wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 11:55 PM EDT

PDB ID	:	2AK4
Title	:	Crystal Structure of SB27 TCR in complex with HLA-B*3508-13mer peptide
Authors	:	Tynan, F.E.; Burrows, S.R.; Buckle, A.M.; Clements, C.S.; Borg, N.A.; Miles, J.J.; Beddoe, T.; Whisstock, J.C.; Wilce, M.C.; Silins, S.L.; Burrows, J.M.; Kjer-Nielsen, L.; Konstenko, L.; Purcell, A.W.; McCluskey, J.; Rossjohn, J.
Deposited on	:	2005-08-03
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

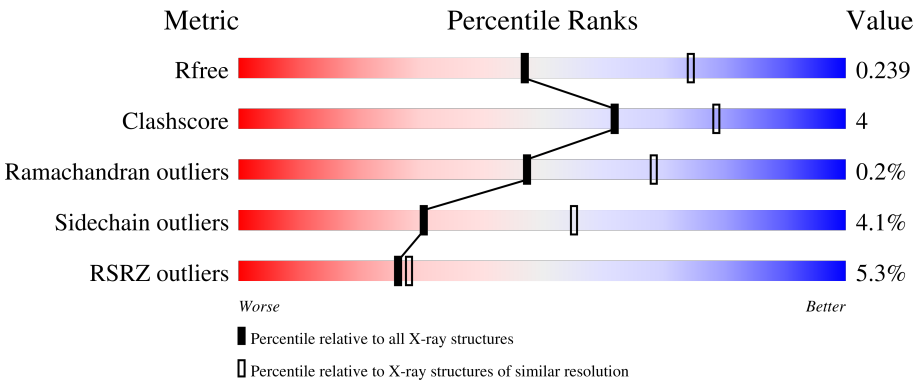
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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 <=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	276	2% 91% 8%
1	F	276	2% 92% 8%
1	K	276	5% 92% 8%
1	Q	276	18% 89% 11%
2	B	99	2% 93% 5% •

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Mol	Chain	Length	Quality of chain
2	G	99	2%, 93%, 5%
2	L	99	2%, 92%, 6%
2	R	99	2%, 91%, 7%
3	C	13	77%, 23%
3	H	13	77%, 23%
3	M	13	8%, 77%, 23%
3	S	13	77%, 23%
4	D	211	6%, 82%, 13%
4	I	211	9%, 84%, 10%
4	N	211	6%, 80%, 15%
4	T	211	8%, 82%, 14%
5	E	245	2%, 81%, 16%
5	J	245	4%, 82%, 14%
5	P	245	3%, 82%, 15%
5	U	245	4%, 80%, 15%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 26609 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-B35 variant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2243	1397	412	427	7	0	0	0
1	F	276	2242	1398	411	426	7	0	0	0
1	K	276	2220	1387	405	421	7	0	0	0
1	Q	276	2239	1397	404	431	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	799	509	134	153	3	0	0	0
2	G	99	818	521	136	158	3	0	0	0
2	L	99	807	514	136	154	3	0	0	0
2	R	99	788	504	133	148	3	0	0	0

- Molecule 3 is a protein called EBV peptide LPEPLPQGQLTAY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	13	101	66	15	20	0	0	0
3	H	13	101	66	15	20	0	0	0
3	M	13	96	63	14	19	0	0	0
3	S	13	97	64	14	19	0	0	0

- Molecule 4 is a protein called SB27 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	204	1575	998	252	319	6	0	0	0
4	I	204	1579	1004	252	316	7	0	0	0
4	N	204	1603	1018	257	321	7	0	0	0
4	T	204	1560	992	248	314	6	0	0	0

- Molecule 5 is a protein called SB27 T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	241	1887	1188	327	363	9	0	0	0
5	J	241	1882	1187	326	360	9	0	0	0
5	P	241	1883	1186	328	360	9	0	0	0
5	U	238	1828	1151	320	348	9	0	0	0

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
6	A	3	3	3	0	0
6	B	1	1	1	0	0
6	C	1	1	1	0	0
6	D	1	1	1	0	0
6	E	1	1	1	0	0
6	F	4	4	4	0	0
6	G	1	1	1	0	0
6	H	1	1	1	0	0
6	J	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	3	Total I 3 3	0	0
6	L	1	Total I 1 1	0	0
6	Q	2	Total I 2 2	0	0
6	R	1	Total I 1 1	0	0
6	S	1	Total I 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	26	Total O 26 26	0	0
7	B	9	Total O 9 9	0	0
7	D	12	Total O 12 12	0	0
7	E	13	Total O 13 13	0	0
7	F	22	Total O 22 22	0	0
7	G	8	Total O 8 8	0	0
7	I	8	Total O 8 8	0	0
7	J	18	Total O 18 18	0	0
7	K	18	Total O 18 18	0	0
7	L	8	Total O 8 8	0	0
7	M	1	Total O 1 1	0	0
7	N	20	Total O 20 20	0	0
7	P	25	Total O 25 25	0	0
7	Q	19	Total O 19 19	0	0

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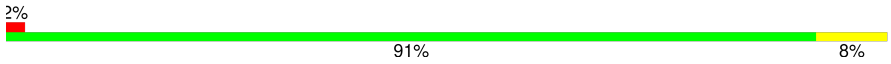
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	R	3	3	3	0	0
			Total	O		
7	S	1	1	1	0	0
			Total	O		
7	T	8	8	8	0	0
			Total	O		
7	U	20	20	20	0	0

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.

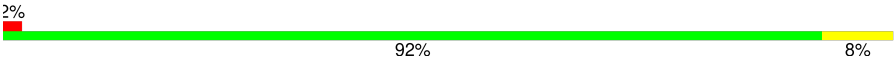
• Molecule 1: HLA-B35 variant

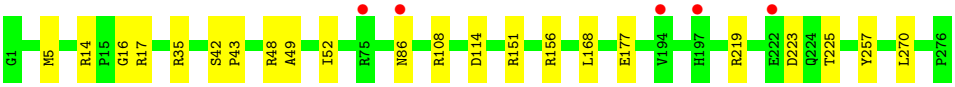
Chain A:



• Molecule 1: HLA-B35 variant

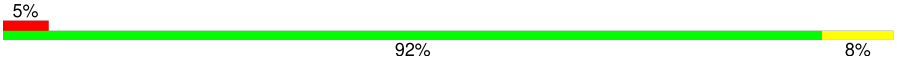
Chain F:

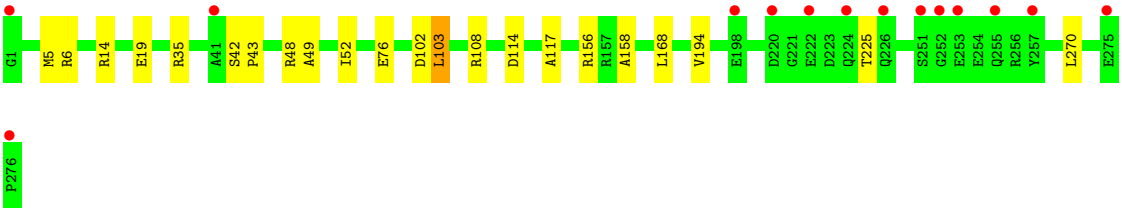




• Molecule 1: HLA-B35 variant

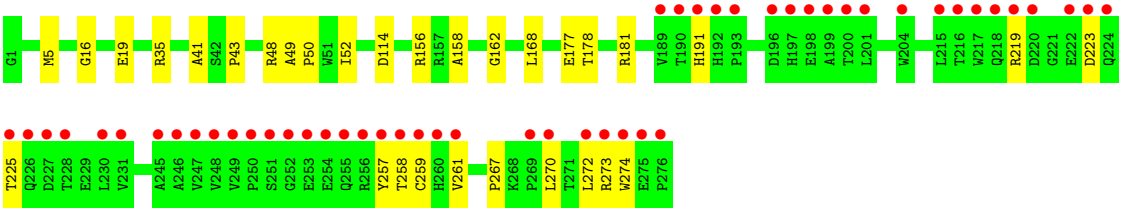
Chain K:



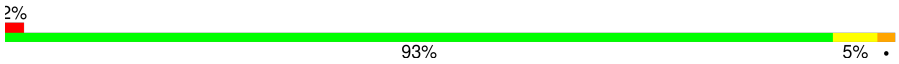


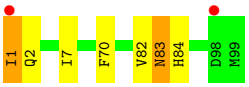
• Molecule 1: HLA-B35 variant

Chain Q:

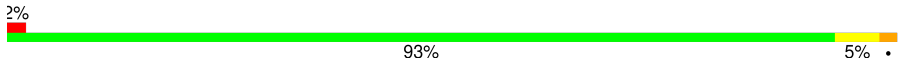


• Molecule 2: Beta-2-microglobulin

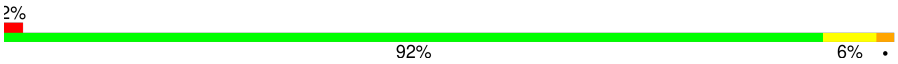
Chain B: 

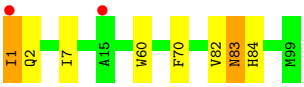


• Molecule 2: Beta-2-microglobulin

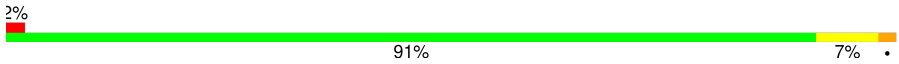
Chain G: 

• Molecule 2: Beta-2-microglobulin

Chain L: 



• Molecule 2: Beta-2-microglobulin

Chain R: 

• Molecule 3: EBV peptide LPEPLPQGQLTAY

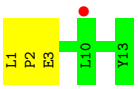
Chain C:

• Molecule 3: EBV peptide LPEPLPQGQLTAY

Chain H:

• Molecule 3: EBV peptide LPEPLPQGQLTAY

Chain M:

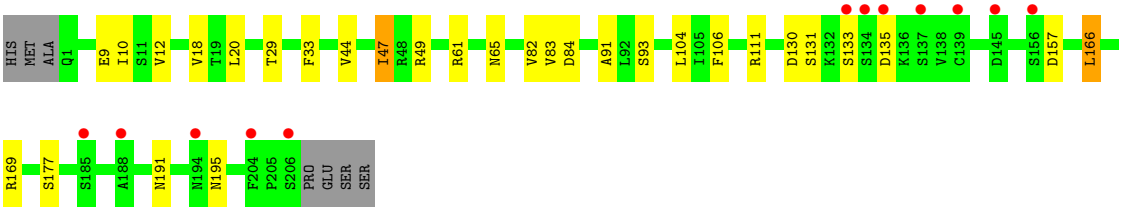


• Molecule 3: EBV peptide LPEPLPQGQLTAY

Chain S:

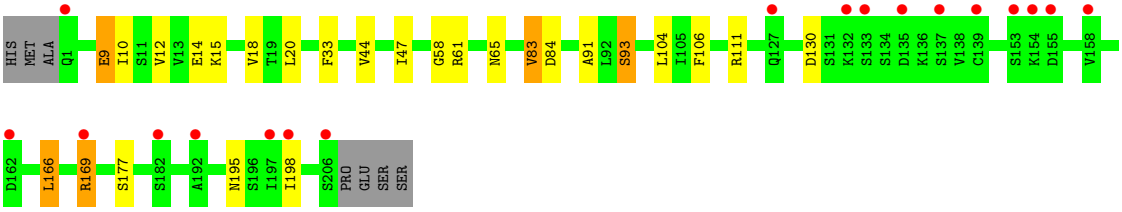
• Molecule 4: SB27 T cell receptor alpha chain

Chain D:



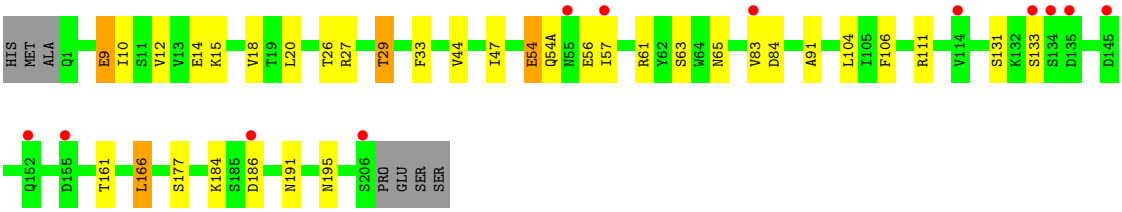
• Molecule 4: SB27 T cell receptor alpha chain

Chain I:



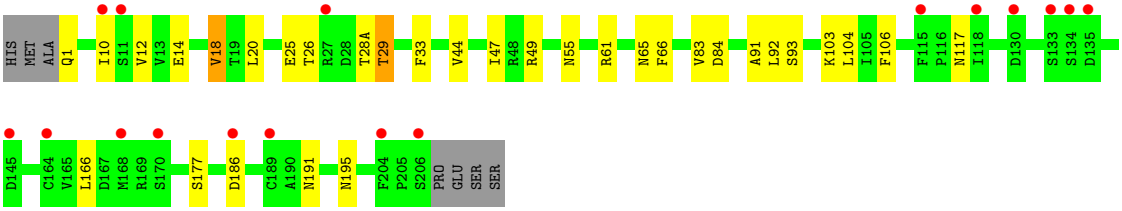
• Molecule 4: SB27 T cell receptor alpha chain

Chain N:



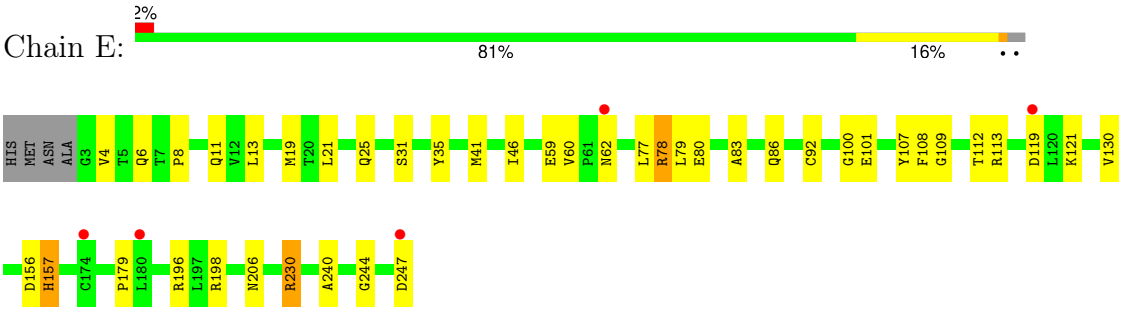
• Molecule 4: SB27 T cell receptor alpha chain

Chain T:



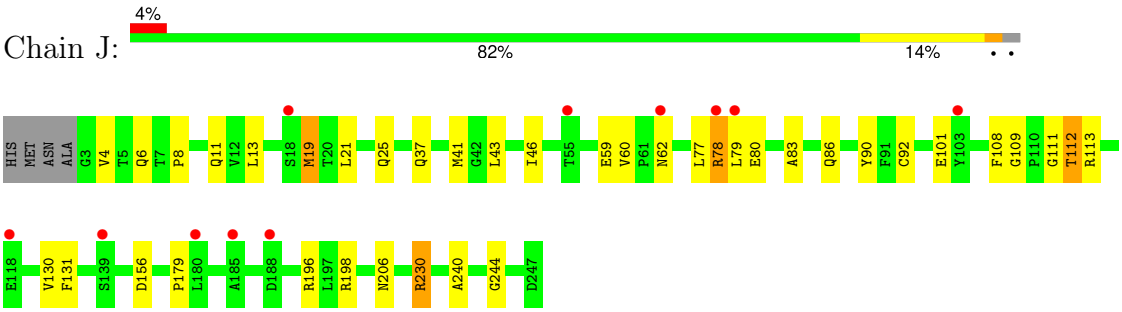
• Molecule 5: SB27 T cell receptor beta chain

Chain E:



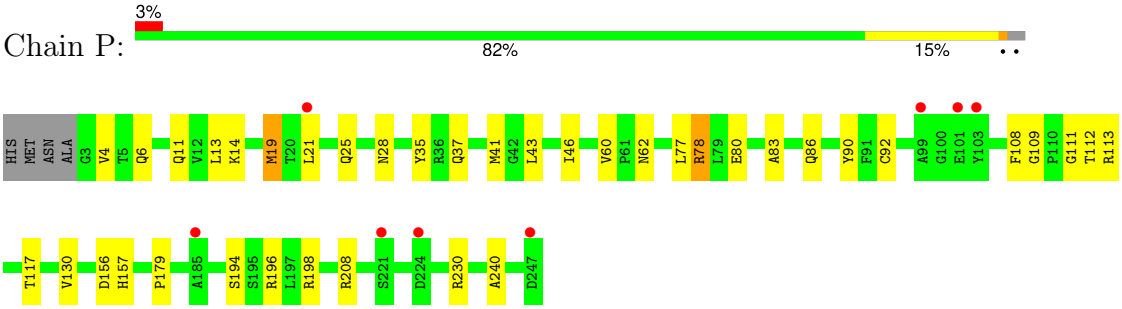
- Molecule 5: SB27 T cell receptor beta chain

Chain J:



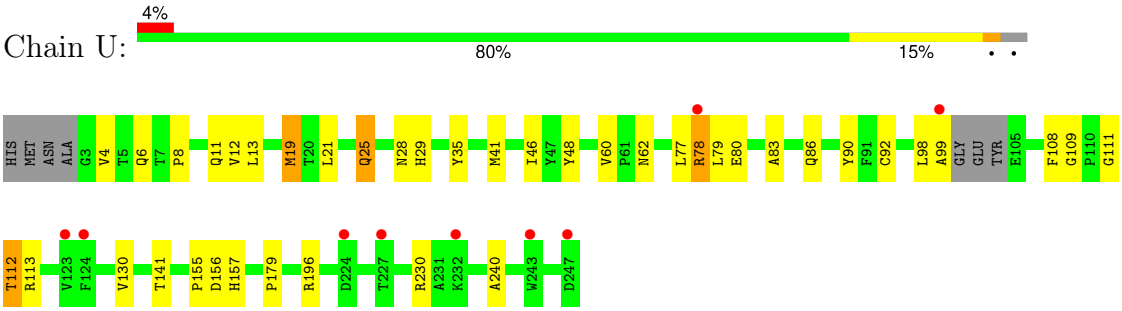
- Molecule 5: SB27 T cell receptor beta chain

Chain P:



- Molecule 5: SB27 T cell receptor beta chain

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.15Å 213.28Å 122.30Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 38.08 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-2.50) 95.3 (38.08-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.246 , 0.278 0.225 , 0.239	Depositor DCC
R_{free} test set	4033 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , -17.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.318 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	26609	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: IOD

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	0.38	0/2306	0.54	0/3137
1	F	0.37	0/2305	0.53	0/3135
1	K	0.38	0/2283	0.55	1/3106 (0.0%)
1	Q	0.36	0/2302	0.52	0/3132
2	B	0.38	0/822	0.50	0/1116
2	G	0.37	0/841	0.50	0/1141
2	L	0.38	0/830	0.51	0/1127
2	R	0.37	0/811	0.49	0/1104
3	C	0.36	0/104	0.44	0/142
3	H	0.33	0/104	0.47	0/142
3	M	0.40	0/99	0.46	0/135
3	S	0.35	0/100	0.44	0/137
4	D	0.39	0/1613	0.53	0/2196
4	I	0.38	0/1617	0.52	0/2202
4	N	0.39	0/1641	0.54	0/2232
4	T	0.39	0/1598	0.54	0/2180
5	E	0.38	0/1939	0.63	2/2641 (0.1%)
5	J	0.37	0/1934	0.52	1/2634 (0.0%)
5	P	0.39	0/1935	0.65	3/2634 (0.1%)
5	U	0.36	0/1878	0.52	1/2562 (0.0%)
All	All	0.38	0/27062	0.54	8/36835 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	247	ASP	CA-C-O	16.16	154.04	120.10
5	P	78	ARG	NE-CZ-NH2	-14.42	113.09	120.30
5	P	78	ARG	NE-CZ-NH1	13.59	127.10	120.30
1	K	103	LEU	CA-CB-CG	7.36	132.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	78	ARG	CD-NE-CZ	5.92	131.89	123.60

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	2243	0	2093	21	0
1	F	2242	0	2093	13	0
1	K	2220	0	2061	13	0
1	Q	2239	0	2077	21	0
2	B	799	0	732	4	0
2	G	818	0	760	4	0
2	L	807	0	747	5	0
2	R	788	0	713	6	0
3	C	101	0	102	2	0
3	H	101	0	102	2	0
3	M	96	0	95	2	0
3	S	97	0	96	2	0
4	D	1575	0	1435	15	0
4	I	1579	0	1449	23	0
4	N	1603	0	1492	19	0
4	T	1560	0	1410	18	0
5	E	1887	0	1766	26	0
5	J	1882	0	1764	28	0
5	P	1883	0	1768	21	0
5	U	1828	0	1688	24	0
6	A	3	0	0	1	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	1	0
6	F	4	0	0	1	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1	0	0	1	0
6	K	3	0	0	0	0
6	L	1	0	0	0	0
6	Q	2	0	0	1	0
6	R	1	0	0	1	0
6	S	1	0	0	0	0
7	A	26	0	0	0	0
7	B	9	0	0	0	0
7	D	12	0	0	1	0
7	E	13	0	0	3	0
7	F	22	0	0	0	0
7	G	8	0	0	0	0
7	I	8	0	0	1	0
7	J	18	0	0	4	0
7	K	18	0	0	1	0
7	L	8	0	0	0	0
7	M	1	0	0	0	0
7	N	20	0	0	0	0
7	P	25	0	0	0	0
7	Q	19	0	0	2	0
7	R	3	0	0	0	0
7	S	1	0	0	0	0
7	T	8	0	0	0	0
7	U	20	0	0	1	0
All	All	26609	0	24443	223	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 4.

The worst 5 of 223 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)
5:P:78:ARG:HD3	5:P:80:GLU:OE2	1.80	0.81
1:A:253:GLU:HG2	4:I:83:VAL:HG21	1.64	0.79
1:A:197:HIS:HB2	4:I:169:ARG:HG3	1.67	0.77
1:Q:162:GLY:HA2	4:T:28(A):THR:HG23	1.74	0.70
5:P:6:GLN:HE21	5:P:109:GLY:HA3	1.57	0.69

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	274/276 (99%)	270 (98%)	4 (2%)	0	100	100
1	F	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
1	K	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
1	Q	274/276 (99%)	267 (97%)	5 (2%)	2 (1%)	22	39
2	B	97/99 (98%)	97 (100%)	0	0	100	100
2	G	97/99 (98%)	97 (100%)	0	0	100	100
2	L	97/99 (98%)	97 (100%)	0	0	100	100
2	R	97/99 (98%)	97 (100%)	0	0	100	100
3	C	11/13 (85%)	11 (100%)	0	0	100	100
3	H	11/13 (85%)	11 (100%)	0	0	100	100
3	M	11/13 (85%)	11 (100%)	0	0	100	100
3	S	11/13 (85%)	11 (100%)	0	0	100	100
4	D	202/211 (96%)	191 (95%)	10 (5%)	1 (0%)	29	48
4	I	202/211 (96%)	194 (96%)	8 (4%)	0	100	100
4	N	202/211 (96%)	189 (94%)	10 (5%)	3 (2%)	10	18
4	T	202/211 (96%)	194 (96%)	8 (4%)	0	100	100
5	E	239/245 (98%)	234 (98%)	5 (2%)	0	100	100
5	J	239/245 (98%)	235 (98%)	4 (2%)	0	100	100
5	P	239/245 (98%)	235 (98%)	4 (2%)	0	100	100
5	U	234/245 (96%)	228 (97%)	6 (3%)	0	100	100
All	All	3287/3376 (97%)	3206 (98%)	75 (2%)	6 (0%)	47	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	N	54	GLU

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Mol	Chain	Res	Type
4	N	56	GLU
4	N	133	SER
1	Q	267	PRO
4	D	130	ASP

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	230/234 (98%)	224 (97%)	6 (3%)	46	72
1	F	229/234 (98%)	223 (97%)	6 (3%)	46	72
1	K	224/234 (96%)	218 (97%)	6 (3%)	44	71
1	Q	228/234 (97%)	224 (98%)	4 (2%)	59	81
2	B	86/94 (92%)	83 (96%)	3 (4%)	36	62
2	G	90/94 (96%)	87 (97%)	3 (3%)	38	64
2	L	88/94 (94%)	85 (97%)	3 (3%)	37	63
2	R	82/94 (87%)	79 (96%)	3 (4%)	34	60
3	C	11/11 (100%)	11 (100%)	0	100	100
3	H	11/11 (100%)	11 (100%)	0	100	100
3	M	10/11 (91%)	10 (100%)	0	100	100
3	S	10/11 (91%)	10 (100%)	0	100	100
4	D	174/195 (89%)	163 (94%)	11 (6%)	18	34
4	I	174/195 (89%)	165 (95%)	9 (5%)	23	44
4	N	180/195 (92%)	169 (94%)	11 (6%)	18	36
4	T	169/195 (87%)	159 (94%)	10 (6%)	19	37
5	E	200/211 (95%)	190 (95%)	10 (5%)	24	46
5	J	199/211 (94%)	190 (96%)	9 (4%)	27	51
5	P	200/211 (95%)	189 (94%)	11 (6%)	21	41
5	U	190/211 (90%)	180 (95%)	10 (5%)	22	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2785/2980 (94%)	2670 (96%)	115 (4%)	30 55

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	14	ARG
5	U	62	ASN
4	N	47	ILE
5	U	41	MET
4	T	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	29	HIS
5	U	157	HIS
4	N	183	ASN
5	U	86	GLN
4	T	113	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	276/276 (100%)	0.40	6 (2%)	62	65	2, 6, 22, 32	0
1	F	276/276 (100%)	0.43	5 (1%)	68	71	2, 6, 23, 33	0
1	K	276/276 (100%)	0.61	14 (5%)	28	29	2, 6, 23, 30	0
1	Q	276/276 (100%)	1.09	51 (18%)	1	1	2, 6, 22, 28	0
2	B	99/99 (100%)	0.23	2 (2%)	65	68	2, 8, 21, 23	0
2	G	99/99 (100%)	0.34	2 (2%)	65	68	2, 8, 21, 23	0
2	L	99/99 (100%)	0.32	2 (2%)	65	68	2, 7, 20, 23	0
2	R	99/99 (100%)	0.31	2 (2%)	65	68	2, 7, 20, 23	0
3	C	13/13 (100%)	0.39	0	100	100	2, 3, 8, 8	0
3	H	13/13 (100%)	0.15	0	100	100	2, 3, 8, 9	0
3	M	13/13 (100%)	0.54	1 (7%)	13	13	2, 3, 5, 8	0
3	S	13/13 (100%)	0.18	0	100	100	2, 3, 5, 8	0
4	D	204/211 (96%)	0.53	12 (5%)	22	23	2, 13, 28, 32	0
4	I	204/211 (96%)	0.70	18 (8%)	10	10	2, 13, 29, 32	0
4	N	204/211 (96%)	0.67	12 (5%)	22	23	2, 13, 29, 32	0
4	T	204/211 (96%)	0.71	17 (8%)	11	11	2, 12, 28, 32	0
5	E	241/245 (98%)	0.42	5 (2%)	63	66	2, 10, 23, 31	0
5	J	241/245 (98%)	0.47	11 (4%)	32	34	3, 10, 23, 30	0
5	P	241/245 (98%)	0.51	8 (3%)	46	50	2, 10, 24, 33	0
5	U	238/245 (97%)	0.54	9 (3%)	40	43	2, 10, 23, 31	0
All	All	3329/3376 (98%)	0.55	177 (5%)	26	28	2, 9, 25, 33	0

The worst 5 of 177 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	252	GLY	14.0
1	Q	255	GLN	9.7
1	Q	227	ASP	8.6
1	Q	199	ALA	8.1
1	Q	249	VAL	7.9

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
6	IOD	R	1018	1/1	0.90	0.14	65,65,65,65	0
6	IOD	L	1017	1/1	0.94	0.11	65,65,65,65	0
6	IOD	J	1022	1/1	0.95	0.12	62,62,62,62	0
6	IOD	C	1013	1/1	0.96	0.04	9,9,9,9	0
6	IOD	G	1020	1/1	0.97	0.12	46,46,46,46	0
6	IOD	B	1016	1/1	0.97	0.17	52,52,52,52	0
6	IOD	S	1015	1/1	0.97	0.03	29,29,29,29	0
6	IOD	E	1021	1/1	0.98	0.12	58,58,58,58	0
6	IOD	Q	1007	1/1	0.98	0.06	3,3,3,3	0
6	IOD	A	1010	1/1	0.98	0.04	12,12,12,12	0
6	IOD	D	1019	1/1	0.98	0.14	52,52,52,52	0
6	IOD	K	1001	1/1	0.99	0.18	3,3,3,3	0
6	IOD	K	1009	1/1	0.99	0.04	13,13,13,13	0
6	IOD	F	1012	1/1	0.99	0.04	32,32,32,32	0
6	IOD	F	1004	1/1	0.99	0.14	5,5,5,5	0
6	IOD	Q	1011	1/1	0.99	0.03	20,20,20,20	0
6	IOD	H	1014	1/1	0.99	0.03	12,12,12,12	0
6	IOD	F	1008	1/1	0.99	0.04	4,4,4,4	0
6	IOD	A	1006	1/1	1.00	0.05	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	IOD	K	1005	1/1	1.00	0.09	3,3,3,3	0
6	IOD	A	1002	1/1	1.00	0.18	3,3,3,3	0
6	IOD	F	1003	1/1	1.00	0.15	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.