



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:02 PM UTC

PDB ID : 5HGA / pdb_00005hga
Title : HLA*A2402 complex with HIV nef138 Y2F-8mer mutant epitope
Authors : Shi, Y.; Qi, J.; Gao, G.F.
Deposited on : 2016-01-08
Resolution : 2.20 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

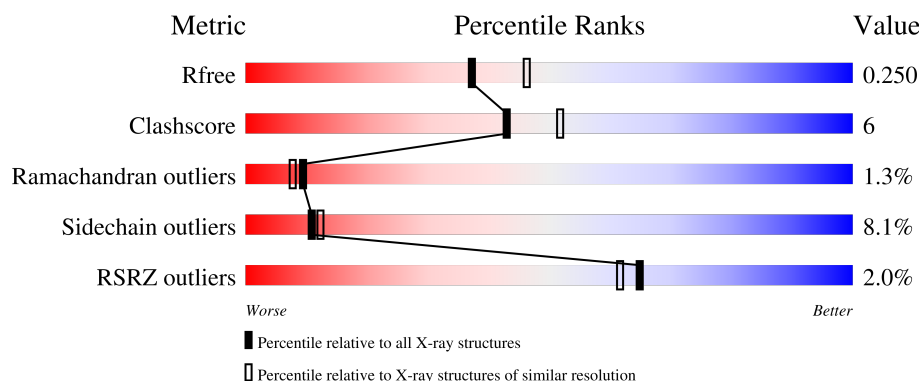
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	% 80% 17% .
1	D	275	% 80% 18% .
2	B	100	6% 80% 16% . .
2	E	100	3% 80% 15% . .
3	C	8	50% 38% 12%

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Mol	Chain	Length	Quality of chain
3	F	8	 62% 25% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6416 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-24 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2221	1382	403	426	10			
1	D	274	Total	C	N	O	S	0	0	0
			2221	1382	403	426	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P05534
D	0	MET	-	initiating methionine	UNP P05534

- 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
			836	533	141	158	4			
2	E	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called 8-mer from Protein Nef.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			74	52	12	10			
3	F	8	Total	C	N	O	0	0	0
			74	52	12	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	PHE	TYR	engineered mutation	UNP P18801
F	2	PHE	TYR	engineered mutation	UNP P18801

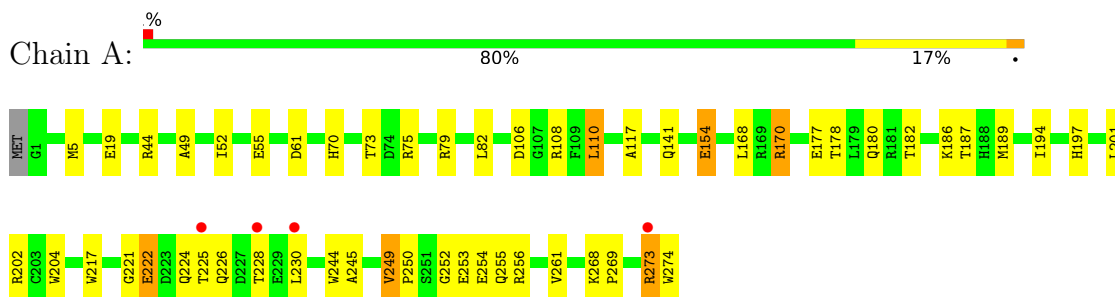
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 62 62	0	0
4	B	14	Total O 14 14	0	0
4	C	8	Total O 8 8	0	0
4	D	53	Total O 53 53	0	0
4	E	14	Total O 14 14	0	0
4	F	3	Total O 3 3	0	0

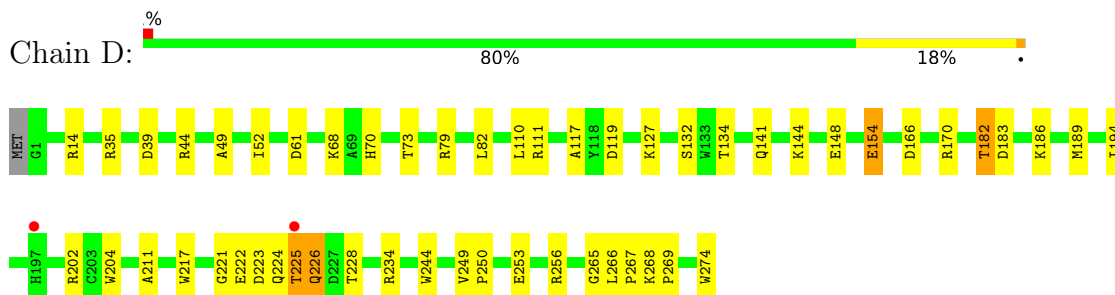
3 Residue-property plots [i](#)

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.

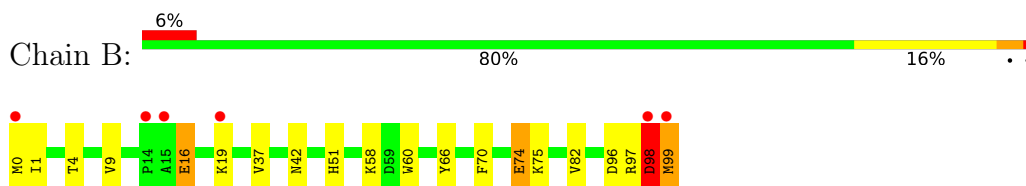
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



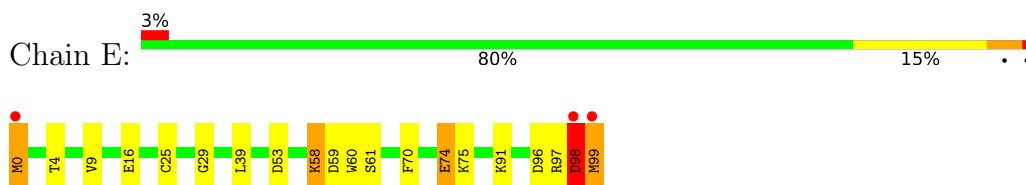
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



- Molecule 2: Beta-2-microglobulin

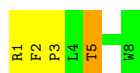


- Molecule 2: Beta-2-microglobulin



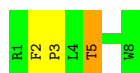
- Molecule 3: 8-mer from Protein Nef

Chain C:  50% 38% 12%



● Molecule 3: 8-mer from Protein Nef

Chain F:  62% 25% 12%



GLOBAL-STATISTICS INFOmissingINFO

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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	0.40	0/2281	0.78	0/3092
1	D	0.40	0/2281	0.78	0/3092
2	B	0.34	0/859	0.73	1/1162 (0.1%)
2	E	0.37	0/859	0.72	0/1162
3	C	0.37	0/78	0.84	0/104
3	F	0.32	0/78	0.82	0/104
All	All	0.39	0/6436	0.77	1/8716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ILE	N-CA-C	5.21	117.90	110.09

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2221	0	2082	29	0
1	D	2221	0	2082	28	1
2	B	836	0	803	10	0
2	E	836	0	803	12	0
3	C	74	0	71	4	0
3	F	74	0	71	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	62	0	0	3	0
4	B	14	0	0	2	1
4	C	8	0	0	2	0
4	D	53	0	0	4	0
4	E	14	0	0	1	0
4	F	3	0	0	0	0
All	All	6416	0	5912	76	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 6.

All (76) 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:252:GLY:O	4:A:301:HOH:O	1.99	0.79
2:B:42:ASN:O	4:B:101:HOH:O	2.07	0.72
2:B:19:LYS:O	4:B:102:HOH:O	2.08	0.71
1:D:211:ALA:O	4:D:301:HOH:O	2.12	0.68
1:A:177:GLU:HG2	1:A:178:THR:HG23	1.78	0.66
1:D:154:GLU:OE2	4:D:302:HOH:O	2.15	0.64
1:D:144:LYS:NZ	1:D:148:GLU:OE2	2.31	0.64
3:C:1:ARG:NH1	4:C:101:HOH:O	2.25	0.64
2:B:96:ASP:O	2:B:98:ASP:N	2.31	0.63
1:D:189:MET:HE3	1:D:217:TRP:HH2	1.65	0.61
1:A:222:GLU:O	1:A:224:GLN:NE2	2.31	0.61
1:A:106:ASP:OD1	4:A:302:HOH:O	2.17	0.58
1:D:111:ARG:NH2	4:D:303:HOH:O	2.27	0.57
2:E:96:ASP:O	2:E:98:ASP:N	2.38	0.56
2:E:99:MET:HB2	4:E:104:HOH:O	2.04	0.56
1:D:44:ARG:NH2	1:D:61:ASP:OD1	2.38	0.55
1:A:255:GLN:O	1:A:273:ARG:NH1	2.34	0.55
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.42	0.55
1:D:234:ARG:HH12	2:E:99:MET:HE2	1.72	0.54
1:D:268:LYS:HG3	1:D:269:PRO:HD2	1.90	0.54
1:A:230:LEU:HD13	1:A:245:ALA:HB2	1.89	0.53
1:D:127:LYS:NZ	1:D:134:THR:OG1	2.30	0.53
1:A:268:LYS:HG3	1:A:269:PRO:HD2	1.91	0.52
1:A:106:ASP:OD1	1:A:108:ARG:HD3	2.12	0.51
2:B:16:GLU:OE1	2:E:59:ASP:HB3	2.12	0.50
1:D:189:MET:HE1	1:D:274:TRP:HB2	1.93	0.49
1:D:119:ASP:HB3	2:E:0:MET:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:OD2	1:A:108:ARG:NH1	2.44	0.48
1:A:189:MET:HE1	1:A:274:TRP:HB2	1.94	0.48
3:C:1:ARG:NH1	4:C:102:HOH:O	2.32	0.48
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.48	0.48
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.96	0.48
1:D:202:ARG:HG2	1:D:204:TRP:NE1	2.29	0.47
1:A:19:GLU:OE1	1:A:75:ARG:HD3	2.15	0.46
1:A:224:GLN:O	1:A:228:THR:HG23	2.15	0.46
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.50	0.46
1:D:234:ARG:NH1	2:E:99:MET:HE2	2.30	0.46
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.97	0.46
1:A:70:HIS:ND1	3:C:5:THR:HG21	2.31	0.46
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.50	0.46
1:A:189:MET:HE3	1:A:217:TRP:HH2	1.81	0.46
2:B:16:GLU:HG3	2:B:19:LYS:HB2	1.98	0.46
1:D:224:GLN:O	1:D:228:THR:HG23	2.16	0.46
1:D:223:ASP:HB3	1:D:225:THR:HG23	1.98	0.46
2:B:74:GLU:OE2	2:B:75:LYS:N	2.49	0.45
2:E:58:LYS:HE3	2:E:58:LYS:H	1.82	0.45
2:E:74:GLU:OE2	2:E:75:LYS:N	2.49	0.44
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.50	0.44
1:A:273:ARG:HG3	1:A:274:TRP:N	2.33	0.44
1:D:49:ALA:O	1:D:52:ILE:HG22	2.18	0.44
2:B:99:MET:HE3	2:B:99:MET:HB3	1.72	0.43
3:F:2:PHE:CG	3:F:3:PRO:HD2	2.54	0.43
1:D:44:ARG:NH2	1:D:61:ASP:HA	2.34	0.43
1:A:154:GLU:OE2	4:A:303:HOH:O	2.21	0.43
1:D:14:ARG:HH22	1:D:39:ASP:CG	2.26	0.43
1:A:187:THR:HG21	1:A:261:VAL:HG21	2.01	0.43
1:A:154:GLU:H	1:A:154:GLU:HG2	1.59	0.42
1:D:35:ARG:HD3	2:E:53:ASP:OD2	2.19	0.42
1:D:154:GLU:HB3	4:D:308:HOH:O	2.18	0.42
1:D:250:PRO:HB2	1:D:253:GLU:HG3	2.01	0.42
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.35	0.42
1:D:182:THR:HG21	1:D:265:GLY:HA2	2.01	0.42
1:D:224:GLN:C	1:D:226:GLN:H	2.27	0.42
2:E:29:GLY:HA2	2:E:61:SER:OG	2.20	0.42
1:D:70:HIS:ND1	3:F:5:THR:HG21	2.35	0.42
1:A:250:PRO:HB2	1:A:253:GLU:HG3	2.01	0.42
3:C:2:PHE:CG	3:C:3:PRO:HD2	2.54	0.42
2:B:37:VAL:HG22	2:B:82:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:O	1:A:52:ILE:HG22	2.20	0.41
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.47	0.41
1:A:249:VAL:HG21	1:A:254:GLU:HG3	2.02	0.41
1:D:127:LYS:HD2	1:D:132:SER:OG	2.21	0.41
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.88	0.41
1:D:266:LEU:HA	1:D:267:PRO:HD2	1.91	0.41
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.56	0.41
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.80	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:166:ASP:OD1	4:B:101:HOH:O[4_445]	2.18	0.02

4.3 Torsion angles ⓘ

4.3.1 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	154/275 (56%)	148 (96%)	4 (3%)	2 (1%)	9	8
1	D	272/275 (99%)	264 (97%)	6 (2%)	2 (1%)	18	19
2	B	98/100 (98%)	95 (97%)	1 (1%)	2 (2%)	6	4
2	E	98/100 (98%)	95 (97%)	1 (1%)	2 (2%)	6	4
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
All	All	634/766 (83%)	614 (97%)	12 (2%)	8 (1%)	9	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	ASP
2	E	98	ASP
1	A	225	THR
2	B	97	ARG
1	D	225	THR
1	A	221	GLY
1	D	221	GLY
2	E	97	ARG

4.3.2 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	230/231 (100%)	213 (93%)	17 (7%)	13	14
1	D	230/231 (100%)	214 (93%)	16 (7%)	14	16
2	B	95/95 (100%)	86 (90%)	9 (10%)	8	8
2	E	95/95 (100%)	85 (90%)	10 (10%)	6	6
3	C	7/7 (100%)	6 (86%)	1 (14%)	3	3
3	F	7/7 (100%)	6 (86%)	1 (14%)	3	3
All	All	664/666 (100%)	610 (92%)	54 (8%)	11	12

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	79	ARG
1	A	82	LEU
1	A	110	LEU
1	A	141	GLN
1	A	154	GLU
1	A	170	ARG
1	A	180	GLN
1	A	182	THR
1	A	186	LYS
1	A	194	ILE

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Mol	Chain	Res	Type
1	A	197	HIS
1	A	222	GLU
1	A	226	GLN
1	A	249	VAL
1	A	256	ARG
1	A	273	ARG
2	B	0	MET
2	B	4	THR
2	B	9	VAL
2	B	16	GLU
2	B	58	LYS
2	B	70	PHE
2	B	74	GLU
2	B	98	ASP
2	B	99	MET
3	C	5	THR
1	D	68	LYS
1	D	73	THR
1	D	79	ARG
1	D	82	LEU
1	D	110	LEU
1	D	141	GLN
1	D	154	GLU
1	D	170	ARG
1	D	182	THR
1	D	183	ASP
1	D	186	LYS
1	D	194	ILE
1	D	222	GLU
1	D	226	GLN
1	D	249	VAL
1	D	256	ARG
2	E	0	MET
2	E	4	THR
2	E	9	VAL
2	E	16	GLU
2	E	58	LYS
2	E	70	PHE
2	E	74	GLU
2	E	91	LYS
2	E	98	ASP
2	E	99	MET

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Mol	Chain	Res	Type
3	F	5	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	141	GLN
1	A	262	GLN
2	B	13	HIS
2	E	13	HIS

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

5.1 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	274/275 (99%)	-0.07	4 (1%) 72 69	15, 31, 68, 106	0
1	D	274/275 (99%)	-0.02	2 (0%) 84 82	17, 33, 64, 85	0
2	B	100/100 (100%)	0.25	6 (6%) 27 24	18, 37, 67, 92	0
2	E	100/100 (100%)	0.04	3 (3%) 52 49	17, 35, 68, 83	0
3	C	8/8 (100%)	-0.24	0 100 100	20, 22, 24, 38	0
3	F	8/8 (100%)	-0.03	0 100 100	21, 25, 29, 42	0
All	All	764/766 (99%)	0.00	15 (1%) 65 62	15, 32, 68, 106	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	0	MET	4.6
2	E	99	MET	4.0
2	B	99	MET	3.6
2	B	0	MET	3.2
1	D	225	THR	3.1
2	E	98	ASP	3.1
2	B	98	ASP	2.8
1	A	230	LEU	2.6
1	A	228	THR	2.4
1	A	225	THR	2.4
1	A	273	ARG	2.3
2	B	15	ALA	2.2
1	D	197	HIS	2.1
2	B	19	LYS	2.1
2	B	14	PRO	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.