



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:12 AM UTC

PDB ID : 8F5A / pdb_00008f5a
Title : Crystal Structure of KS1 TCR in complex with HLA-B*57:01-TW10
Authors : Chatzileontiadou, D.S.M.; Lobos, C.A.; Gras, S.
Deposited on : 2022-11-12
Resolution : 1.95 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
Mogul : 2022.3.0, CSD as543be (2022)
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

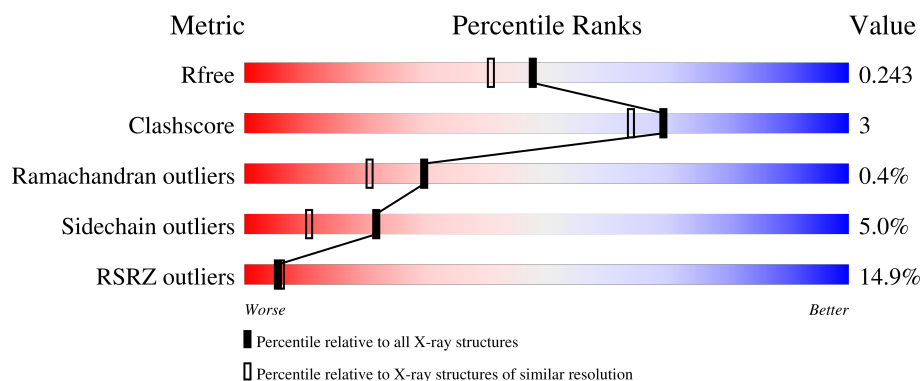
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	278	15% 86% 14% .
2	B	99	15% 85% 15%
3	C	208	17% 88% 6% ..
4	D	239	13% 87% 13%
5	E	10	100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7086 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 heavy chain HLA-B*57:01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	5	0
			2255	1413	408	425	9			

- 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	1	0
			833	532	140	158	3			

- Molecule 3 is a protein called KS1 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	203	Total	C	N	O	S	0	2	0
			1516	947	256	304	9			

- Molecule 4 is a protein called KS1 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	238	Total	C	N	O	S	0	8	0
			1907	1205	333	363	6			

- Molecule 5 is a protein called TW10 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	10	Total	C	N	O	0	0	0
			82	51	13	18			

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	188	Total	O	0	0
			188	188		
9	B	50	Total	O	0	0
			50	50		
9	C	109	Total	O	0	0
			109	109		

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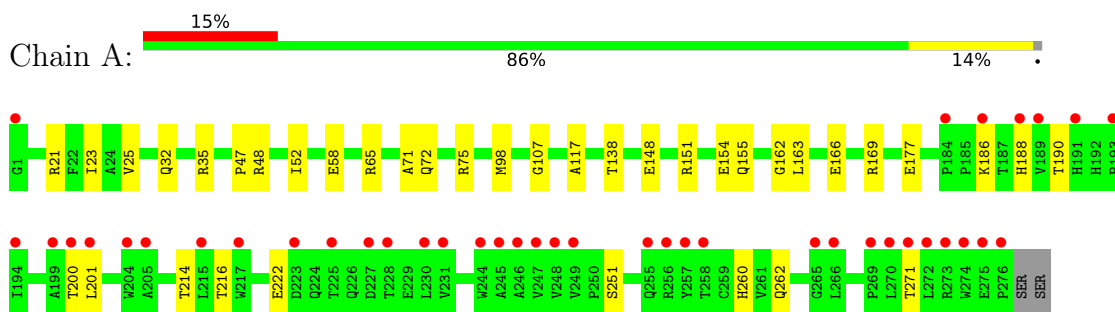
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	130	Total 130	O 130	0	0
9	E	9	Total 9	O 9	0	0

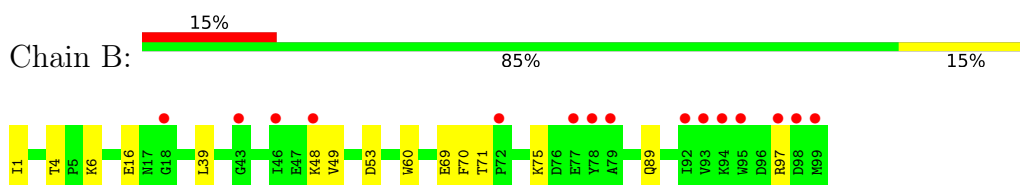
3 Residue-property plots [i](#)

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.

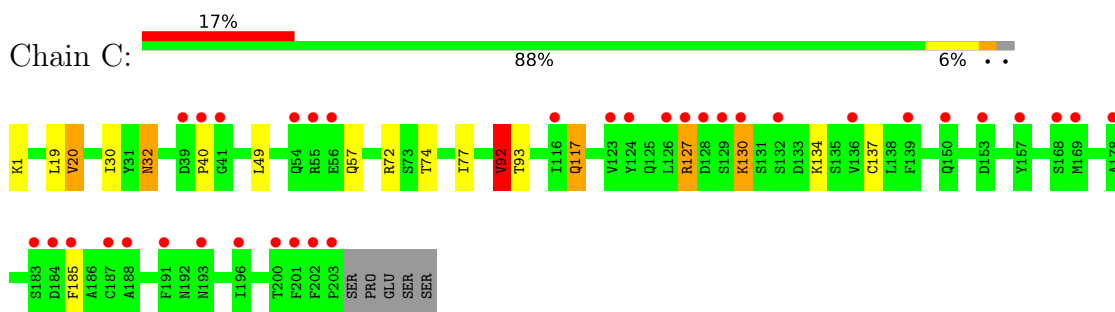
- Molecule 1: heavy chain HLA-B*57:01



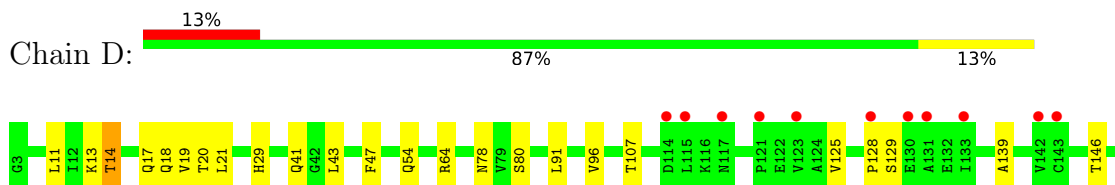
- Molecule 2: Beta-2-microglobulin

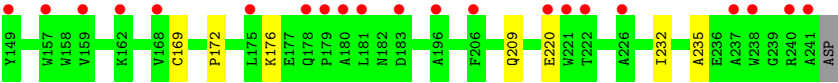


- Molecule 3: KS1 TCR alpha chain



- Molecule 4: KS1 TCR beta chain





- Molecule 5: TW10 peptide

Chain E:

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.02Å 55.80Å 122.71Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	46.63 – 1.95 46.63 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.63-1.95) 100.0 (46.63-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.202 , 0.237 0.207 , 0.243	Depositor DCC
R_{free} test set	3406 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ACT, CL

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	0.76	1/2332 (0.0%)	0.94	0/3171
2	B	0.64	0/859	0.99	2/1162 (0.2%)
3	C	0.72	0/1549	1.01	2/2107 (0.1%)
4	D	0.68	0/1983	0.97	0/2699
5	E	0.82	0/83	0.96	0/111
All	All	0.71	1/6806 (0.0%)	0.97	4/9250 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	MET	SD-CE	-5.85	1.65	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	32	ASN	CA-CB-CG	5.83	118.43	112.60
3	C	92	VAL	N-CA-CB	-5.61	102.25	111.44
2	B	70	PHE	CA-CB-CG	5.40	119.20	113.80
2	B	71	THR	CB-CA-C	5.33	117.28	110.34

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	2255	0	2143	18	0
2	B	833	0	803	5	0
3	C	1516	0	1451	12	0
4	D	1907	0	1818	16	0
5	E	82	0	78	0	0
6	A	4	0	3	1	0
7	A	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	188	0	0	1	0
9	B	50	0	0	0	0
9	C	109	0	0	0	0
9	D	130	0	0	0	0
9	E	9	0	0	0	0
All	All	7086	0	6296	45	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 3.

All (45) 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:65:ARG:HH12	4:D:54:GLN:HE21	1.13	0.91
1:A:65:ARG:NH1	4:D:54:GLN:HE21	1.89	0.71
3:C:32:ASN:HB2	3:C:93:THR:HG22	1.73	0.70
4:D:14:THR:O	4:D:17:GLN:HG2	1.95	0.66
1:A:48:ARG:HD2	2:B:53:ASP:OD2	1.94	0.66
1:A:214:THR:HB	1:A:262:GLN:HB3	1.83	0.60
4:D:13:LYS:HG3	4:D:19:VAL:CG1	2.33	0.57
4:D:21:LEU:HD22	4:D:107:THR:HG21	1.86	0.57
1:A:65:ARG:HH12	4:D:54:GLN:NE2	1.92	0.55
3:C:20:VAL:HG13	3:C:74:THR:HG23	1.90	0.54
1:A:188:HIS:CE1	1:A:190:THR:HG23	2.42	0.54
6:A:301:ACT:H2	9:A:438:HOH:O	2.06	0.54
2:B:48:LYS:NZ	2:B:69:GLU:H	2.06	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.53
4:D:209:GLN:HG3	4:D:232:ILE:HG23	1.91	0.52
1:A:107:GLY:O	1:A:169:ARG:NH2	2.42	0.51
3:C:32:ASN:HB2	3:C:93:THR:CG2	2.40	0.51
4:D:125:VAL:HG23	4:D:235:ALA:HB3	1.92	0.51
3:C:19:LEU:HD11	3:C:77:ILE:HD12	1.94	0.49
4:D:128:PRO:HG2	4:D:139:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:ARG:HB2	4:D:80:SER:HB2	1.93	0.49
1:A:21:ARG:NE	1:A:23:ILE:HD11	2.27	0.49
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.79	0.47
1:A:260:HIS:CE1	1:A:271:THR:HG22	2.49	0.47
2:B:48:LYS:HZ3	2:B:69:GLU:H	1.63	0.47
4:D:29:HIS:HA	4:D:96:VAL:HB	1.97	0.47
3:C:127:ARG:NH1	3:C:130:LYS:HB3	2.30	0.47
3:C:40:PRO:HG3	4:D:172:PRO:HB3	1.98	0.46
4:D:43:LEU:HD21	4:D:91:LEU:HD12	1.97	0.46
4:D:13:LYS:HG3	4:D:19:VAL:HG12	1.98	0.45
3:C:137:CYS:SG	3:C:185:PHE:CE2	3.09	0.45
1:A:162:GLY:O	1:A:166:GLU:HG3	2.17	0.44
1:A:260:HIS:CE1	1:A:271:THR:CG2	3.00	0.44
1:A:25[A]:VAL:HG13	1:A:32:GLN:HG3	2.00	0.43
3:C:49:LEU:O	3:C:57:GLN:HG3	2.18	0.42
4:D:128:PRO:CG	4:D:139:ALA:HB1	2.49	0.42
1:A:71:ALA:O	1:A:75:ARG:HG3	2.20	0.42
3:C:130:LYS:HB3	3:C:130:LYS:HE3	1.86	0.42
1:A:151:ARG:HD2	1:A:154:GLU:OE2	2.20	0.41
2:B:39:LEU:HB2	2:B:49:VAL:HG21	2.02	0.41
3:C:117:GLN:NE2	3:C:117:GLN:H	2.19	0.41
3:C:30:ILE:HD13	3:C:92:VAL:HG22	2.03	0.41
1:A:47:PRO:HB3	1:A:52:ILE:HG23	2.03	0.40
3:C:134:LYS:HE3	4:D:146:THR:HG21	2.02	0.40
1:A:72[A]:GLN:NE2	1:A:75:ARG:HH11	2.19	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	279/278 (100%)	271 (97%)	7 (2%)	1 (0%)	30 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	98/99 (99%)	94 (96%)	4 (4%)	0	100	100
3	C	203/208 (98%)	195 (96%)	6 (3%)	2 (1%)	12	5
4	D	244/239 (102%)	237 (97%)	7 (3%)	0	100	100
5	E	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	832/834 (100%)	804 (97%)	25 (3%)	3 (0%)	30	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	127	ARG
1	A	251	SER
3	C	130	LYS

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	233/232 (100%)	220 (94%)	13 (6%)	19	8
2	B	95/94 (101%)	88 (93%)	7 (7%)	13	4
3	C	167/183 (91%)	162 (97%)	5 (3%)	36	27
4	D	210/207 (101%)	198 (94%)	12 (6%)	18	8
5	E	9/9 (100%)	9 (100%)	0	100	100
All	All	714/725 (98%)	677 (95%)	37 (5%)	22	9

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	58	GLU
1	A	138[A]	THR
1	A	138[B]	THR
1	A	148	GLU

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Mol	Chain	Res	Type
1	A	155	GLN
1	A	163	LEU
1	A	177	GLU
1	A	186	LYS
1	A	200	THR
1	A	201	LEU
1	A	216	THR
1	A	222	GLU
2	B	1	ILE
2	B	4	THR
2	B	6	LYS
2	B	16	GLU
2	B	75	LYS
2	B	89	GLN
2	B	97	ARG
3	C	1	LYS
3	C	20	VAL
3	C	72	ARG
3	C	92	VAL
3	C	117	GLN
4	D	11	LEU
4	D	14	THR
4	D	18	GLN
4	D	20	THR
4	D	41	GLN
4	D	47	PHE
4	D	78[A]	ASN
4	D	78[B]	ASN
4	D	129	SER
4	D	169	CYS
4	D	176	LYS
4	D	220	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	155	GLN
1	A	188	HIS
1	A	192	HIS
1	A	224	GLN
1	A	260	HIS

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Mol	Chain	Res	Type
2	B	13	HIS
3	C	117	GLN
3	C	125	GLN
4	D	41	GLN
4	D	54	GLN
4	D	211	GLN
4	D	223	GLN
4	D	231	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ACT	A	301	-	3,3,3	0.97	0	3,3,3	0.99	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	ACT	1	0

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	276/278 (99%)	0.65	41 (14%) 5 6	11, 35, 86, 93	5 (1%)
2	B	99/99 (100%)	0.98	15 (15%) 5 6	25, 49, 73, 78	1 (1%)
3	C	203/208 (97%)	1.00	35 (17%) 4 4	20, 49, 79, 91	3 (1%)
4	D	238/239 (99%)	0.83	32 (13%) 7 8	14, 48, 77, 88	9 (3%)
5	E	10/10 (100%)	-0.60	0 100 100	19, 21, 24, 29	0
All	All	826/834 (99%)	0.81	123 (14%) 5 6	11, 43, 81, 93	18 (2%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	183	ASP	4.7
3	C	127	ARG	4.5
3	C	126	LEU	4.3
1	A	248	VAL	4.2
3	C	169	MET	4.2
4	D	180	ALA	4.1
1	A	257	TYR	4.0
3	C	55	ARG	4.0
1	A	249	VAL	4.0
3	C	128	ASP	4.0
1	A	217	TRP	3.9
1	A	247	VAL	3.9
1	A	270	LEU	3.8
1	A	201	LEU	3.8
4	D	181	LEU	3.7
4	D	226	ALA	3.7
1	A	204	TRP	3.7
3	C	129	SER	3.6
3	C	40	PRO	3.6
3	C	196	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	272	LEU	3.5
1	A	225	THR	3.5
1	A	230	LEU	3.4
1	A	205	ALA	3.3
1	A	269	PRO	3.3
4	D	241	ALA	3.3
3	C	202	PHE	3.3
3	C	187	CYS	3.3
4	D	221	TRP	3.3
1	A	215	LEU	3.2
2	B	43	GLY	3.2
1	A	189	VAL	3.2
3	C	183	SER	3.1
1	A	193	PRO	3.1
4	D	128	PRO	3.1
1	A	194	ILE	3.0
1	A	200	THR	3.0
3	C	54	GLN	3.0
3	C	150	GLN	3.0
2	B	99	MET	3.0
3	C	153	ASP	2.9
2	B	95	TRP	2.9
4	D	196	ALA	2.9
1	A	1	GLY	2.8
2	B	46	ILE	2.8
2	B	77	GLU	2.8
3	C	130	LYS	2.8
4	D	237	ALA	2.7
1	A	191	HIS	2.7
3	C	191	PHE	2.7
2	B	92	ILE	2.7
1	A	223	ASP	2.7
1	A	255	GLN	2.7
1	A	188	HIS	2.7
4	D	131	ALA	2.6
4	D	238[A]	TRP	2.6
4	D	115	LEU	2.6
1	A	227	ASP	2.6
2	B	98	ASP	2.6
1	A	199	ALA	2.6
1	A	186	LYS	2.6
2	B	48	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	228	THR	2.6
1	A	276	PRO	2.5
2	B	78	TYR	2.5
4	D	157	TRP	2.5
3	C	41	GLY	2.5
2	B	93	VAL	2.5
4	D	220	GLU	2.5
1	A	274	TRP	2.5
3	C	124	TYR	2.4
3	C	132	SER	2.4
2	B	79	ALA	2.4
1	A	244	TRP	2.4
1	A	273	ARG	2.4
4	D	143	CYS	2.4
3	C	178	ALA	2.4
3	C	56	GLU	2.4
4	D	142	VAL	2.4
3	C	157	TYR	2.4
3	C	193	ASN	2.4
1	A	231	VAL	2.4
3	C	185	PHE	2.3
3	C	136	VAL	2.3
1	A	256	ARG	2.3
3	C	39	ASP	2.3
4	D	123	VAL	2.3
2	B	18	GLY	2.3
1	A	266	LEU	2.3
3	C	200	THR	2.3
4	D	175	LEU	2.3
3	C	203	PRO	2.2
4	D	130	GLU	2.2
3	C	168	SER	2.2
3	C	184	ASP	2.2
4	D	179	PRO	2.2
4	D	206	PHE	2.2
4	D	240	ARG	2.2
4	D	159	VAL	2.2
1	A	245	ALA	2.2
1	A	275	GLU	2.2
4	D	168	VAL	2.2
2	B	72	PRO	2.2
1	A	246	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	188	ALA	2.2
2	B	97	ARG	2.2
1	A	265	GLY	2.1
4	D	162	LYS	2.1
4	D	178	GLN	2.1
2	B	94	LYS	2.1
3	C	201	PHE	2.1
1	A	258	THR	2.1
1	A	271	THR	2.1
4	D	222	THR	2.1
3	C	116	ILE	2.0
3	C	139	PHE	2.0
4	D	117	ASN	2.0
4	D	114	ASP	2.0
4	D	133	ILE	2.0
4	D	149	TYR	2.0
1	A	184	PRO	2.0
4	D	121	PRO	2.0
3	C	123	VAL	2.0

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](#)

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($\text{\AA}^2$)	Q<0.9
8	CL	C	301	1/1	0.81	0.19	80,80,80,80	0
7	NA	A	302	1/1	0.82	0.16	67,67,67,67	0
6	ACT	A	301	4/4	0.85	0.17	44,45,45,46	0
8	CL	D	301	1/1	0.87	0.21	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.