression tag	UNP P55210
D	309	HIS	-	expression tag	UNP P55210
D	310	HIS	-	expression tag	UNP P55210
D	311	HIS	-	expression tag	UNP P55210

- Molecule 3 is a protein called ACE-1MH-ASP-PF5-PHE-1U8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
3	E	6	Total 58	C 37	F 5	N 6	O 10	0	0	0
3	F	6	Total 58	C 37	F 5	N 6	O 10	0	0	0

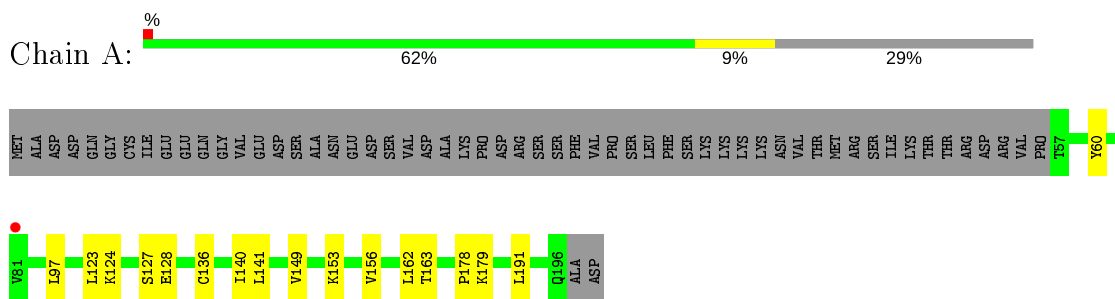
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	17	Total 17	O 17	0	0
4	C	29	Total 29	O 29	0	0
4	D	16	Total 16	O 16	0	0
4	E	1	Total 1	O 1	0	0

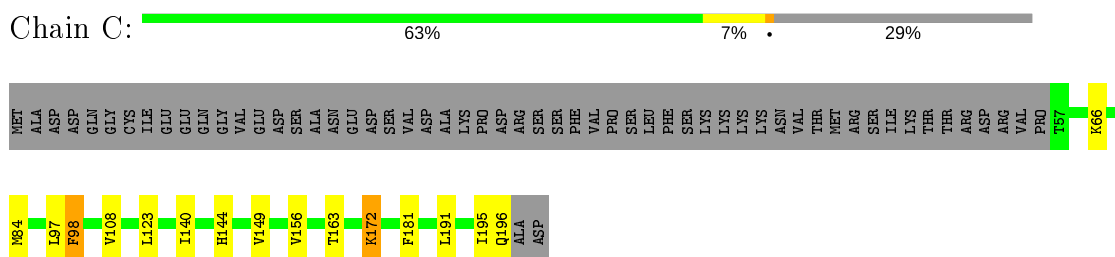
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

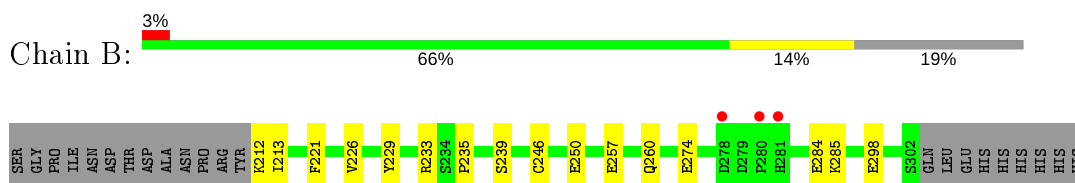
- Molecule 1: Caspase-7 subunit p20



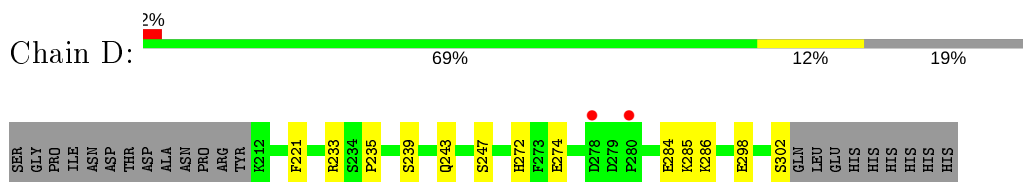
- Molecule 1: Caspase-7 subunit p20



- Molecule 2: Caspase-7 subunit p11

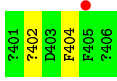


- Molecule 2: Caspase-7 subunit p11



- Molecule 3: ACE-1MH-ASP-PF5-PHE-1U8





- Molecule 3: ACE-1MH-ASP-PF5-PHE-1U8

Chain F:  67% 33%

A horizontal bar chart for Chain F. The bar is divided into two segments: a green segment on the left representing 67% and a yellow segment on the right representing 33%.



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.31Å 88.31Å 186.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.23 – 2.35 48.23 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.23-2.35) 99.8 (48.23-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, R_{free}	0.195 , 0.236 0.195 , 0.235	Depositor DCC
R_{free} test set	1922 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtrriage
Anisotropy	0.587	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3829	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 1MH, PF5, ACE, 1U8

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	0.41	0/1098	0.55	0/1477
1	C	0.44	0/1110	0.59	0/1491
2	B	0.35	0/759	0.51	0/1029
2	D	0.40	0/749	0.57	0/1016
3	E	0.40	0/18	0.26	0/21
3	F	0.55	0/18	0.39	0/21
All	All	0.41	0/3752	0.56	0/5055

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	1081	0	1036	9	0
1	C	1093	0	1061	13	0
2	B	737	0	704	11	0
2	D	727	0	696	10	0
3	E	58	0	29	2	0
3	F	58	0	29	2	0
4	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	17	0	0	0	0
4	C	29	0	0	0	0
4	D	16	0	0	1	0
4	E	1	0	0	0	0
All	All	3829	0	3555	37	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 5.

All (37) 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:191:LEU:HD22	2:B:285:LYS:HG3	1.72	0.70
1:C:149:VAL:HG22	1:C:156:VAL:HG22	1.73	0.69
2:D:233:ARG:HA	2:D:239:SER:HA	1.80	0.63
2:B:246:CYS:O	2:B:250:GLU:HG3	1.98	0.63
1:A:163:THR:HG21	2:B:221:PHE:HE2	1.65	0.62
1:C:98:PHE:HB2	1:C:108:VAL:HG11	1.81	0.62
1:C:97:LEU:HD13	1:C:140:ILE:HG21	1.84	0.60
2:D:274:GLU:HG2	2:D:284:GLU:HA	1.84	0.59
2:B:233:ARG:HA	2:B:239:SER:HA	1.84	0.59
2:D:239:SER:O	2:D:243:GLN:HG2	2.04	0.57
2:B:212:LYS:HA	1:C:196:GLN:HA	1.88	0.56
1:A:149:VAL:CG1	1:A:156:VAL:HB	2.37	0.55
1:C:191:LEU:HD22	2:D:285:LYS:HG3	1.89	0.53
1:C:84:MET:HB3	1:C:144:HIS:CD2	2.46	0.51
2:D:286:LYS:HD3	4:D:409:HOH:O	2.11	0.51
1:C:163:THR:HG21	2:D:221:PHE:CE2	2.47	0.50
1:A:149:VAL:HG13	1:A:156:VAL:HB	1.92	0.49
1:C:163:THR:HG21	2:D:221:PHE:HE2	1.80	0.47
3:E:402:1MH:H4	3:E:402:1MH:H10	1.45	0.47
1:A:123:LEU:HD22	1:A:162:LEU:HB3	1.97	0.47
1:C:172:LYS:HE2	1:C:172:LYS:H	1.82	0.45
1:C:172:LYS:CE	1:C:172:LYS:H	2.29	0.45
2:D:235:PRO:HG3	3:F:404:PF5:FD2	2.06	0.45
2:B:235:PRO:HG3	3:E:404:PF5:FE2	2.07	0.45
1:A:124:LYS:NZ	1:A:128:GLU:OE2	2.46	0.45
1:A:60:TYR:CD1	1:A:178:PRO:HD3	2.51	0.45
2:D:272:HIS:O	2:D:272:HIS:ND1	2.49	0.45
1:C:163:THR:HG22	1:C:181:PHE:CE2	2.52	0.44
2:B:213:ILE:N	1:C:195:ILE:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:CYS:HB3	1:A:178:PRO:HG2	2.01	0.42
1:C:123:LEU:HD23	1:C:123:LEU:HA	1.80	0.42
2:B:260:GLN:NE2	2:D:298:GLU:OE2	2.34	0.42
2:B:257:GLU:HG3	2:B:298:GLU:HB3	2.02	0.42
2:B:226:VAL:HG23	2:B:229:TYR:CD1	2.56	0.41
2:B:274:GLU:HG2	2:B:284:GLU:HA	2.03	0.41
3:F:402:1MH:H4	3:F:402:1MH:H10	1.79	0.41
1:A:97:LEU:HD13	1:A:140:ILE:HG21	2.03	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	138/198 (70%)	135 (98%)	3 (2%)	0	100	100
1	C	139/198 (70%)	136 (98%)	3 (2%)	0	100	100
2	B	89/113 (79%)	89 (100%)	0	0	100	100
2	D	89/113 (79%)	84 (94%)	5 (6%)	0	100	100
3	E	2/6 (33%)	2 (100%)	0	0	100	100
3	F	2/6 (33%)	2 (100%)	0	0	100	100
All	All	459/634 (72%)	448 (98%)	11 (2%)	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	115/172 (67%)	111 (96%)	4 (4%)	36	44
1	C	118/172 (69%)	115 (98%)	3 (2%)	47	58
2	B	80/103 (78%)	80 (100%)	0	100	100
2	D	78/103 (76%)	76 (97%)	2 (3%)	46	56
3	E	2/2 (100%)	2 (100%)	0	100	100
3	F	2/2 (100%)	2 (100%)	0	100	100
All	All	395/554 (71%)	386 (98%)	9 (2%)	50	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	141	LEU
1	A	153	LYS
1	A	179	LYS
1	C	66	LYS
1	C	98	PHE
1	C	172	LYS
2	D	247	SER
2	D	302	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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$
3	1U8	E	406	1,3	4,8,20	0.85	0	2,10,27	0.60	0
3	1MH	E	402	3	10,11,12	0.88	0	10,13,15	1.54	3 (30%)
3	PF5	E	404	3	15,16,17	1.00	0	19,23,25	1.29	4 (21%)
3	PF5	F	404	3	15,16,17	0.86	0	19,23,25	1.47	4 (21%)
3	1MH	F	402	3	10,11,12	0.90	0	10,13,15	1.50	3 (30%)
3	1U8	F	406	1,3	4,8,20	0.72	0	2,10,27	0.56	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
3	1U8	E	406	1,3	-	0/5/8/17	-
3	1MH	E	402	3	-	5/5/6/8	0/1/1/1
3	PF5	E	404	3	-	0/5/6/8	0/1/1/1
3	PF5	F	404	3	-	0/5/6/8	0/1/1/1
3	1MH	F	402	3	-	2/5/6/8	0/1/1/1
3	1U8	F	406	1,3	-	0/5/8/17	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	F	404	PF5	CD2-CG-CD1	4.16	120.82	115.90
3	E	404	PF5	CD2-CG-CD1	3.69	120.27	115.90
3	E	402	1MH	C6-CB-CA	-2.99	108.05	114.10
3	F	402	1MH	C6-CB-CA	-2.89	108.24	114.10
3	F	404	PF5	CG-CD2-CE2	-2.49	119.42	122.37
3	F	404	PF5	CG-CD1-CE1	-2.44	119.48	122.37
3	F	404	PF5	CB-CG-CD1	-2.34	118.83	122.03
3	E	404	PF5	CB-CG-CD1	-2.24	118.97	122.03
3	E	404	PF5	CG-CD2-CE2	-2.18	119.80	122.37
3	E	404	PF5	CG-CD1-CE1	-2.15	119.83	122.37
3	F	402	1MH	C11-C6-C7	2.14	120.25	117.10
3	E	402	1MH	C9-N8-C7	2.12	120.51	116.85
3	E	402	1MH	C6-C7-N8	-2.05	119.70	123.72
3	F	402	1MH	C6-C7-N8	-2.00	119.81	123.72

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	402	1MH	O-C-CA-CB
3	E	402	1MH	C-CA-CB-C6
3	E	402	1MH	C11-C6-CB-CA
3	E	402	1MH	C7-C6-CB-CA
3	E	402	1MH	N-CA-CB-C6
3	F	402	1MH	C11-C6-CB-CA
3	F	402	1MH	C7-C6-CB-CA

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	1MH	1	0
3	E	404	PF5	1	0
3	F	404	PF5	1	0
3	F	402	1MH	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	140/198 (70%)	-0.28	1 (0%) 87 92	35, 47, 61, 75	0
1	C	140/198 (70%)	-0.07	0 100 100	32, 39, 55, 70	0
2	B	91/113 (80%)	-0.11	3 (3%) 46 59	32, 44, 76, 84	0
2	D	91/113 (80%)	-0.16	2 (2%) 62 72	33, 42, 73, 88	0
3	E	2/6 (33%)	1.20	1 (50%) 0 0	61, 61, 61, 67	0
3	F	2/6 (33%)	-0.38	0 100 100	52, 52, 52, 60	0
All	All	466/634 (73%)	-0.16	7 (1%) 73 81	32, 43, 64, 88	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	278	ASP	3.1
2	D	278	ASP	3.1
2	D	280	PRO	3.0
1	A	81	VAL	2.3
2	B	280	PRO	2.2
2	B	281	HIS	2.0
3	E	405	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	1MH	E	402	11/12	0.74	0.29	74,84,89,92	0
3	1MH	F	402	11/12	0.77	0.32	65,80,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PF5	E	404	16/17	0.92	0.23	55,76,91,95	0
3	PF5	F	404	16/17	0.94	0.16	48,62,81,86	0
3	1U8	E	406	9/20	0.97	0.12	42,48,53,53	0
3	1U8	F	406	9/20	0.97	0.09	36,39,41,42	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.