



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:28 AM UTC

PDB ID : 3O6F / pdb_00003o6f
Title : Crystal structure of a human autoimmune TCR MS2-3C8 bound to MHC class II self-ligand MBP/HLA-DR4
Authors : Yin, Y.; Li, Y.; Martin, R.; Mariuzza, R.A.
Deposited on : 2010-07-29
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

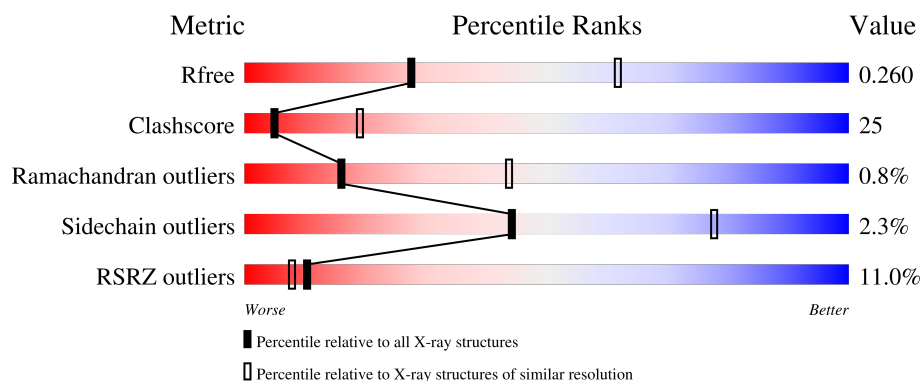
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	182	8% 51% 44% ..
1	E	182	5% 66% 31% ..
2	B	221	6% 48% 37% . 12%
2	F	221	6% 60% 31% 5% 5%
3	C	206	17% 62% 28% . 7%

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Mol	Chain	Length	Quality of chain
3	G	206	21% 54% 35% 9%
4	D	245	5% 58% 40%
4	H	245	17% 42% 55%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12887 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1446	940	232	269	5			
1	E	179	Total	C	N	O	S	0	0	0
			1456	947	237	267	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1578	1001	271	301	5			
2	F	210	Total	C	N	O	S	0	0	0
			1671	1054	294	318	5			

- Molecule 3 is a protein called T-cell receptor alpha chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	191	Total	C	N	O	S	4	0	0
			1441	897	241	296	7			
3	G	188	Total	C	N	O	S	0	0	0
			1448	902	247	291	8			

- Molecule 4 is a protein called T-cell receptor beta-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1919	1210	327	374	8			
4	H	243	Total	C	N	O	S	0	0	0
			1901	1201	324	369	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	189	SER	CYS	engineered mutation	UNP A0A5B9
H	189	SER	CYS	engineered mutation	UNP A0A5B9

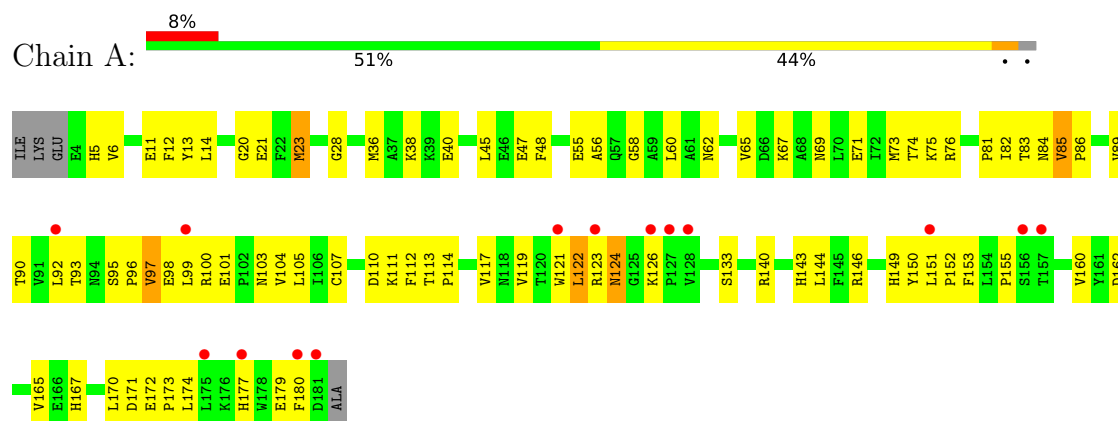
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	3	Total O 3 3	0	0
5	C	8	Total O 8 8	0	0
5	D	4	Total O 4 4	0	0
5	E	1	Total O 1 1	0	0
5	F	4	Total O 4 4	0	0
5	G	5	Total O 5 5	0	0

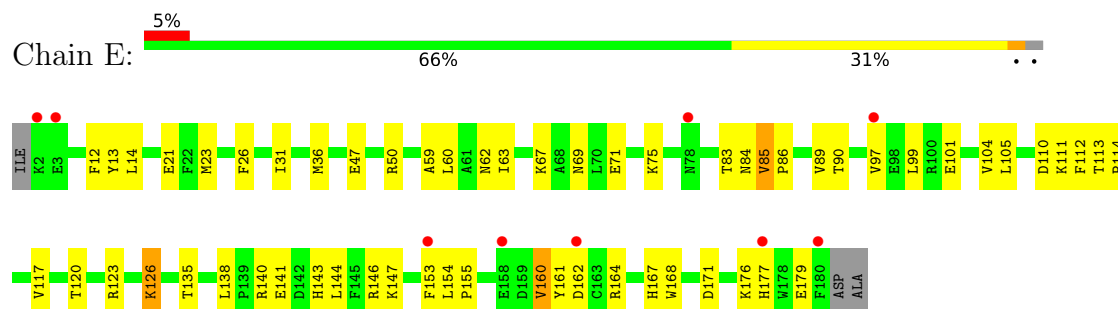
3 Residue-property plots [i](#)

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.

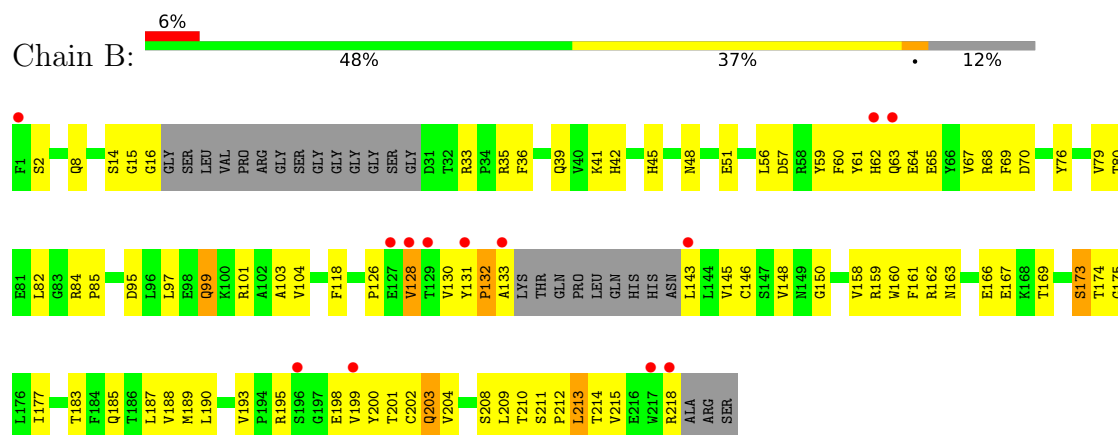
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

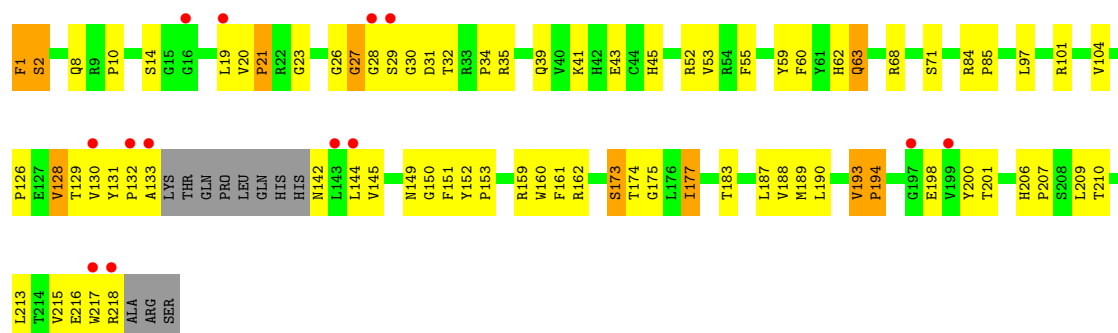


- Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain



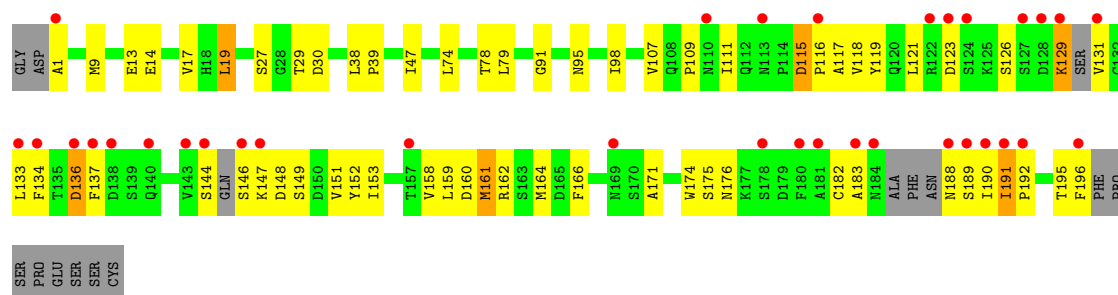
- Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain

Chain F: 



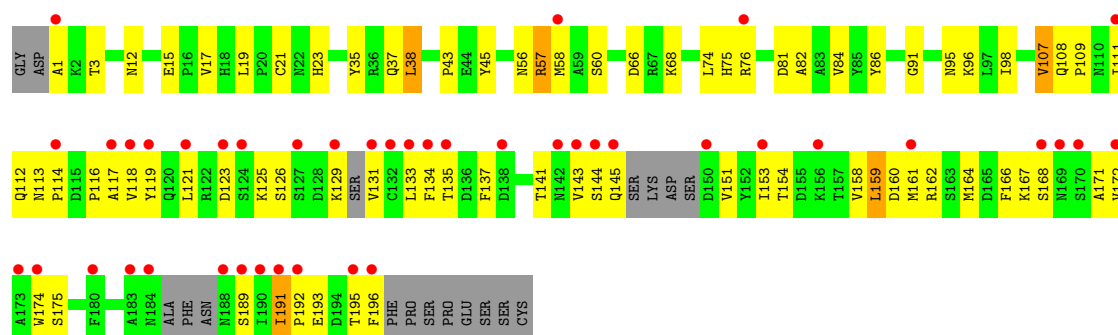
- Molecule 3: T-cell receptor alpha chain C region

Chain C: 



- Molecule 3: T-cell receptor alpha chain C region

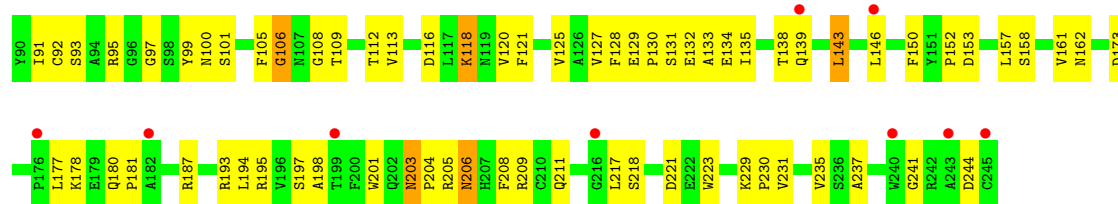
Chain G: 



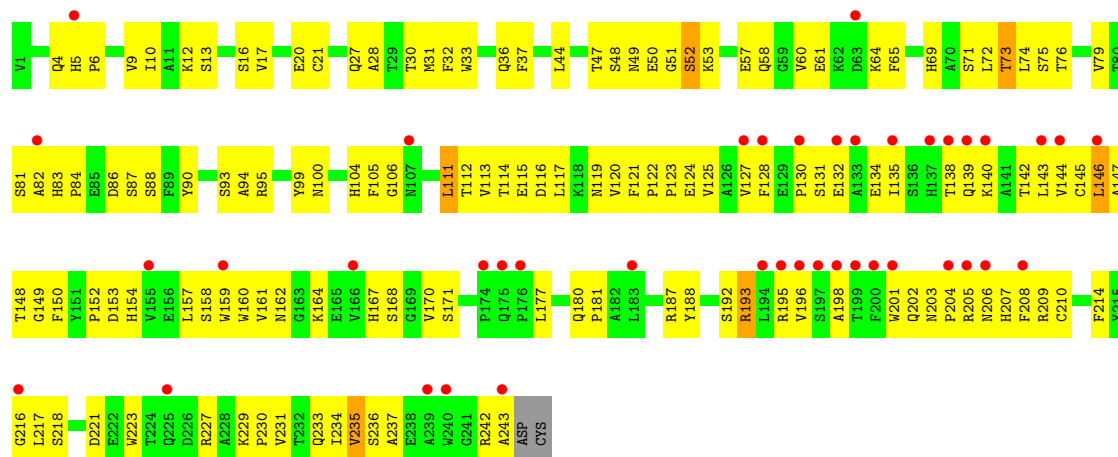
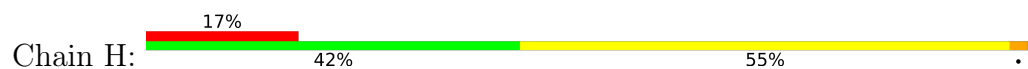
- Molecule 4: T-cell receptor beta-1 chain C region

Chain D: 





● Molecule 4: T-cell receptor beta-1 chain C region



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.48Å 218.40Å 98.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.80 49.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.20-2.80) 99.8 (49.20-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.239 , 0.279 (Not available) , 0.260	Depositor DCC
R_{free} test set	2782 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12887	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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](#)

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	0.58	0/1491	1.02	12/2036 (0.6%)
1	E	0.62	0/1501	1.00	9/2048 (0.4%)
2	B	0.62	0/1622	1.03	2/2204 (0.1%)
2	F	0.74	0/1717	1.04	8/2330 (0.3%)
3	C	0.68	0/1469	1.09	7/2005 (0.3%)
3	G	0.60	0/1476	1.00	9/2008 (0.4%)
4	D	0.58	0/1972	1.01	12/2690 (0.4%)
4	H	0.55	0/1954	1.01	7/2666 (0.3%)
All	All	0.62	0/13202	1.02	66/17987 (0.4%)

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
2	F	0	1

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	193	VAL	CA-C-N	9.14	131.27	119.84
2	F	193	VAL	C-N-CA	9.14	131.27	119.84
1	E	85	VAL	CA-C-N	7.88	125.41	119.66
1	E	85	VAL	C-N-CA	7.88	125.41	119.66
3	C	115	ASP	CA-C-N	7.29	127.34	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	68	ARG	Sidechain

5.2 Too-close contacts

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	1446	0	1370	90	0
1	E	1456	0	1393	51	0
2	B	1578	0	1451	88	0
2	F	1671	0	1552	73	0
3	C	1441	0	1333	71	0
3	G	1448	0	1377	74	0
4	D	1919	0	1809	113	0
4	H	1901	0	1794	145	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	8	0	0	0	0
5	D	4	0	0	0	0
5	E	1	0	0	0	0
5	F	4	0	0	3	0
5	G	5	0	0	1	0
All	All	12887	0	12079	626	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 25.

The worst 5 of 626 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:D:135:ILE:HD11	4:D:198:ALA:CB	1.58	1.30
3:C:121:LEU:CD2	4:D:131:SER:N	2.08	1.17
4:D:128:PHE:CE2	4:D:146:LEU:HD12	1.80	1.16
4:D:135:ILE:HD11	4:D:198:ALA:HB2	1.17	1.15
3:C:121:LEU:HD21	4:D:131:SER:H	1.16	1.09

There are no symmetry-related clashes.

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	176/182 (97%)	160 (91%)	15 (8%)	1 (1%)	21	51
1	E	177/182 (97%)	164 (93%)	13 (7%)	0	100	100
2	B	189/221 (86%)	176 (93%)	11 (6%)	2 (1%)	11	36
2	F	206/221 (93%)	185 (90%)	17 (8%)	4 (2%)	6	22
3	C	183/206 (89%)	162 (88%)	20 (11%)	1 (0%)	24	55
3	G	180/206 (87%)	154 (86%)	25 (14%)	1 (1%)	21	51
4	D	243/245 (99%)	225 (93%)	18 (7%)	0	100	100
4	H	241/245 (98%)	210 (87%)	28 (12%)	3 (1%)	10	34
All	All	1595/1708 (93%)	1436 (90%)	147 (9%)	12 (1%)	16	44

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	2	SER
4	H	235	VAL
2	B	132	PRO
2	B	2	SER
4	H	146	LEU

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	159/166 (96%)	156 (98%)	3 (2%)	50	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	160/166 (96%)	158 (99%)	2 (1%)	61	86
2	B	167/189 (88%)	164 (98%)	3 (2%)	51	82
2	F	176/189 (93%)	172 (98%)	4 (2%)	44	78
3	C	159/183 (87%)	155 (98%)	4 (2%)	42	76
3	G	163/183 (89%)	157 (96%)	6 (4%)	30	65
4	D	212/216 (98%)	205 (97%)	7 (3%)	33	69
4	H	209/216 (97%)	205 (98%)	4 (2%)	50	81
All	All	1405/1508 (93%)	1372 (98%)	33 (2%)	44	78

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	159	LEU
4	H	53	LYS
4	H	193	ARG
4	D	143	LEU
4	D	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	233	GLN
4	H	49	ASN
1	E	143	HIS
3	G	75	HIS
1	E	84	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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	178/182 (97%)	0.55	14 (7%) 18 13	32, 66, 117, 124	0
1	E	179/182 (98%)	0.33	9 (5%) 34 26	27, 51, 98, 108	0
2	B	195/221 (88%)	0.29	13 (6%) 24 17	29, 54, 93, 133	0
2	F	210/221 (95%)	0.14	13 (6%) 26 20	26, 48, 93, 116	0
3	C	191/206 (92%)	0.68	34 (17%) 4 3	24, 50, 128, 139	1 (0%)
3	G	188/206 (91%)	0.89	43 (22%) 2 1	28, 68, 137, 147	0
4	D	245/245 (100%)	0.37	12 (4%) 35 27	34, 57, 95, 125	0
4	H	243/245 (99%)	1.16	41 (16%) 4 3	30, 92, 128, 143	0
All	All	1629/1708 (95%)	0.56	179 (10%) 10 8	24, 60, 124, 147	1 (0%)

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	131	VAL	7.8
4	H	243	ALA	6.1
3	C	143	VAL	5.9
3	G	190	ILE	5.4
2	B	133	ALA	5.1

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 oligosaccharides 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.