



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:56 am GMT

PDB ID : 3BZE
Title : The human non-classical major histocompatibility complex molecule HLA-E
Authors : Hoare, H.L.; Sullivan, L.C.; Ely, L.K.; Beddoe, T.; Henderson, K.N.; Lin, J.; Clements, C.S.; Reid, H.H.; Brooks, A.G.; Rossjohn, J.
Deposited on : 2008-01-17
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

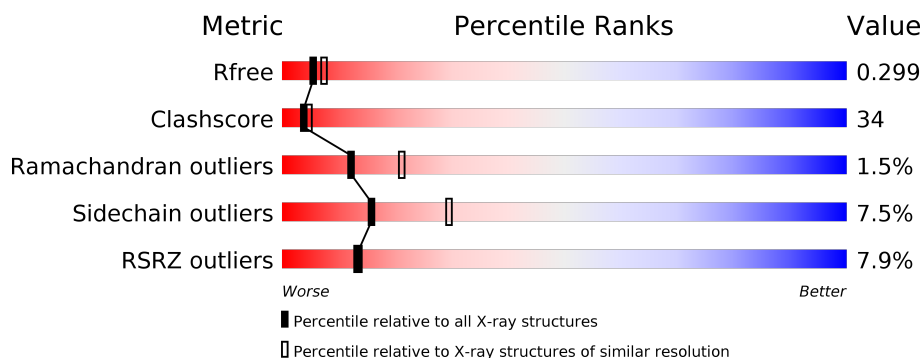
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	273	<div> <div>5%</div> <div>62%</div> <div>31%</div> <div>5%</div> </div>
1	C	273	<div> <div>16%</div> <div>42%</div> <div>45%</div> <div>12%</div> </div>
1	E	273	<div> <div>3%</div> <div>57%</div> <div>35%</div> <div>5%</div> </div>
1	G	273	<div> <div>7%</div> <div>59%</div> <div>35%</div> <div>5%</div> </div>
2	B	100	<div> <div>5%</div> <div>70%</div> <div>25%</div> <div>5%</div> </div>
2	D	100	<div> <div>4%</div> <div>59%</div> <div>38%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	100	<div><div></div><div>6%</div><div>61%</div><div>36%</div><div></div></div>
2	H	100	<div><div></div><div>4%</div><div>56%</div><div>37%</div><div>7%</div></div>
3	P	9	<div><div></div><div>11%</div><div>89%</div><div>11%</div></div>
3	Q	9	<div><div></div><div>89%</div><div>67%</div><div>33%</div></div>
3	R	9	<div><div></div><div>11%</div><div>78%</div><div>22%</div></div>
3	S	9	<div><div></div><div>44%</div><div>67%</div><div>33%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12744 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, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2234	1396	401	430	7			
1	C	273	Total	C	N	O	S	0	0	0
			2234	1396	401	430	7			
1	E	267	Total	C	N	O	S	0	0	0
			2187	1370	392	418	7			
1	G	273	Total	C	N	O	S	0	0	0
			2234	1396	401	430	7			

- 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
			837	533	141	159	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	F	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769
D	0	MET	-	INITIATING METHIONINE	UNP P61769
F	0	MET	-	INITIATING METHIONINE	UNP P61769
H	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called leader peptide of HLA class I histocompatibility antigen, alpha chain G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total 73	C 49	N 12	O 11	S 1	0	0	0
3	Q	9	Total 73	C 49	N 12	O 11	S 1	0	0	0
3	R	9	Total 73	C 49	N 12	O 11	S 1	0	0	0
3	S	9	Total 73	C 49	N 12	O 11	S 1	0	0	0

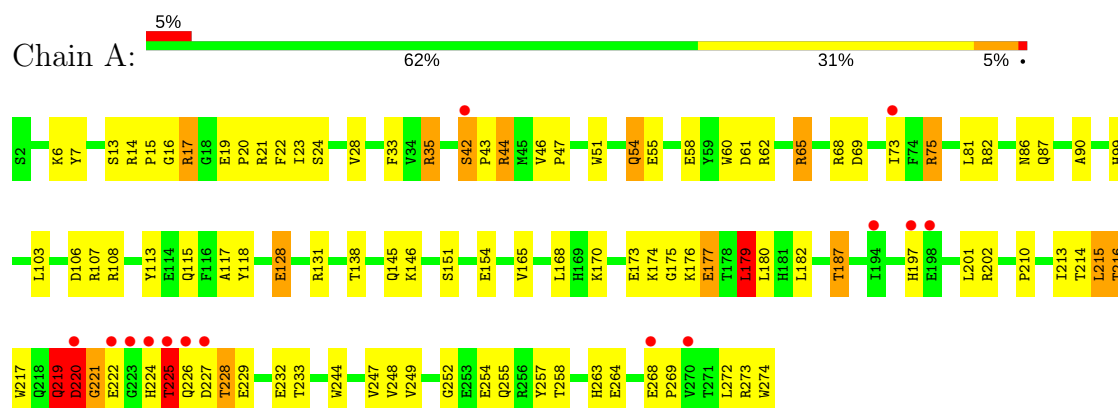
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	20	Total 20	O 20	0	0
4	C	48	Total 48	O 48	0	0
4	D	11	Total 11	O 11	0	0
4	E	20	Total 20	O 20	0	0
4	F	10	Total 10	O 10	0	0
4	G	44	Total 44	O 44	0	0
4	H	12	Total 12	O 12	0	0
4	P	3	Total 3	O 3	0	0
4	Q	1	Total 1	O 1	0	0
4	R	1	Total 1	O 1	0	0
4	S	1	Total 1	O 1	0	0

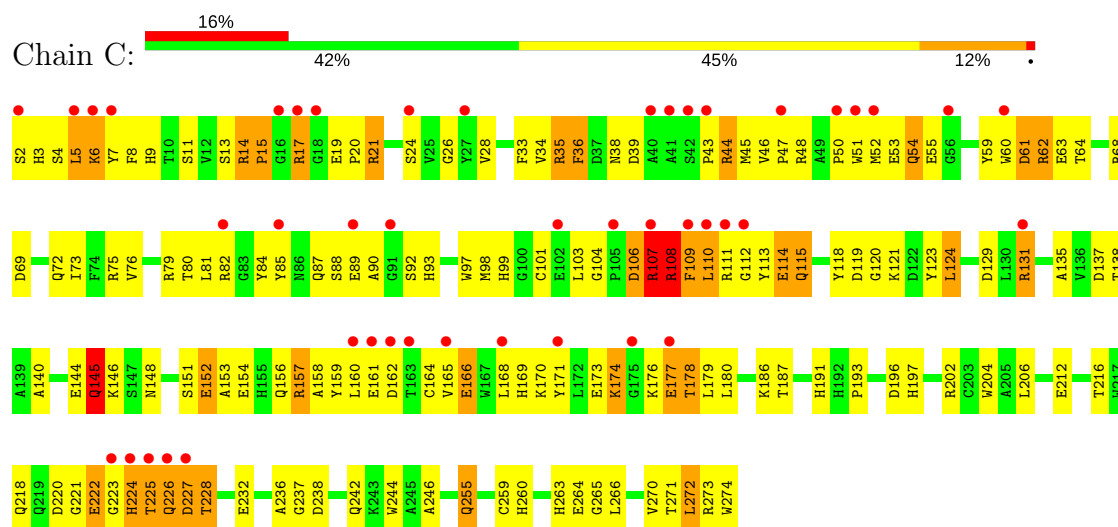
3 Residue-property plots [i](#)

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.

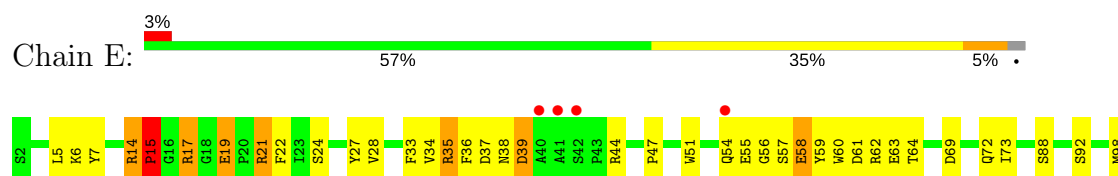
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

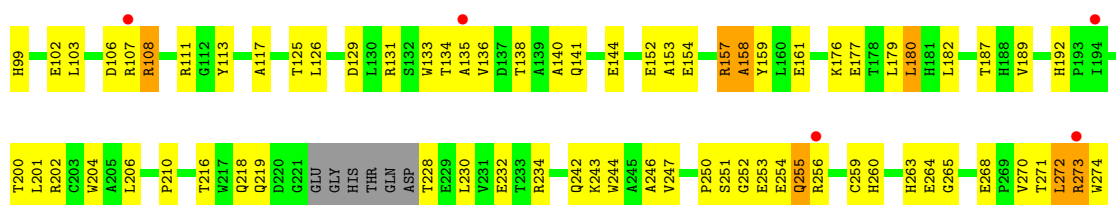


- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

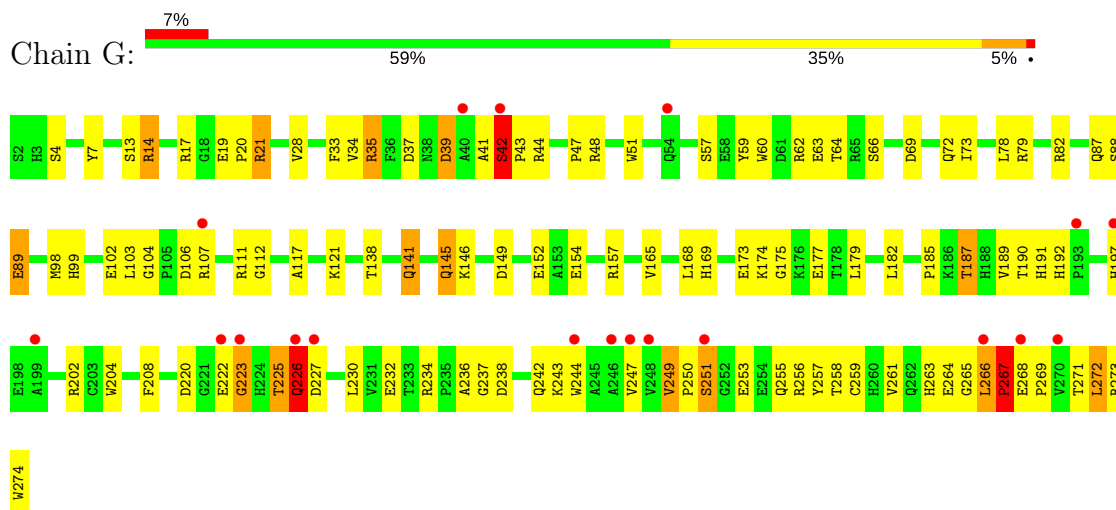


- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

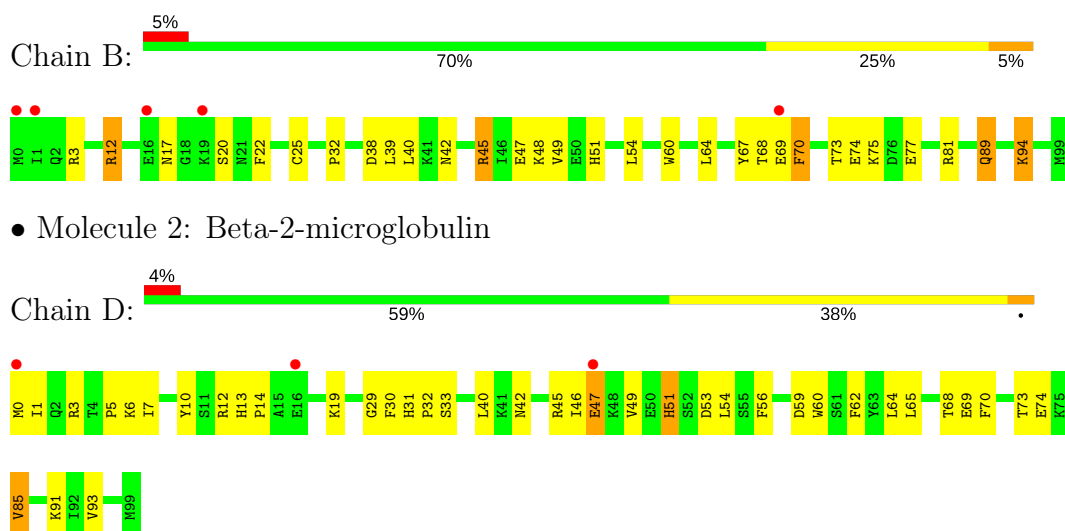




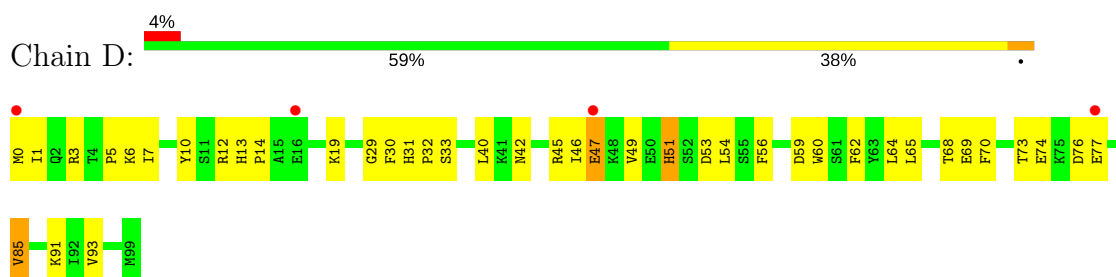
• Molecule 1: HLA class I histocompatibility antigen, alpha chain E



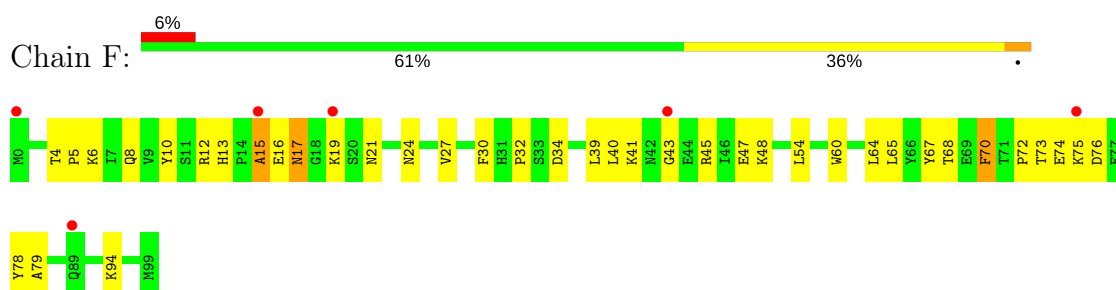
• Molecule 2: Beta-2-microglobulin



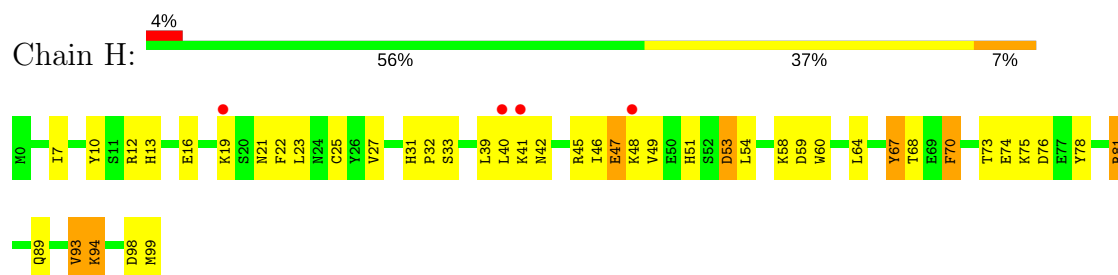
• Molecule 2: Beta-2-microglobulin



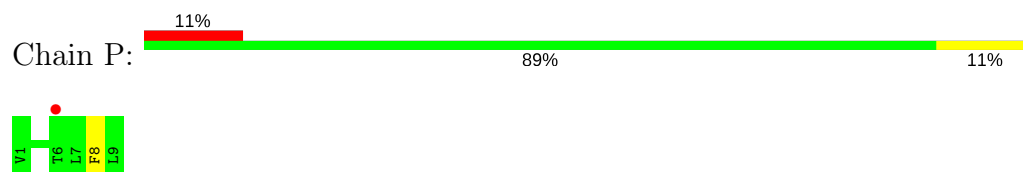
• Molecule 2: Beta-2-microglobulin



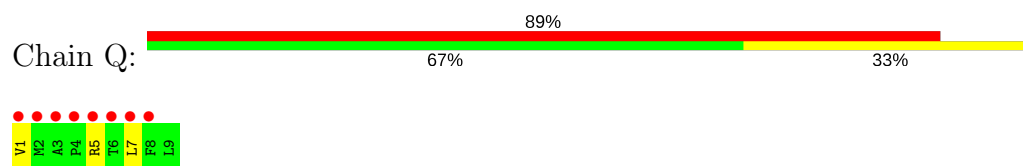
- Molecule 2: Beta-2-microglobulin



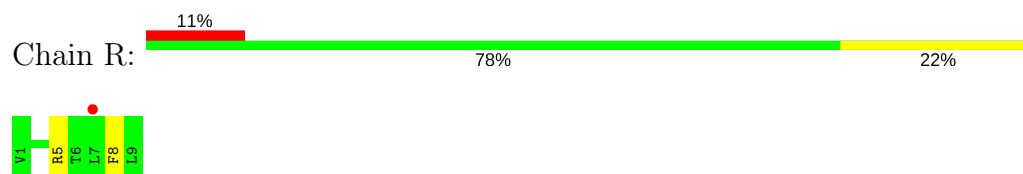
- Molecule 3: leader peptide of HLA class I histocompatibility antigen, alpha chain G



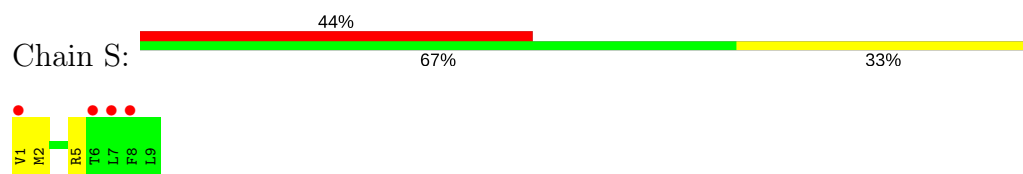
- Molecule 3: leader peptide of HLA class I histocompatibility antigen, alpha chain G



- Molecule 3: leader peptide of HLA class I histocompatibility antigen, alpha chain G



- Molecule 3: leader peptide of HLA class I histocompatibility antigen, alpha chain G



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.78Å 73.35Å 131.53Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 29.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.50) 98.6 (29.93-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.296 0.255 , 0.299	Depositor DCC
R_{free} test set	3195 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12744	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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

5.1 Standard geometry

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	0.61	4/2300 (0.2%)	0.89	13/3127 (0.4%)
1	C	0.50	0/2300	0.82	11/3127 (0.4%)
1	E	0.47	1/2251 (0.0%)	0.77	5/3059 (0.2%)
1	G	0.54	1/2300 (0.0%)	0.83	14/3127 (0.4%)
2	B	0.47	0/860	0.67	0/1162
2	D	0.46	0/860	0.71	1/1162 (0.1%)
2	F	0.61	1/860 (0.1%)	0.74	0/1162
2	H	0.58	0/860	0.73	0/1162
3	P	0.57	0/74	0.84	0/98
3	Q	0.59	0/74	0.93	0/98
3	R	0.54	0/74	0.88	0/98
3	S	0.62	0/74	0.91	0/98
All	All	0.54	7/12887 (0.1%)	0.80	44/17480 (0.3%)

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	C	0	2
1	G	1	3
All	All	1	5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ARG	CA-C	-6.35	1.36	1.52
1	A	44	ARG	N-CA	-6.21	1.33	1.46
1	G	226	GLN	N-CA	-5.68	1.34	1.46
2	F	15	ALA	N-CA	-5.54	1.35	1.46
1	E	158	ALA	N-CA	-5.41	1.35	1.46

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	GLN	C-N-CA	-13.92	86.91	121.70
1	E	273	ARG	CB-CA-C	13.78	137.96	110.40
1	A	215	LEU	N-CA-CB	-12.62	85.15	110.40
1	C	228	THR	N-CA-CB	-10.92	89.56	110.30
2	D	47	GLU	CB-CA-C	9.28	128.95	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	42	SER	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	ARG	Peptide
1	C	227	ASP	Mainchain
1	G	223	GLY	Peptide
1	G	226	GLN	Mainchain
1	G	267	PRO	Mainchain

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	2234	0	2072	116	0
1	C	2234	0	2066	284	2
1	E	2187	0	2035	105	0
1	G	2234	0	2072	130	1
2	B	837	0	803	42	2
2	D	837	0	803	45	0
2	F	837	0	803	49	0
2	H	837	0	803	73	0
3	P	73	0	83	1	0
3	Q	73	0	83	4	0
3	R	73	0	83	5	0
3	S	73	0	83	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	44	0	0	14	0
4	B	20	0	0	12	0
4	C	48	0	0	45	0
4	D	11	0	0	6	0
4	E	20	0	0	9	0
4	F	10	0	0	10	0
4	G	44	0	0	24	4
4	H	12	0	0	4	0
4	P	3	0	0	0	0
4	Q	1	0	0	2	0
4	R	1	0	0	3	0
4	S	1	0	0	0	0
All	All	12744	0	11789	820	5

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 34.

The worst 5 of 820 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:C:223:GLY:HA2	1:C:224:HIS:CG	1.45	1.46
1:A:224:HIS:HB2	1:A:225:THR:CB	1.54	1.37
2:F:4:THR:HG23	4:F:107:HOH:O	1.21	1.34
1:G:249:VAL:CG1	1:G:250:PRO:HD2	1.55	1.33
1:G:146:LYS:HE2	4:G:285:HOH:O	1.18	1.31

All (5) 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)
2:B:77:GLU:OE2	4:G:309:HOH:O[2_646]	1.37	0.83
1:G:17:ARG:NH2	1:G:149:ASP:OD1[2_646]	1.50	0.70
1:C:145:GLN:CB	4:G:295:HOH:O[2_646]	1.56	0.64
1:C:145:GLN:NE2	4:G:295:HOH:O[2_646]	2.04	0.16
2:B:77:GLU:CD	4:G:309:HOH:O[2_646]	2.07	0.13

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	271/273 (99%)	241 (89%)	26 (10%)	4 (2%)	12	21
1	C	271/273 (99%)	231 (85%)	32 (12%)	8 (3%)	5	7
1	E	263/273 (96%)	235 (89%)	24 (9%)	4 (2%)	12	21
1	G	271/273 (99%)	243 (90%)	24 (9%)	4 (2%)	12	21
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	D	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	18	32
2	F	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	18	32
2	H	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
3	P	7/9 (78%)	7 (100%)	0	0	100	100
3	Q	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	S	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1496/1528 (98%)	1337 (89%)	137 (9%)	22 (2%)	12	21

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	224	HIS
1	C	226	GLN
1	G	267	PRO
1	A	225	THR
1	C	225	THR

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	236/236 (100%)	220 (93%)	16 (7%)	18	34
1	C	236/236 (100%)	210 (89%)	26 (11%)	7	13
1	E	231/236 (98%)	210 (91%)	21 (9%)	11	21
1	G	236/236 (100%)	219 (93%)	17 (7%)	17	31
2	B	95/95 (100%)	90 (95%)	5 (5%)	26	48
2	D	95/95 (100%)	93 (98%)	2 (2%)	59	83
2	F	95/95 (100%)	90 (95%)	5 (5%)	26	48
2	H	95/95 (100%)	86 (90%)	9 (10%)	10	19
3	P	8/8 (100%)	8 (100%)	0	100	100
3	Q	8/8 (100%)	8 (100%)	0	100	100
3	R	8/8 (100%)	8 (100%)	0	100	100
3	S	8/8 (100%)	8 (100%)	0	100	100
All	All	1351/1356 (100%)	1250 (92%)	101 (8%)	16	29

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	255	GLN
1	E	54	GLN
2	H	47	GLU
2	D	51	HIS
1	E	17	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	127	ASN
1	C	263	HIS
1	G	263	HIS
1	C	145	GLN
1	C	226	GLN

5.3.3 RNA ⓘ

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 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 ⓘ

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	273/273 (100%)	0.35	14 (5%) 29 30	13, 25, 48, 79	0
1	C	273/273 (100%)	0.97	45 (16%) 2 2	6, 27, 56, 72	0
1	E	267/273 (97%)	0.40	9 (3%) 46 48	11, 25, 47, 58	0
1	G	273/273 (100%)	0.52	19 (6%) 17 17	12, 26, 43, 63	0
2	B	100/100 (100%)	0.22	5 (5%) 30 31	14, 24, 43, 53	0
2	D	100/100 (100%)	0.36	4 (4%) 39 41	13, 26, 42, 82	0
2	F	100/100 (100%)	0.49	6 (6%) 23 23	14, 27, 42, 62	0
2	H	100/100 (100%)	0.44	4 (4%) 39 41	17, 27, 37, 44	0
3	P	9/9 (100%)	1.17	1 (11%) 6 5	23, 24, 28, 29	0
3	Q	9/9 (100%)	3.20	8 (88%) 0 0	19, 22, 25, 26	0
3	R	9/9 (100%)	1.06	1 (11%) 6 5	12, 21, 25, 26	0
3	S	9/9 (100%)	1.96	4 (44%) 0 0	14, 16, 21, 24	0
All	All	1522/1528 (99%)	0.54	120 (7%) 13 13	6, 26, 47, 82	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	THR	9.5
1	C	107	ARG	6.9
2	D	0	MET	6.6
1	A	223	GLY	6.5
1	A	224	HIS	6.3

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

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

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.