



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:41 PM UTC

PDB ID : 8WUL / pdb_00008wul
Title : Crystal structure of affinity enhanced TCR in complex with HLA-A*11:01 bound to KRAS-G12V peptide (VVGAVGVGK)
Authors : Zhang, M.Y.; Luo, L.J.; Xu, W.; Guan, F.H.; Wang, X.Y.; Zhu, P.; Zhang, J.H.; Zhou, X.Y.; Wang, F.; Ye, S.
Deposited on : 2023-10-20
Resolution : 2.36 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
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

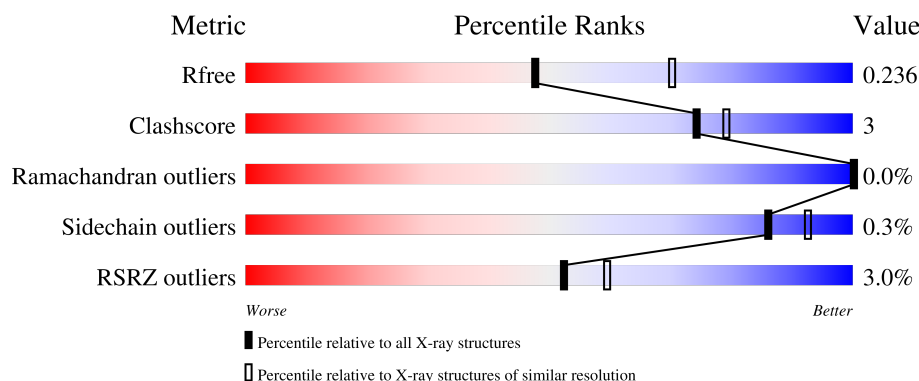
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	198	4% 79% 9% 12%
1	C	198	3% 80% 8% 12%
1	E	198	3% 77% 12% 11%
1	G	198	5% 76% 13% 11%
2	B	239	2% 91% 8%

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Mol	Chain	Length	Quality of chain
2	D	239	91% 9%
2	F	239	95% 5%
2	H	239	91% 9%
3	I	274	88% 12%
3	L	274	92% 8%
3	O	274	93% 7%
3	R	274	94% 6%
4	J	99	87% 13%
4	M	99	91% 8%
4	P	99	95% 5%
4	S	99	90% 10%
5	K	9	89% 11%
5	N	9	78% 22%
5	Q	9	100%
5	T	9	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26016 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 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	175	Total	C	N	O	S	0	0	0
			1362	850	232	269	11			
1	A	175	Total	C	N	O	S	0	0	0
			1362	850	232	269	11			
1	E	176	Total	C	N	O	S	0	0	0
			1371	855	234	271	11			
1	G	177	Total	C	N	O	S	0	0	0
			1380	860	236	273	11			

- Molecule 2 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	239	Total	C	N	O	S	0	0	0
			1923	1219	335	359	10			
2	B	237	Total	C	N	O	S	0	0	0
			1909	1211	333	355	10			
2	F	239	Total	C	N	O	S	0	0	0
			1923	1219	335	359	10			
2	H	238	Total	C	N	O	S	0	0	0
			1915	1215	334	356	10			

- Molecule 3 is a protein called MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
3	I	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
3	O	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
3	R	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
4	J	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
4	P	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
4	S	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

- Molecule 5 is a protein called KRAS-G12V nonamer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	9	Total	C	N	O	0	0	0
			54	35	10	9			
5	K	9	Total	C	N	O	0	0	0
			54	35	10	9			
5	Q	9	Total	C	N	O	0	0	0
			54	35	10	9			
5	T	9	Total	C	N	O	0	0	0
			54	35	10	9			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	14	Total	O	0	0
			14	14		
6	D	26	Total	O	0	0
			26	26		
6	A	18	Total	O	0	0
			18	18		
6	B	29	Total	O	0	0
			29	29		
6	E	20	Total	O	0	0
			20	20		
6	F	26	Total	O	0	0
			26	26		
6	G	18	Total	O	0	0
			18	18		
6	H	32	Total	O	0	0
			32	32		
6	L	33	Total	O	0	0
			33	33		

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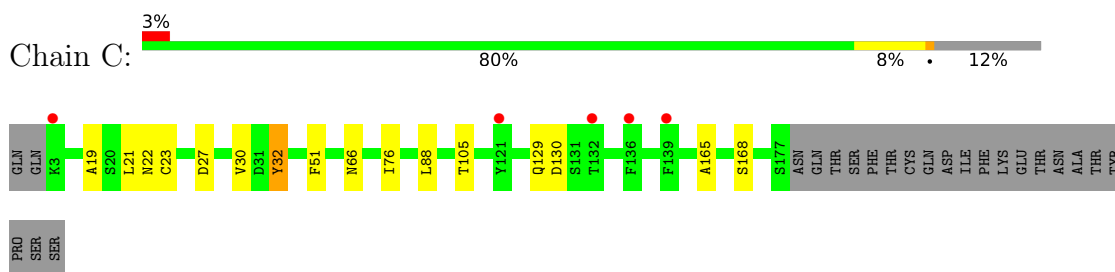
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	12	Total 12	O 12	0	0
6	N	1	Total 1	O 1	0	0
6	I	31	Total 31	O 31	0	0
6	J	3	Total 3	O 3	0	0
6	O	51	Total 51	O 51	0	0
6	P	26	Total 26	O 26	0	0
6	R	53	Total 53	O 53	0	0
6	S	10	Total 10	O 10	0	0

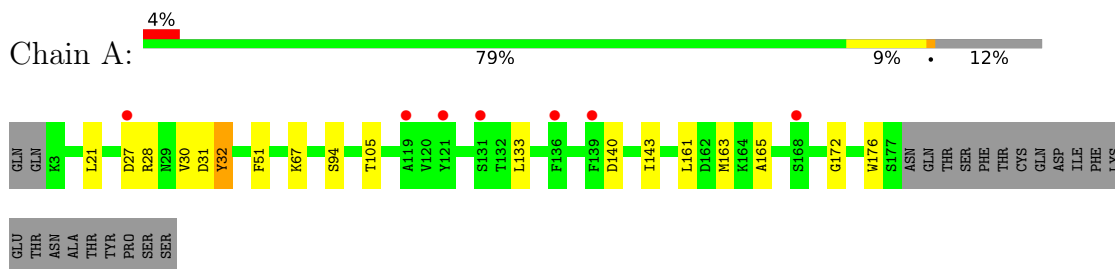
3 Residue-property plots [i](#)

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.

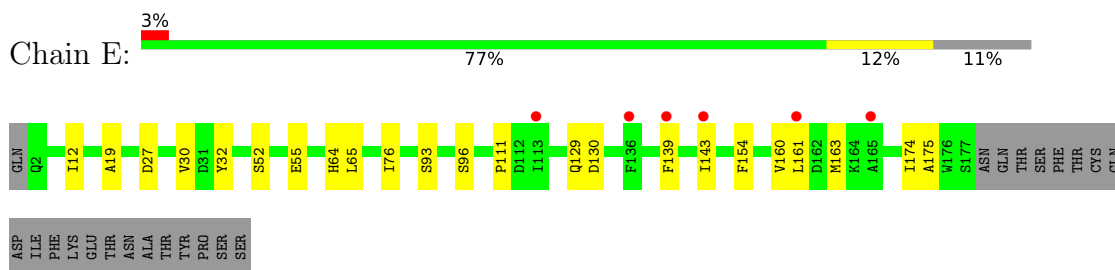
- Molecule 1: TCR alpha chain



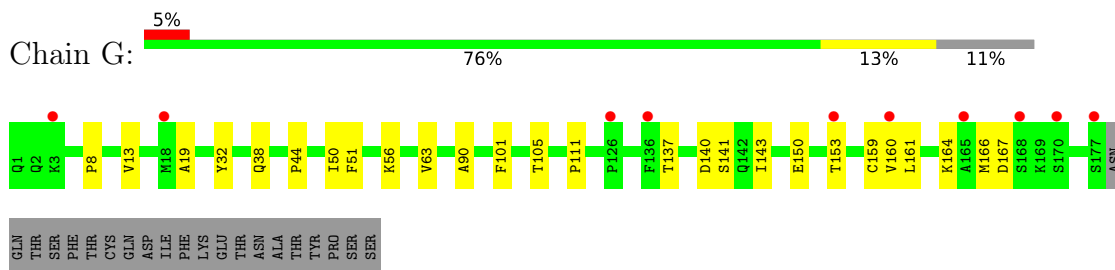
- Molecule 1: TCR alpha chain



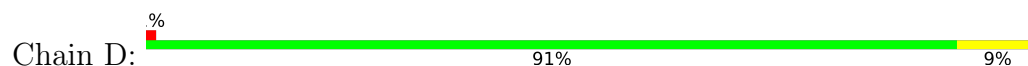
- Molecule 1: TCR alpha chain



- Molecule 1: TCR alpha chain



- Molecule 2: TCR beta chain



- Molecule 2: TCR beta chain



- Molecule 2: TCR beta chain



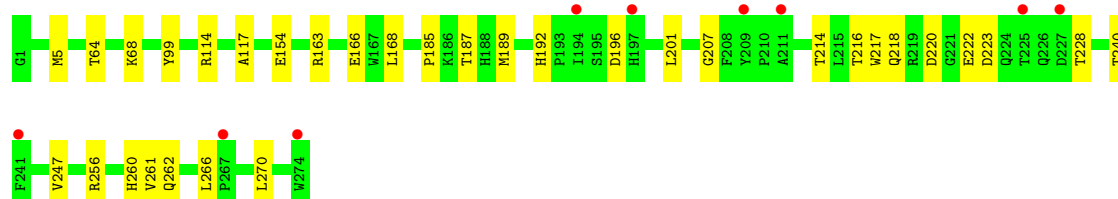
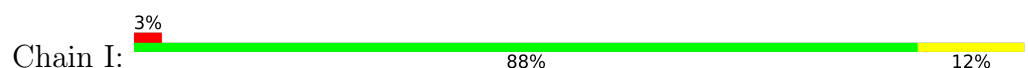
- Molecule 2: TCR beta chain



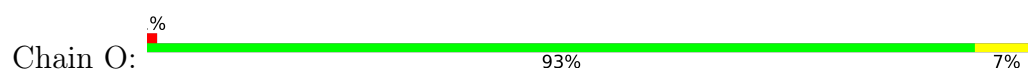
- Molecule 3: MHC class I antigen



- Molecule 3: MHC class I antigen

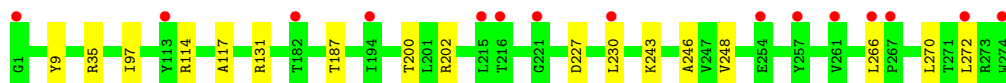
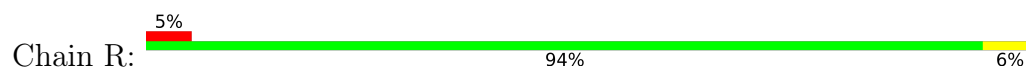


- Molecule 3: MHC class I antigen





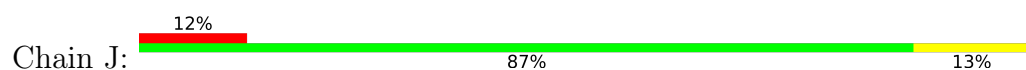
- Molecule 3: MHC class I antigen



- Molecule 4: Beta-2-microglobulin



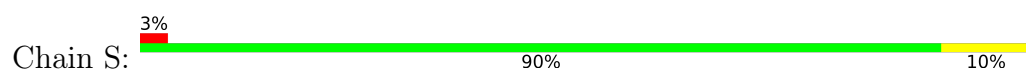
- Molecule 4: Beta-2-microglobulin



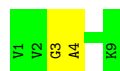
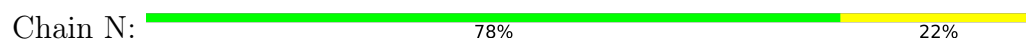
- Molecule 4: Beta-2-microglobulin



- Molecule 4: Beta-2-microglobulin



- Molecule 5: KRAS-G12V nonamer peptide



- Molecule 5: KRAS-G12V nonamer peptide

Chain K:  89% 11%



- Molecule 5: KRAS-G12V nonamer peptide

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: KRAS-G12V nonamer peptide

Chain T:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.75Å 96.33Å 123.12Å 94.56° 90.63° 93.20°	Depositor
Resolution (Å)	29.67 – 2.36 29.67 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.67-2.36) 97.9 (29.67-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.36Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.190 , 0.235 0.192 , 0.236	Depositor DCC
R_{free} test set	8042 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26016	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7639e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.09	0/1393	0.29	0/1885
1	C	0.10	0/1393	0.29	0/1885
1	E	0.10	0/1402	0.30	0/1897
1	G	0.10	0/1411	0.30	0/1909
2	B	0.10	0/1963	0.28	0/2659
2	D	0.10	0/1977	0.29	0/2679
2	F	0.09	0/1977	0.29	0/2679
2	H	0.10	0/1969	0.29	0/2668
3	I	0.10	0/2296	0.30	0/3117
3	L	0.10	0/2296	0.30	0/3117
3	O	0.11	0/2296	0.31	0/3117
3	R	0.11	0/2296	0.30	0/3117
4	J	0.10	0/851	0.31	0/1152
4	M	0.10	0/851	0.32	0/1152
4	P	0.11	0/851	0.32	0/1152
4	S	0.10	0/851	0.32	0/1152
5	K	0.10	0/53	0.33	0/70
5	N	0.08	0/53	0.33	0/70
5	Q	0.13	0/53	0.33	0/70
5	T	0.08	0/53	0.27	0/70
All	All	0.10	0/26285	0.30	0/35617

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 [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	1362	0	1313	10	0
1	C	1362	0	1313	9	0
1	E	1371	0	1321	12	0
1	G	1380	0	1332	16	0
2	B	1909	0	1843	12	0
2	D	1923	0	1856	12	0
2	F	1923	0	1856	9	0
2	H	1915	0	1852	14	0
3	I	2235	0	2085	21	0
3	L	2235	0	2085	16	0
3	O	2235	0	2085	11	0
3	R	2235	0	2085	10	0
4	J	828	0	794	8	0
4	M	828	0	794	6	0
4	P	828	0	794	3	0
4	S	828	0	794	6	0
5	K	54	0	65	0	0
5	N	54	0	65	3	0
5	Q	54	0	65	0	0
5	T	54	0	65	0	0
6	A	18	0	0	0	0
6	B	29	0	0	1	0
6	C	14	0	0	0	0
6	D	26	0	0	0	0
6	E	20	0	0	0	0
6	F	26	0	0	0	0
6	G	18	0	0	0	0
6	H	32	0	0	0	0
6	I	31	0	0	0	0
6	J	3	0	0	0	0
6	L	33	0	0	0	0
6	M	12	0	0	0	0
6	N	1	0	0	0	0
6	O	51	0	0	0	0
6	P	26	0	0	0	0
6	R	53	0	0	1	0
6	S	10	0	0	0	0
All	All	26016	0	24462	157	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 (157) 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)
2:B:23:GLN:HE21	2:B:30:MET:HE2	1.46	0.79
1:G:159:CYS:HB3	2:H:188:ARG:HH12	1.51	0.76
3:R:200:THR:HG22	3:R:248:VAL:HG12	1.74	0.69
3:L:32:GLN:NE2	4:M:53:ASP:OD2	2.27	0.66
1:C:66:ASN:ND2	1:E:12:ILE:O	2.29	0.65
1:C:21:LEU:HD22	1:C:105:THR:HG21	1.80	0.64
4:M:36:GLU:HG3	4:M:83:ASN:HB3	1.80	0.63
2:H:179:SER:HG	2:H:182:SER:HG	1.45	0.61
3:L:189:MET:HE3	3:L:217:TRP:HH2	1.66	0.61
1:A:31:ASP:HA	1:A:67:LYS:HD3	1.82	0.61
3:R:266:LEU:HD13	3:R:270:LEU:HD13	1.83	0.60
4:J:39:LEU:HD23	4:J:80:CYS:HB3	1.83	0.60
3:L:189:MET:HE2	3:L:201:LEU:HD22	1.83	0.60
3:O:189:MET:HE2	3:O:274:TRP:HB2	1.84	0.59
3:O:220:ASP:OD2	3:O:256:ARG:NH1	2.35	0.59
1:G:111:PRO:HG3	1:G:160:VAL:HG11	1.85	0.59
3:O:114:ARG:NH1	3:O:116:ASP:OD1	2.36	0.59
3:R:230:LEU:HD11	3:R:243:LYS:HE2	1.85	0.58
4:P:39:LEU:HD23	4:P:80:CYS:HB3	1.84	0.58
2:D:192:SER:HB2	2:D:195:PHE:H	1.69	0.57
1:G:137:THR:OG1	2:H:190:ARG:NH2	2.38	0.57
4:J:19:LYS:NZ	4:J:20:SER:O	2.37	0.57
3:I:214:THR:HB	3:I:262:GLN:HB2	1.87	0.57
4:S:39:LEU:HD23	4:S:80:CYS:HB3	1.86	0.57
3:L:35:ARG:HH11	3:L:48:ARG:HH21	1.51	0.56
1:G:140:ASP:HB3	1:G:143:ILE:HD13	1.88	0.56
3:O:189:MET:HE3	3:O:201:LEU:HB3	1.88	0.55
2:B:34:ARG:HH21	2:B:44:MET:HE3	1.70	0.55
1:C:165:ALA:HB3	1:C:168:SER:HB2	1.88	0.54
4:J:20:SER:HA	4:J:71:THR:HG22	1.89	0.54
1:C:32:TYR:HB3	1:C:51:PHE:HA	1.89	0.54
1:E:55:GLU:HG3	1:E:64:HIS:CD2	2.42	0.54
3:R:131:ARG:NH1	6:R:302:HOH:O	2.41	0.54
2:D:224:LYS:HG3	2:D:226:VAL:HG13	1.89	0.54
3:I:220:ASP:OD2	3:I:256:ARG:NH2	2.41	0.53
1:A:32:TYR:HB3	1:A:51:PHE:HA	1.91	0.53
3:I:218:GLN:HG2	3:I:223:ASP:HA	1.90	0.53
3:L:5:MET:HB2	3:L:168:LEU:HD13	1.90	0.53
4:M:45:ARG:NH1	4:M:47:GLU:OE1	2.42	0.53
1:A:21:LEU:HD22	1:A:105:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:189:MET:HE3	3:I:217:TRP:HH2	1.74	0.52
2:H:171:THR:HG23	2:H:187:SER:HB2	1.90	0.52
1:A:28:ARG:NH1	3:I:166:GLU:OE2	2.41	0.52
3:I:196:ASP:OD1	3:I:196:ASP:N	2.40	0.52
3:I:216:THR:HB	3:I:260:HIS:HB2	1.92	0.51
1:C:19:ALA:HB3	1:C:76:ILE:HB	1.92	0.51
3:R:227:ASP:HB3	3:R:248:VAL:HG22	1.93	0.51
3:L:216:THR:HG23	3:L:260:HIS:HB2	1.93	0.51
1:E:111:PRO:HG3	1:E:160:VAL:HG11	1.92	0.50
2:F:139:LYS:HD2	2:F:190:ARG:HH21	1.76	0.50
1:G:150:GLU:HB3	1:G:153:THR:HG22	1.93	0.50
1:G:38:GLN:HB3	1:G:44:PRO:HA	1.92	0.50
1:C:27:ASP:HB3	1:C:30:VAL:HG23	1.94	0.50
3:R:187:THR:HG22	3:R:272:LEU:HD22	1.93	0.50
2:D:19:LEU:HD22	2:D:108:THR:HG21	1.93	0.49
1:E:93:SER:O	1:E:96:SER:OG	2.30	0.49
2:D:153:HIS:HB3	2:D:210:HIS:HB2	1.93	0.49
2:B:57:THR:HG22	2:B:59:SER:H	1.77	0.49
2:B:150:PHE:HA	6:B:303:HOH:O	2.11	0.49
3:L:35:ARG:HG2	3:L:48:ARG:HG2	1.94	0.49
1:C:129:GLN:HG3	1:C:130:ASP:H	1.76	0.49
2:B:128:GLU:OE1	2:B:237:ARG:NH2	2.38	0.49
1:E:19:ALA:HB3	1:E:76:ILE:HB	1.93	0.49
2:H:211:GLY:H	2:H:227:THR:HG22	1.77	0.49
2:D:22:GLU:OE1	2:D:71:HIS:NE2	2.46	0.49
4:P:45:ARG:NH2	4:P:47:GLU:OE2	2.46	0.48
3:O:200:THR:HG22	3:O:248:VAL:HG22	1.95	0.48
2:F:215:GLU:N	2:F:215:GLU:OE1	2.44	0.48
3:L:109:PHE:HB2	3:L:165:VAL:HG21	1.94	0.48
1:G:50:ILE:HD12	1:G:63:VAL:HG13	1.95	0.48
2:H:153:HIS:HB3	2:H:210:HIS:HB2	1.95	0.48
3:I:189:MET:HE2	3:I:201:LEU:HD22	1.96	0.48
3:I:5:MET:HB2	3:I:168:LEU:HD13	1.95	0.47
2:F:81:PRO:HA	2:F:112:VAL:HB	1.97	0.47
1:A:27:ASP:HB3	1:A:30:VAL:HG23	1.96	0.47
2:H:237:ARG:NH1	2:H:238:ALA:O	2.47	0.47
1:G:32:TYR:HB3	1:G:51:PHE:HA	1.95	0.47
3:I:187:THR:HG21	3:I:261:VAL:HG21	1.97	0.47
3:I:99:TYR:HB3	3:I:114:ARG:HG3	1.97	0.47
3:I:192:HIS:NE2	4:J:98:ASP:O	2.48	0.47
3:R:117:ALA:HB2	4:S:60:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:HB3	1:A:143:ILE:HG23	1.97	0.46
2:B:22:GLU:OE1	2:B:24:TYR:OH	2.28	0.46
3:I:117:ALA:HB2	4:J:60:TRP:CE2	2.50	0.46
2:D:171:THR:HG23	2:D:187:SER:HB2	1.98	0.45
4:J:37:VAL:HG22	4:J:82:VAL:HG22	1.97	0.45
3:O:117:ALA:HB2	4:P:60:TRP:CE2	2.50	0.45
2:D:81:PRO:HA	2:D:112:VAL:HB	1.99	0.45
1:A:172:GLY:HA3	2:B:188:ARG:NH1	2.32	0.45
2:H:19:LEU:HD22	2:H:108:THR:HG21	1.99	0.45
1:E:139:PHE:HB2	1:E:143:ILE:HD12	1.98	0.45
3:I:207:GLY:HA2	3:I:240:THR:HB	1.99	0.45
1:G:56:LYS:HB3	1:G:63:VAL:HG12	1.99	0.45
2:H:122:PRO:HB3	2:H:149:PHE:HB3	1.99	0.45
2:H:22:GLU:OE1	2:H:24:TYR:OH	2.28	0.44
3:I:266:LEU:HD13	3:I:270:LEU:HD13	1.99	0.44
3:R:9:TYR:HB2	3:R:97:ILE:HB	1.99	0.44
1:G:90:ALA:HB2	1:G:101:PHE:CD1	2.53	0.44
3:O:219:ARG:HE	3:O:256:ARG:HH11	1.65	0.44
2:B:81:PRO:HA	2:B:112:VAL:HB	2.00	0.44
3:I:64:THR:HG22	3:I:68:LYS:HE2	1.98	0.44
3:R:35:ARG:HD3	4:S:53:ASP:CG	2.42	0.44
4:S:23:LEU:O	4:S:67:TYR:HA	2.18	0.44
2:D:122:PRO:HB3	2:D:149:PHE:HB3	1.98	0.44
1:C:22:ASN:OD1	1:C:23:CYS:N	2.51	0.43
3:I:228:THR:HA	3:I:247:VAL:HG12	1.99	0.43
1:G:140:ASP:OD1	1:G:141:SER:N	2.52	0.43
2:F:198:ASN:HB3	2:F:201:ASN:ND2	2.33	0.43
1:G:161:LEU:HD23	2:H:188:ARG:NE	2.33	0.43
3:R:202:ARG:HG3	3:R:246:ALA:HB2	2.01	0.43
3:O:9:TYR:CE2	3:O:70:GLN:HG2	2.54	0.43
1:A:163:MET:C	1:A:165:ALA:H	2.27	0.43
2:B:41:LEU:HD23	2:B:41:LEU:HA	1.84	0.43
3:I:185:PRO:HD2	3:I:266:LEU:HG	2.01	0.43
1:A:94:SER:O	3:I:163:ARG:HD2	2.19	0.42
1:E:129:GLN:HG2	1:E:130:ASP:H	1.82	0.42
1:E:174:ILE:HD11	2:F:188:ARG:HH12	1.84	0.42
3:L:228:THR:HG22	3:L:247:VAL:HG12	2.01	0.42
3:O:219:ARG:HE	3:O:256:ARG:NH1	2.16	0.42
3:O:230:LEU:HD11	3:O:243:LYS:HE3	2.01	0.42
3:L:35:ARG:HH11	3:L:48:ARG:NH2	2.15	0.42
1:G:164:LYS:HB3	1:G:164:LYS:HE2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:ARG:NH2	5:N:4:ALA:O	2.53	0.42
1:E:52:SER:C	1:E:65:LEU:HD23	2.45	0.42
1:E:163:MET:HE1	2:F:139:LYS:HD3	2.01	0.41
2:D:202:HIS:HB3	2:D:235:TRP:CD1	2.55	0.41
1:G:8:PRO:O	1:G:105:THR:OG1	2.30	0.41
1:G:166:MET:HG3	1:G:167:ASP:H	1.85	0.41
2:H:41:LEU:HD23	2:H:41:LEU:HA	1.88	0.41
2:B:123:LYS:HE3	2:B:123:LYS:HB2	1.91	0.41
3:L:192:HIS:NE2	4:M:98:ASP:O	2.52	0.41
3:I:222:GLU:OE1	3:I:222:GLU:N	2.52	0.41
2:F:202:HIS:CE1	2:F:233:GLU:HB3	2.55	0.41
1:A:133:LEU:HB3	1:A:176:TRP:HB3	2.03	0.41
3:L:159:TYR:CE1	5:N:3:GLY:HA3	2.55	0.41
3:L:220:ASP:OD2	3:L:256:ARG:NH1	2.54	0.41
3:I:154:GLU:OE1	3:I:154:GLU:N	2.48	0.41
4:S:6:LYS:O	4:S:27:VAL:HA	2.20	0.41
2:B:172:ASP:HB2	2:B:185:LEU:HD12	2.03	0.41
2:H:211:GLY:N	2:H:227:THR:HG22	2.36	0.41
3:L:117:ALA:HB2	4:M:60:TRP:CE2	2.55	0.41
3:O:5:MET:HB2	3:O:168:LEU:HD13	2.03	0.41
3:L:99:TYR:CE1	5:N:4:ALA:HB2	2.56	0.41
2:B:122:PRO:HB3	2:B:149:PHE:HB3	2.03	0.40
3:L:15:PRO:HB3	3:L:89:GLU:O	2.22	0.40
1:C:88:LEU:HD13	2:D:41:LEU:HD12	2.04	0.40
2:F:41:LEU:HD23	2:F:41:LEU:HA	1.90	0.40
1:G:13:VAL:HG21	1:G:19:ALA:HB2	2.03	0.40
1:E:27:ASP:HB3	1:E:30:VAL:HG23	2.04	0.40
4:M:96:ASP:HB3	4:M:99:MET:HE3	2.03	0.40
4:S:20:SER:HA	4:S:71:THR:HG22	2.04	0.40
2:D:121:PRO:HD3	2:D:225:PRO:HB3	2.03	0.40
2:H:43:PHE:CZ	2:H:46:SER:HB2	2.57	0.40
1:E:154:PHE:O	1:E:175:ALA:HA	2.22	0.40
2:F:177:LYS:HE3	2:F:180:ASN:HA	2.04	0.40
4:J:6:LYS:O	4:J:27:VAL:HA	2.21	0.40
4:J:73:THR:O	4:J:97:ARG:NH2	2.54	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	173/198 (87%)	166 (96%)	7 (4%)	0	100	100
1	C	173/198 (87%)	170 (98%)	3 (2%)	0	100	100
1	E	174/198 (88%)	171 (98%)	3 (2%)	0	100	100
1	G	175/198 (88%)	170 (97%)	5 (3%)	0	100	100
2	B	235/239 (98%)	228 (97%)	7 (3%)	0	100	100
2	D	237/239 (99%)	226 (95%)	11 (5%)	0	100	100
2	F	237/239 (99%)	226 (95%)	11 (5%)	0	100	100
2	H	236/239 (99%)	227 (96%)	9 (4%)	0	100	100
3	I	272/274 (99%)	267 (98%)	5 (2%)	0	100	100
3	L	272/274 (99%)	267 (98%)	5 (2%)	0	100	100
3	O	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
3	R	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
4	J	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
4	M	97/99 (98%)	97 (100%)	0	0	100	100
4	P	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
4	S	97/99 (98%)	97 (100%)	0	0	100	100
5	K	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	0
5	N	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	Q	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	T	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	3144/3276 (96%)	3054 (97%)	89 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	3	GLY

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	156/178 (88%)	154 (99%)	2 (1%)	61	76
1	C	156/178 (88%)	155 (99%)	1 (1%)	78	87
1	E	157/178 (88%)	155 (99%)	2 (1%)	61	76
1	G	158/178 (89%)	158 (100%)	0	100	100
2	B	210/211 (100%)	210 (100%)	0	100	100
2	D	211/211 (100%)	211 (100%)	0	100	100
2	F	211/211 (100%)	211 (100%)	0	100	100
2	H	210/211 (100%)	210 (100%)	0	100	100
3	I	231/231 (100%)	231 (100%)	0	100	100
3	L	231/231 (100%)	231 (100%)	0	100	100
3	O	231/231 (100%)	230 (100%)	1 (0%)	84	91
3	R	231/231 (100%)	230 (100%)	1 (0%)	84	91
4	J	94/94 (100%)	94 (100%)	0	100	100
4	M	94/94 (100%)	93 (99%)	1 (1%)	65	79
4	P	94/94 (100%)	94 (100%)	0	100	100
4	S	94/94 (100%)	94 (100%)	0	100	100
5	K	5/5 (100%)	5 (100%)	0	100	100
5	N	5/5 (100%)	5 (100%)	0	100	100
5	Q	5/5 (100%)	5 (100%)	0	100	100
5	T	5/5 (100%)	5 (100%)	0	100	100
All	All	2789/2876 (97%)	2781 (100%)	8 (0%)	86	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	TYR
1	A	32	TYR
1	A	161	LEU

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Mol	Chain	Res	Type
1	E	32	TYR
1	E	161	LEU
4	M	36	GLU
3	O	35	ARG
3	R	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	71	HIS
2	D	93	GLN
1	A	22	ASN
1	A	71	HIS
2	B	63	GLN
2	B	75	GLN
1	E	5	GLN
1	E	66	ASN
1	E	80	GLN
1	E	142	GLN
2	F	75	GLN
2	F	197	HIS
1	G	38	GLN
1	G	144	ASN
2	H	35	GLN
2	H	75	GLN
2	H	93	GLN
3	L	188	HIS
4	M	13	HIS
3	I	191	HIS
3	O	188	HIS

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 ⓘ

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	175/198 (88%)	0.48	7 (4%) 42 48	42, 74, 150, 211	0
1	C	175/198 (88%)	0.36	5 (2%) 53 60	44, 70, 132, 180	0
1	E	176/198 (88%)	0.55	6 (3%) 48 55	42, 70, 168, 230	0
1	G	177/198 (89%)	0.48	10 (5%) 30 35	41, 74, 153, 212	0
2	B	237/239 (99%)	0.35	5 (2%) 63 68	36, 75, 123, 146	0
2	D	239/239 (100%)	0.19	3 (1%) 75 79	39, 65, 105, 151	0
2	F	239/239 (100%)	0.42	4 (1%) 69 74	41, 76, 126, 176	0
2	H	238/239 (99%)	0.24	5 (2%) 63 68	37, 67, 126, 168	0
3	I	274/274 (100%)	0.21	9 (3%) 49 56	37, 65, 131, 165	0
3	L	274/274 (100%)	0.12	1 (0%) 88 91	39, 66, 100, 137	0
3	O	274/274 (100%)	0.02	4 (1%) 72 77	34, 57, 98, 121	0
3	R	274/274 (100%)	0.31	15 (5%) 30 36	39, 63, 140, 179	0
4	J	99/99 (100%)	0.85	12 (12%) 8 10	49, 90, 125, 152	0
4	M	99/99 (100%)	0.12	4 (4%) 42 48	46, 68, 93, 115	0
4	P	99/99 (100%)	-0.05	1 (1%) 79 83	39, 59, 88, 107	0
4	S	99/99 (100%)	0.40	3 (3%) 52 59	53, 78, 110, 121	0
5	K	9/9 (100%)	-0.18	0 100 100	40, 44, 52, 53	0
5	N	9/9 (100%)	0.05	0 100 100	43, 44, 51, 53	0
5	Q	9/9 (100%)	-0.11	0 100 100	36, 41, 46, 47	0
5	T	9/9 (100%)	0.14	0 100 100	44, 48, 54, 56	0
All	All	3184/3276 (97%)	0.29	94 (2%) 52 59	34, 68, 129, 230	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	176	TYR	4.6
4	J	1	ILE	4.5
1	E	136	PHE	4.0
4	J	99	MET	3.8
2	B	176	TYR	3.7
1	G	165	ALA	3.6
2	H	238	ALA	3.4
2	H	176	TYR	3.3
3	R	272	LEU	3.2
4	J	80	CYS	3.2
3	I	225	THR	3.2
1	A	139	PHE	3.2
3	I	194	ILE	3.0
2	D	176	TYR	3.0
3	I	267	PRO	2.9
2	F	188	ARG	2.9
1	E	165	ALA	2.9
3	R	257	TYR	2.8
3	R	215	LEU	2.8
3	R	230	LEU	2.8
1	C	139	PHE	2.8
1	E	113	ILE	2.8
4	J	71	THR	2.8
3	R	267	PRO	2.7
4	S	80	CYS	2.7
1	E	161	LEU	2.7
4	J	49	VAL	2.7
2	B	58	ALA	2.6
1	A	121	TYR	2.6
3	R	261	VAL	2.6
1	G	136	PHE	2.6
3	I	211	ALA	2.6
1	A	136	PHE	2.6
3	R	266	LEU	2.6
3	R	113	TYR	2.6
1	A	119	ALA	2.5
1	A	27	ASP	2.5
3	I	241	PHE	2.5
4	J	24	ASN	2.5
1	G	153	THR	2.5
1	C	136	PHE	2.5
1	A	131	SER	2.5
4	J	22	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	18	MET	2.5
1	E	143	ILE	2.4
4	P	1	ILE	2.4
3	I	209	TYR	2.4
1	C	3	LYS	2.4
2	H	1	LYS	2.4
1	G	160	VAL	2.4
3	I	197	HIS	2.3
4	J	40	LEU	2.3
2	D	58	ALA	2.3
4	M	1	ILE	2.3
4	J	38	ASP	2.3
1	G	170	SER	2.3
3	L	209	TYR	2.3
3	R	194	ILE	2.3
4	M	80	CYS	2.2
1	G	168	SER	2.2
2	H	165	VAL	2.2
3	R	221	GLY	2.2
2	B	181	TYR	2.2
4	J	46	ILE	2.2
1	E	139	PHE	2.2
1	G	126	PRO	2.2
4	S	14	PRO	2.2
2	F	1	LYS	2.2
3	R	1	GLY	2.2
2	F	24	TYR	2.1
4	J	45	ARG	2.1
3	I	227	ASP	2.1
1	G	3	LYS	2.1
2	B	131	LYS	2.1
3	R	254	GLU	2.1
4	S	1	ILE	2.1
1	A	168	SER	2.1
3	O	55	GLU	2.1
1	C	121	TYR	2.1
3	I	274	TRP	2.1
3	R	274	TRP	2.1
4	M	18	GLY	2.1
1	G	177	SER	2.1
3	R	216	THR	2.1
4	M	19	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	O	230	LEU	2.0
2	H	2	ILE	2.0
2	D	24	TYR	2.0
4	J	37	VAL	2.0
1	C	132	THR	2.0
3	O	225	THR	2.0
3	R	182	THR	2.0
2	B	237	ARG	2.0
3	O	57	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.