



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:03 AM GMT

PDB ID : 3KPS
Title : Crystal Structure of the LC13 TCR in complex with HLA B*4405 bound to EEYLQAFTY a self peptide from the ABCD3 protein
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Deposited on : 2009-11-16
Resolution : 2.70 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

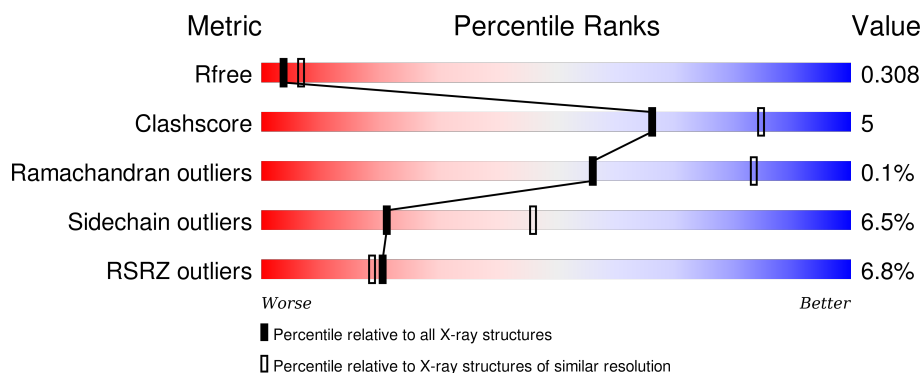
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	276	<div> <div>12%</div> <div>87%</div> <div>12%</div> </div>
2	B	99	<div> <div>12%</div> <div>83%</div> <div>17%</div> </div>
3	C	9	<div> <div>56%</div> <div>33%</div> <div>11%</div> </div>
4	D	201	<div> <div>3%</div> <div>83%</div> <div>13%</div> </div>
5	E	241	<div> <div>2%</div> <div>84%</div> <div>15%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6684 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, B-44 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2259	1408	407	437	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TYR	ASP	VARIANT	UNP P30481

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called EEYLQAFTY, self peptide from the ATP binding cassette protein ABCD3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			83	55	10	18			

- Molecule 4 is a protein called LC13 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1567	975	267	317	8			

- Molecule 5 is a protein called LC13 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1919	1209	335	371	4			

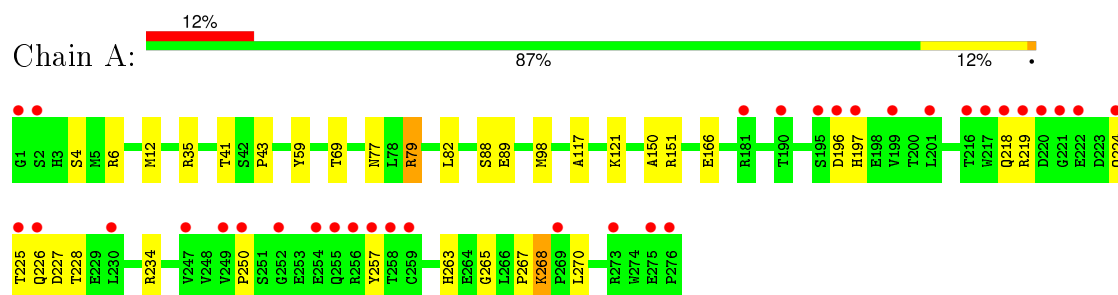
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	B	4	Total 4	O 4	0	0
6	C	1	Total 1	O 1	0	0
6	D	6	Total 6	O 6	0	0
6	E	13	Total 13	O 13	0	0

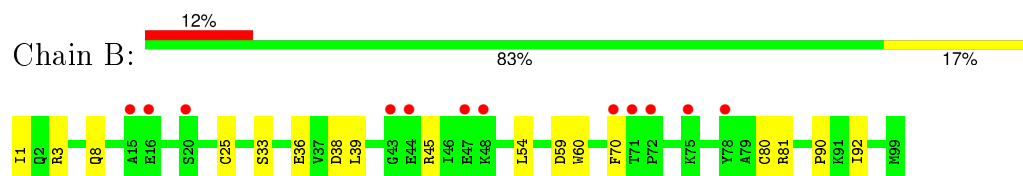
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, B-44 alpha chain



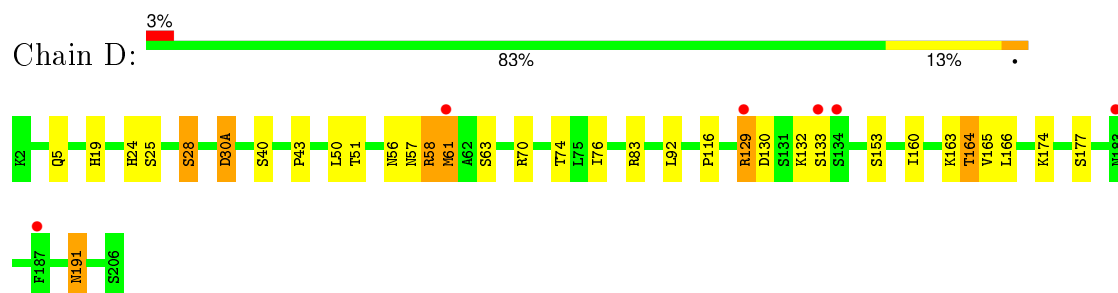
- Molecule 2: Beta-2-microglobulin



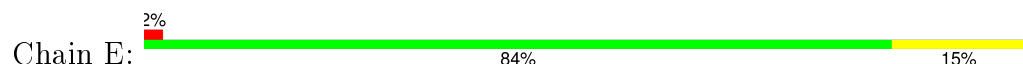
- Molecule 3: EEYLQAFTY, self peptide from the ATP binding cassette protein ABCD3

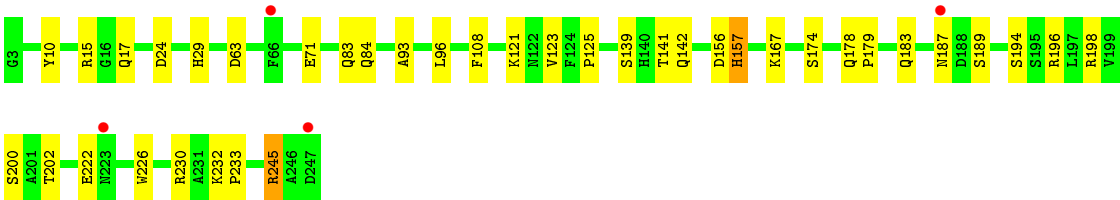


- Molecule 4: LC13 TCR alpha chain



- Molecule 5: LC13 TCR beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.52Å 54.24Å 121.77Å 90.00° 114.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.4 (50.00-2.70) 91.4 (50.04-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.269 0.241 , 0.308	Depositor DCC
R_{free} test set	1112 reflections (5.45%)	DCC
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21528 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6684	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/2320	0.59	0/3154
2	B	0.42	0/852	0.59	0/1152
3	C	0.57	0/85	0.65	0/113
4	D	0.47	0/1603	0.66	0/2181
5	E	0.49	0/1971	0.60	0/2681
All	All	0.47	0/6831	0.61	0/9281

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

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	2259	0	2128	19	0
2	B	829	0	794	9	0
3	C	83	0	72	7	0
4	D	1567	0	1492	21	0
5	E	1919	0	1820	18	0
6	A	3	0	0	0	0
6	B	4	0	0	0	0
6	C	1	0	0	0	0
6	D	6	0	0	1	0
6	E	13	0	0	1	0
All	All	6684	0	6306	64	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 (64) 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:164:THR:HB	5:E:174:SER:OG	1.77	0.82
4:D:57:ASN:HB3	4:D:58:ARG:O	1.85	0.75
1:A:267:PRO:HB2	1:A:268:LYS:HE2	1.68	0.73
1:A:263:HIS:CD2	1:A:265:GLY:H	2.11	0.68
4:D:56:ASN:ND2	4:D:63:SER:OG	2.30	0.65
4:D:163:LYS:HA	4:D:177:SER:O	1.97	0.63
1:A:59:TYR:CE1	3:C:1:GLU:HG2	2.36	0.61
4:D:57:ASN:CB	4:D:58:ARG:O	2.47	0.61
4:D:28:SER:O	4:D:70:ARG:NH2	2.34	0.61
5:E:156:ASP:OD1	5:E:179:PRO:HG2	2.02	0.60
5:E:178:GLN:NE2	5:E:178:GLN:HA	2.17	0.60
1:A:267:PRO:HB2	1:A:268:LYS:CE	2.32	0.59
4:D:153:SER:HB3	4:D:160:ILE:CD1	2.32	0.59
3:C:5:GLN:HA	3:C:5:GLN:HE21	1.68	0.59
1:A:197:HIS:O	1:A:250:PRO:HA	2.02	0.58
1:A:219:ARG:HB2	1:A:257:TYR:CE2	2.39	0.58
4:D:28:SER:HB2	4:D:30(A):ASP:OD2	2.03	0.58
4:D:153:SER:HB3	4:D:160:ILE:HD12	1.85	0.58
4:D:58:ARG:O	4:D:61:MET:HG2	2.04	0.57
1:A:77:ASN:ND2	3:C:9:TYR:H	2.04	0.56
1:A:59:TYR:HE1	3:C:1:GLU:HG2	1.70	0.55
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.89	0.54
1:A:234:ARG:HH11	2:B:8:GLN:NE2	2.05	0.54
2:B:38:ASP:HB2	2:B:81:ARG:HB3	1.90	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.43	0.54
2:B:3:ARG:NH2	2:B:59:ASP:O	2.41	0.53
4:D:51:THR:HG22	4:D:70:ARG:HD3	1.90	0.53
5:E:10:TYR:HB3	5:E:157:HIS:CD2	2.44	0.52
1:A:41:THR:O	1:A:43:PRO:HD3	2.10	0.52
3:C:5:GLN:HA	3:C:5:GLN:NE2	2.25	0.52
1:A:69:THR:HG21	3:C:4:LEU:HD21	1.92	0.51
4:D:43:PRO:HD2	5:E:108:PHE:CG	2.47	0.50
5:E:93:ALA:HB2	5:E:108:PHE:CD2	2.47	0.50
1:A:4:SER:HB2	1:A:6:ARG:NH1	2.27	0.50
2:B:80:CYS:O	2:B:92:ILE:HA	2.12	0.49
5:E:245:ARG:O	5:E:245:ARG:HG2	2.13	0.48
4:D:164:THR:HG23	6:D:212:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:123:VAL:O	5:E:230:ARG:NH2	2.48	0.47
5:E:141:THR:O	5:E:142:GLN:HB2	2.15	0.47
4:D:129:ARG:HH11	4:D:129:ARG:HG2	1.80	0.46
5:E:156:ASP:C	5:E:157:HIS:HD1	2.19	0.46
1:A:121:LYS:HG3	2:B:1:ILE:HG23	1.97	0.45
4:D:116:PRO:HG3	4:D:165:VAL:HG13	1.99	0.45
5:E:226:TRP:HB2	5:E:232:LYS:HG3	1.98	0.45
5:E:178:GLN:HA	5:E:179:PRO:HD3	1.87	0.45
5:E:125:PRO:HD3	5:E:233:PRO:HB3	1.99	0.45
5:E:167:LYS:HB2	6:E:251:HOH:O	2.17	0.45
3:C:5:GLN:CA	3:C:5:GLN:NE2	2.79	0.45
4:D:130:ASP:HB3	4:D:133:SER:O	2.17	0.44
4:D:166:LEU:O	4:D:174:LYS:HA	2.17	0.44
1:A:150:ALA:O	1:A:151:ARG:HB2	2.18	0.44
4:D:166:LEU:HD11	5:E:198:ARG:HB3	1.99	0.44
4:D:50:LEU:O	4:D:70:ARG:NH1	2.49	0.44
1:A:82:LEU:HD13	1:A:89:GLU:HG2	2.00	0.43
5:E:183:GLN:O	5:E:189:SER:HB2	2.19	0.43
4:D:191:ASN:C	4:D:191:ASN:HD22	2.22	0.43
1:A:218:GLN:O	1:A:257:TYR:HA	2.18	0.43
2:B:33:SER:HB2	2:B:54:LEU:HD21	2.00	0.42
2:B:38:ASP:OD1	2:B:45:ARG:NE	2.53	0.42
1:A:224:GLN:C	1:A:226:GLN:N	2.74	0.41
1:A:79:ARG:O	1:A:82:LEU:HB2	2.20	0.41
5:E:15:ARG:HD3	5:E:83:GLN:OE1	2.19	0.41
5:E:178:GLN:HE21	5:E:178:GLN:HA	1.85	0.41
4:D:19:HIS:HD2	4:D:76:ILE:HG12	1.86	0.40

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	274/276 (99%)	258 (94%)	16 (6%)	0	100	100
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	199/201 (99%)	185 (93%)	13 (6%)	1 (0%)	34	63
5	E	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
All	All	816/826 (99%)	765 (94%)	50 (6%)	1 (0%)	56	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	61	MET

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	237/237 (100%)	225 (95%)	12 (5%)	29	59
2	B	94/94 (100%)	91 (97%)	3 (3%)	46	77
3	C	8/8 (100%)	7 (88%)	1 (12%)	6	13
4	D	180/180 (100%)	166 (92%)	14 (8%)	16	35
5	E	207/207 (100%)	190 (92%)	17 (8%)	14	32
All	All	726/726 (100%)	679 (94%)	47 (6%)	21	46

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	35	ARG
1	A	79	ARG
1	A	88	SER
1	A	98	MET
1	A	166	GLU
1	A	196	ASP

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Mol	Chain	Res	Type
1	A	225	THR
1	A	227	ASP
1	A	228	THR
1	A	268	LYS
1	A	270	LEU
2	B	36	GLU
2	B	70	PHE
2	B	90	PRO
3	C	5	GLN
4	D	5	GLN
4	D	24	HIS
4	D	25	SER
4	D	28	SER
4	D	30(A)	ASP
4	D	40	SER
4	D	58	ARG
4	D	74	THR
4	D	83	ARG
4	D	92	LEU
4	D	129	ARG
4	D	132	LYS
4	D	164	THR
4	D	191	ASN
5	E	17	GLN
5	E	24	ASP
5	E	29	HIS
5	E	63	ASP
5	E	71	GLU
5	E	84	GLN
5	E	96	LEU
5	E	121	LYS
5	E	139	SER
5	E	157	HIS
5	E	187	ASN
5	E	194	SER
5	E	196	ARG
5	E	200	SER
5	E	202	THR
5	E	222	GLU
5	E	245	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	77	ASN
1	A	263	HIS
2	B	8	GLN
3	C	5	GLN
4	D	19	HIS
4	D	33	HIS
4	D	56	ASN
4	D	115	HIS
4	D	191	ASN
5	E	29	HIS
5	E	51	ASN
5	E	80	GLN
5	E	122	ASN
5	E	223	ASN
5	E	236	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 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	276/276 (100%)	0.76	34 (12%) 5 4	17, 35, 47, 56	1 (0%)
2	B	99/99 (100%)	0.78	12 (12%) 6 4	29, 40, 50, 56	0
3	C	9/9 (100%)	0.65	0 100 100	33, 36, 38, 42	0
4	D	201/201 (100%)	0.50	6 (2%) 54 54	27, 38, 49, 65	0
5	E	241/241 (100%)	0.29	4 (1%) 73 74	25, 35, 48, 59	0
All	All	826/826 (100%)	0.56	56 (6%) 20 19	17, 36, 49, 65	1 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	PRO	5.0
1	A	197	HIS	4.9
1	A	195	SER	4.4
1	A	199	VAL	3.9
1	A	181	ARG	3.6
2	B	48	LYS	3.6
1	A	1	GLY	3.6
1	A	259	CYS	3.6
2	B	71	THR	3.6
1	A	252	GLY	3.5
2	B	75	LYS	3.4
1	A	218	GLN	3.4
1	A	219	ARG	3.3
4	D	187	PHE	3.3
1	A	250	PRO	3.1
1	A	217	TRP	3.0
5	E	247	ASP	2.8
1	A	275	GLU	2.8
2	B	16	GLU	2.7
5	E	223	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	2	SER	2.7
4	D	134	SER	2.7
1	A	225	THR	2.7
1	A	222	GLU	2.7
2	B	43	GLY	2.6
2	B	72	PRO	2.6
1	A	196	ASP	2.6
1	A	273	ARG	2.6
2	B	70	PHE	2.6
1	A	216	THR	2.6
1	A	226	GLN	2.5
1	A	255	GLN	2.5
1	A	269	PRO	2.5
4	D	129	ARG	2.5
1	A	220	ASP	2.5
2	B	44	GLU	2.5
1	A	221	GLY	2.4
1	A	224	GLN	2.4
1	A	201	LEU	2.3
1	A	249	VAL	2.3
4	D	61	MET	2.3
2	B	15	ALA	2.3
1	A	257	TYR	2.3
1	A	258	THR	2.2
1	A	256	ARG	2.2
4	D	183	ASN	2.2
2	B	20	SER	2.2
2	B	47	GLU	2.2
4	D	133	SER	2.2
5	E	187	ASN	2.2
1	A	230	LEU	2.1
1	A	247	VAL	2.1
1	A	254	GLU	2.1
2	B	78	TYR	2.0
5	E	66	PHE	2.0
1	A	190	THR	2.0

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.