



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:07 PM UTC

PDB ID : 8V4Z / pdb_00008v4z
Title : Crystal structure of a HLA-B*35:01-NP7 with D1 TCR
Authors : Littler, D.R.; Rossjohn, J.
Deposited on : 2023-11-29
Resolution : 2.40 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

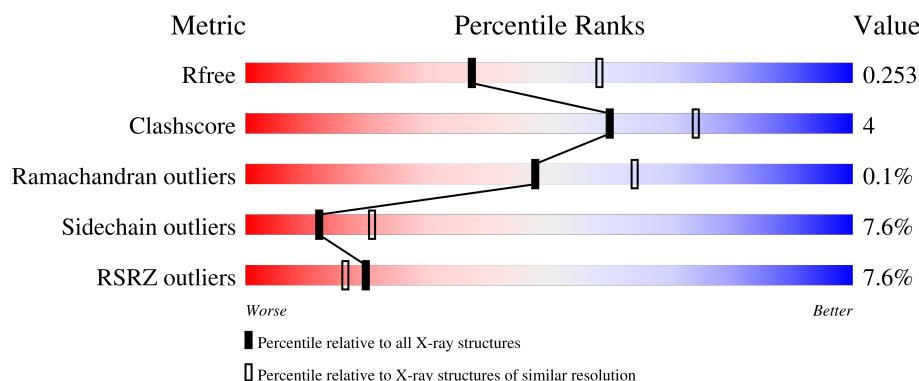
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	276	7% 83% 13% ..
1	F	276	6% 82% 13% ..
1	K	276	3% 83% 14% ..
1	P	276	8% 84% 12% ..
2	B	100	21% 59% 27% 11% ..

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Mol	Chain	Length	Quality of chain
2	G	100	
2	L	100	
2	Q	100	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	197	
4	I	197	
4	N	197	
4	S	197	
5	E	242	
5	J	242	
5	O	242	
5	T	242	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27408 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	2	0
			2252	1403	413	429	7			
1	F	273	Total	C	N	O	S	0	3	0
			2260	1408	414	430	8			
1	K	274	Total	C	N	O	S	0	4	0
			2277	1418	416	434	9			
1	P	274	Total	C	N	O	S	0	3	0
			2269	1413	415	433	8			

- 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			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	L	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	Q	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called LEU-PRO-PHE-GLU-LYS-SER-THR-ILE-MET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	H	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	M	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			
3	R	9	Total	C	N	O	S	0	0	0
			74	49	10	14	1			

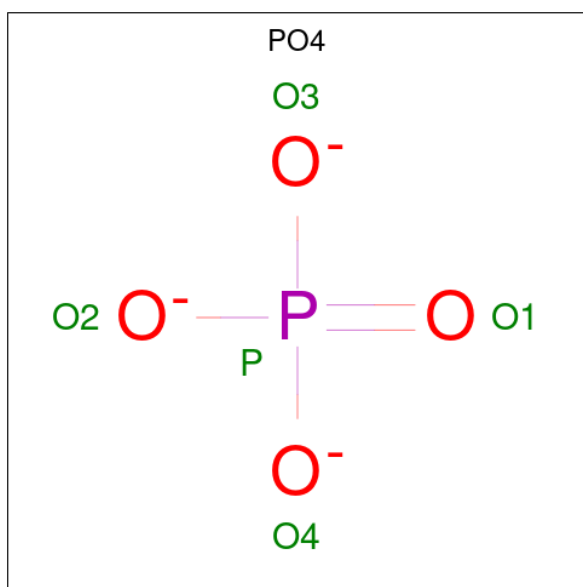
- Molecule 4 is a protein called D1 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	2	0
			1545	970	249	316	10			
4	I	197	Total	C	N	O	S	0	2	0
			1545	970	249	316	10			
4	N	197	Total	C	N	O	S	0	2	0
			1545	970	249	316	10			
4	S	197	Total	C	N	O	S	0	2	0
			1545	970	249	316	10			

- Molecule 5 is a protein called D1 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			
5	J	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			
5	O	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			
5	T	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			5	4	1		
6	I	1	Total	O	P	0	0
			5	4	1		
6	N	1	Total	O	P	0	0
			5	4	1		
6	S	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	56	Total	O	0	0
			56	56		
7	B	5	Total	O	0	0
			5	5		
7	C	4	Total	O	0	0
			4	4		
7	D	64	Total	O	0	0
			64	64		
7	E	52	Total	O	0	0
			52	52		
7	F	89	Total	O	0	0
			89	89		
7	G	11	Total	O	0	0
			11	11		
7	H	2	Total	O	0	0
			2	2		

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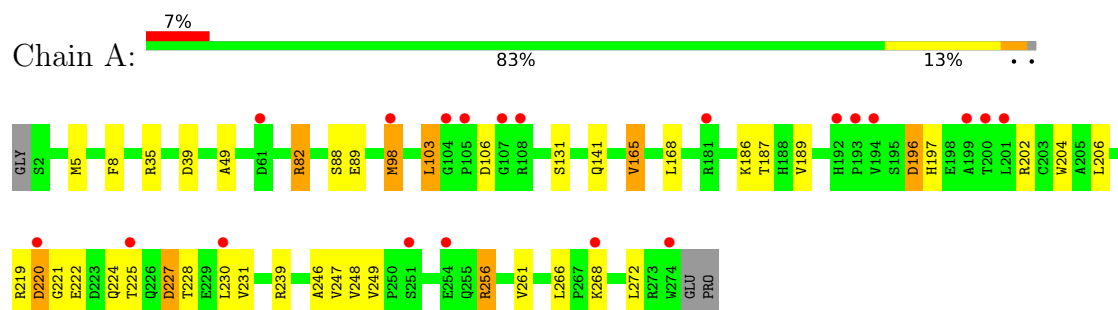
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	33	Total 33	O 33	0	0
7	J	63	Total 63	O 63	0	0
7	K	121	Total 121	O 121	0	0
7	L	19	Total 19	O 19	0	0
7	M	6	Total 6	O 6	0	0
7	N	62	Total 62	O 62	0	0
7	O	106	Total 106	O 106	0	0
7	P	15	Total 15	O 15	0	0
7	Q	1	Total 1	O 1	0	0
7	R	2	Total 2	O 2	0	0
7	S	40	Total 40	O 40	0	0
7	T	19	Total 19	O 19	0	0

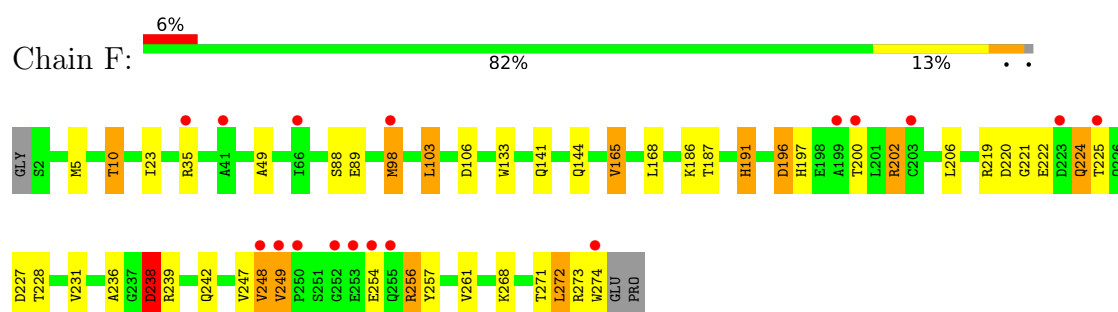
3 Residue-property plots [i](#)

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.

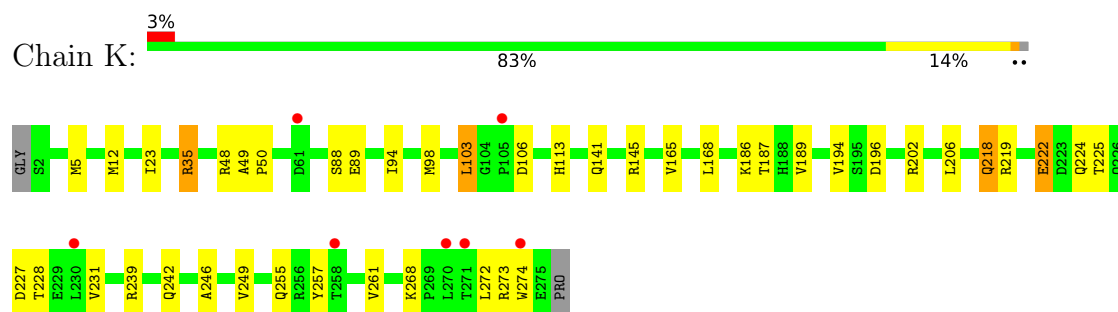
- Molecule 1: MHC class I antigen



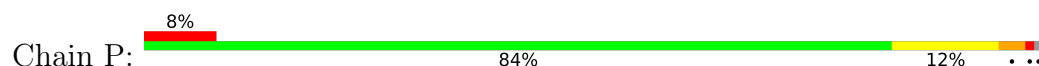
- Molecule 1: MHC class I antigen

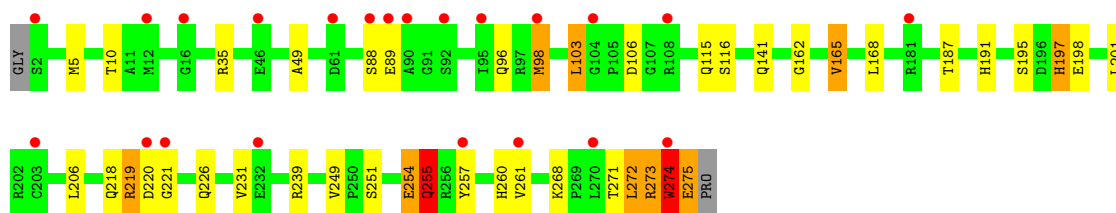


- Molecule 1: MHC class I antigen

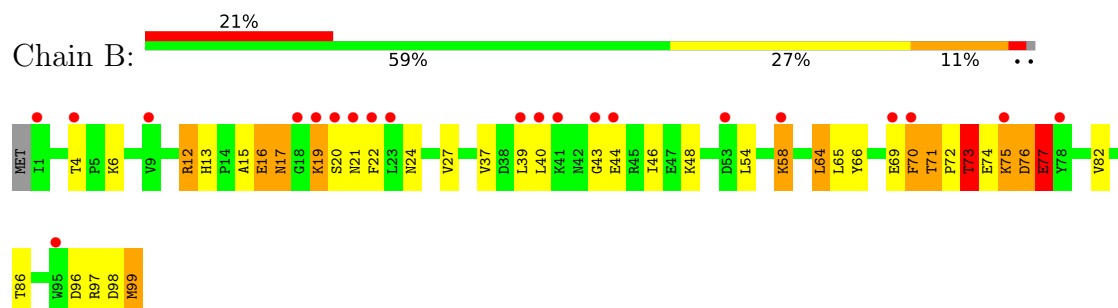


- Molecule 1: MHC class I antigen

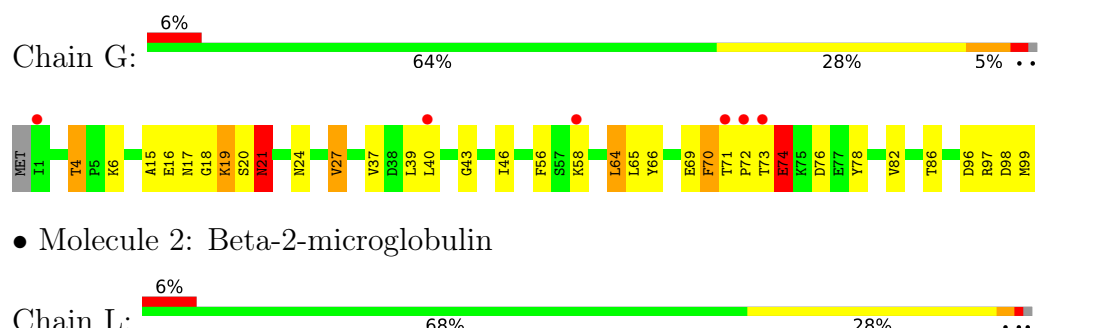




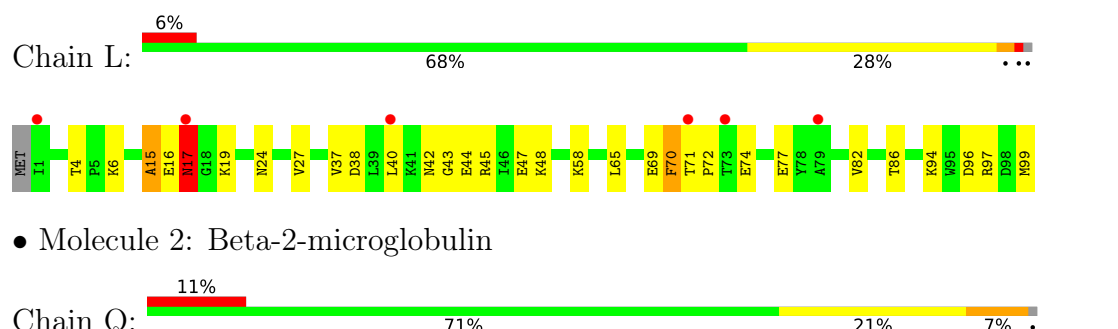
• Molecule 2: Beta-2-microglobulin



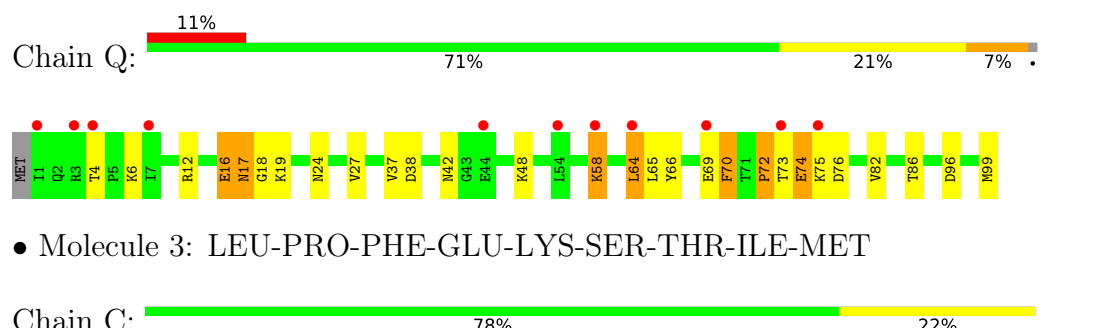
• Molecule 2: Beta-2-microglobulin



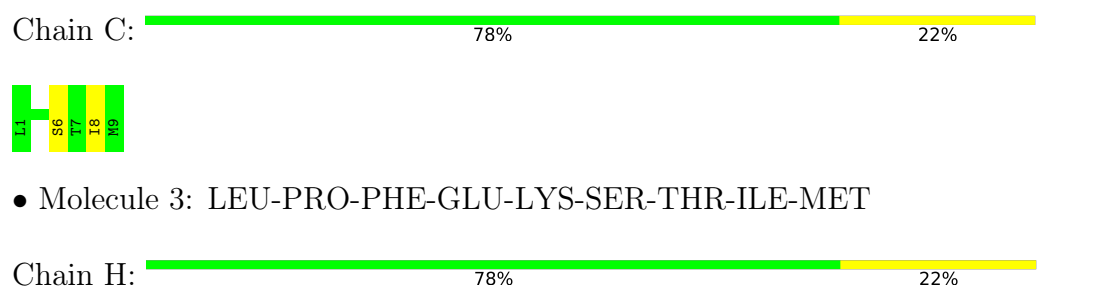
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 3: LEU-PRO-PHE-GLU-LYS-SER-THR-ILE-MET



• Molecule 3: LEU-PRO-PHE-GLU-LYS-SER-THR-ILE-MET



- Molecule 3: LEU-PRO-PHE-GLU-LYS-SER-THR-ILE-MET

Chain M: 78% 22%



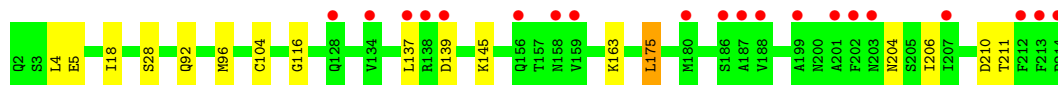
- Molecule 3: LEU-PRO-PHE-GLU-LYS-SER-THR-ILE-MET

Chain R: 78% 22%



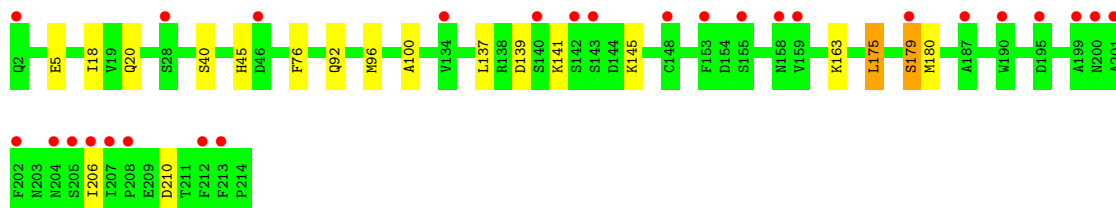
- Molecule 4: D1 TCR alpha chain

Chain D: 10% 91% 8%



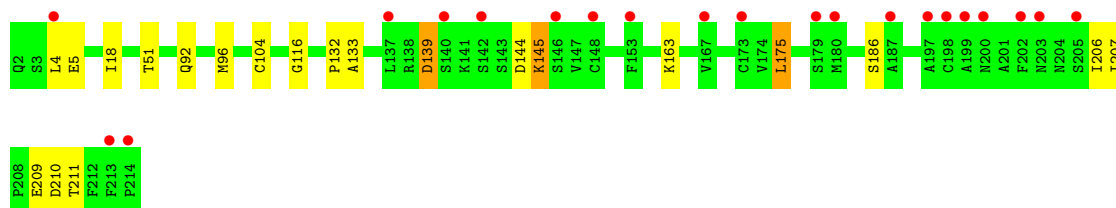
- Molecule 4: D1 TCR alpha chain

Chain I: 14% 90% 9%



- Molecule 4: D1 TCR alpha chain

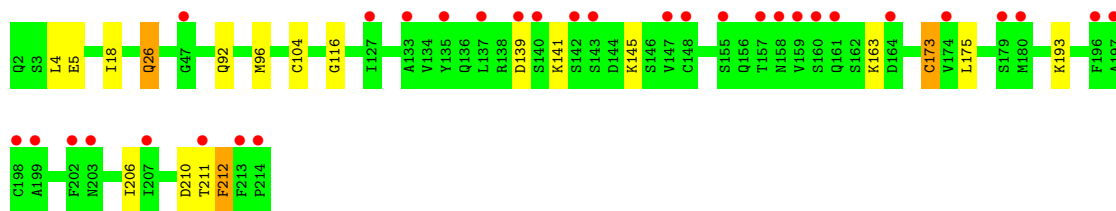
Chain N: 11% 89% 9%



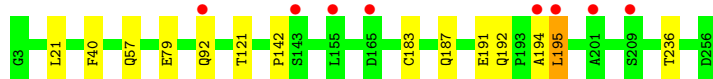
- Molecule 4: D1 TCR alpha chain

Chain S: 16% 90% 8%





● Molecule 5: D1 TCR beta chain



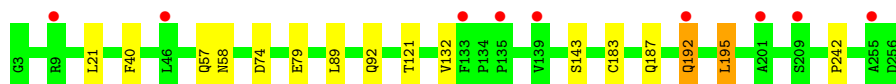
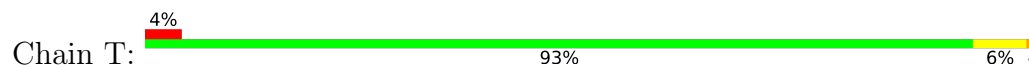
● Molecule 5: D1 TCR beta chain



● Molecule 5: D1 TCR beta chain



● Molecule 5: D1 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.99Å 190.21Å 250.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 2.40 49.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.06-2.40) 99.9 (49.06-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.218 , 0.252 0.219 , 0.253	Depositor DCC
R_{free} test set	7342 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtrriage
Anisotropy	0.580	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27408	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.48 % 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 2.6128e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.71	0/2314	1.21	6/3146 (0.2%)
1	F	0.69	0/2322	1.19	5/3156 (0.2%)
1	K	0.70	0/2339	1.17	0/3178
1	P	0.71	0/2331	1.26	9/3168 (0.3%)
2	B	0.81	0/852	1.34	12/1152 (1.0%)
2	G	0.71	0/852	1.24	6/1152 (0.5%)
2	L	0.73	0/852	1.60	12/1152 (1.0%)
2	Q	0.70	0/852	1.17	3/1152 (0.3%)
3	C	0.63	0/75	1.02	0/98
3	H	0.67	0/75	0.99	0/98
3	M	0.62	0/75	1.03	0/98
3	R	0.66	0/75	1.00	0/98
4	D	0.70	0/1579	1.05	1/2139 (0.0%)
4	I	0.69	0/1579	1.04	2/2139 (0.1%)
4	N	0.70	0/1579	1.05	1/2139 (0.0%)
4	S	0.69	0/1579	1.07	2/2139 (0.1%)
5	E	0.68	0/1994	1.05	3/2712 (0.1%)
5	J	0.65	0/1994	1.03	3/2712 (0.1%)
5	O	0.72	0/1994	1.07	2/2712 (0.1%)
5	T	0.67	0/1994	1.05	3/2712 (0.1%)
All	All	0.70	0/27306	1.15	70/37052 (0.2%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	17	ASN	N-CA-C	31.32	149.23	111.33
1	P	219	ARG	CB-CA-C	14.24	145.51	113.33
1	P	219	ARG	N-CA-C	-13.04	89.46	109.79
2	B	77	GLU	N-CA-C	12.67	128.96	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	16	GLU	N-CA-C	-11.16	91.47	108.99
2	B	17	ASN	N-CA-C	9.25	121.37	111.28
5	O	81	PRO	N-CA-C	9.13	125.98	113.65
1	P	220	ASP	N-CA-CB	-8.31	96.44	110.49
2	Q	70	PHE	CA-CB-CG	8.21	122.01	113.80
4	S	212	PHE	CA-CB-CG	8.15	121.95	113.80
1	P	274	TRP	N-CA-C	-8.00	97.19	108.23
2	L	17	ASN	CB-CA-C	-7.94	97.19	110.68
2	L	16	GLU	CB-CA-C	7.92	126.80	109.94
2	G	76	ASP	CA-CB-CG	7.91	120.50	112.60
2	L	15	ALA	N-CA-C	7.70	121.03	109.25
2	L	74	GLU	CA-C-N	-7.34	111.07	122.37
2	L	74	GLU	C-N-CA	-7.34	111.07	122.37
1	F	196	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	196	ASP	CA-CB-CG	7.24	119.84	112.60
2	B	70	PHE	CA-CB-CG	6.86	120.66	113.80
2	G	70	PHE	CA-CB-CG	6.86	120.66	113.80
2	Q	18	GLY	CA-C-N	6.74	131.35	121.31
2	Q	18	GLY	C-N-CA	6.74	131.35	121.31
1	P	255	GLN	N-CA-C	-6.64	104.66	112.89
2	G	74	GLU	CB-CG-CD	6.54	123.72	112.60
2	G	21	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	220	ASP	CA-CB-CG	6.42	119.02	112.60
1	F	238	ASP	N-CA-C	-6.32	100.22	109.63
1	A	221	GLY	N-CA-C	6.30	124.05	115.30
2	L	16	GLU	CA-C-N	6.25	128.94	120.38
2	L	16	GLU	C-N-CA	6.25	128.94	120.38
2	L	71	THR	CA-C-N	-6.23	114.23	120.21
2	L	71	THR	C-N-CA	-6.23	114.23	120.21
2	B	54	LEU	N-CA-C	6.13	118.17	108.67
2	B	16	GLU	N-CA-C	-5.72	99.69	109.24
5	T	79	GLU	CA-C-N	5.51	127.13	122.28
5	T	79	GLU	C-N-CA	5.51	127.13	122.28
4	D	139	ASP	CA-CB-CG	5.43	118.03	112.60
2	B	22	PHE	CA-CB-CG	5.41	119.21	113.80
4	I	139	ASP	CA-CB-CG	5.38	117.98	112.60
4	N	139	ASP	CA-CB-CG	5.32	117.92	112.60
2	B	17	ASN	CA-C-N	5.28	126.93	120.22
2	B	17	ASN	C-N-CA	5.28	126.93	120.22
5	E	79	GLU	CA-C-N	5.27	127.27	122.37
5	E	79	GLU	C-N-CA	5.27	127.27	122.37
2	G	18	GLY	CA-C-N	-5.26	116.00	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	18	GLY	C-N-CA	-5.26	116.00	122.84
5	T	40	PHE	CA-CB-CG	5.26	119.06	113.80
2	B	21	ASN	CA-C-N	5.25	130.05	122.44
2	B	21	ASN	C-N-CA	5.25	130.05	122.44
5	J	79	GLU	CA-C-N	5.24	127.25	122.37
5	J	79	GLU	C-N-CA	5.24	127.25	122.37
4	S	139	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	227	ASP	CA-CB-CG	5.22	117.82	112.60
5	E	40	PHE	CA-CB-CG	5.20	119.00	113.80
2	B	73	THR	N-CA-C	5.20	116.86	108.08
2	L	70	PHE	N-CA-C	5.17	117.67	109.50
1	P	165	VAL	CA-C-N	5.10	127.43	120.54
1	P	165	VAL	C-N-CA	5.10	127.43	120.54
2	B	77	GLU	N-CA-CB	-5.10	102.25	109.85
1	F	165	VAL	CA-C-N	5.09	127.42	120.54
1	F	165	VAL	C-N-CA	5.09	127.42	120.54
5	J	40	PHE	CA-CB-CG	5.09	118.89	113.80
5	O	40	PHE	CA-CB-CG	5.07	118.87	113.80
4	I	76	PHE	CA-CB-CG	5.07	118.87	113.80
1	P	162	GLY	CA-C-N	5.04	127.28	120.38
1	P	162	GLY	C-N-CA	5.04	127.28	120.38
1	A	165	VAL	CA-C-N	5.02	127.32	120.54
1	A	165	VAL	C-N-CA	5.02	127.32	120.54
1	F	248	VAL	CB-CA-C	5.00	116.94	111.08

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	2252	0	2113	16	0
1	F	2260	0	2123	21	0
1	K	2277	0	2135	22	0
1	P	2269	0	2129	30	0
2	B	829	0	794	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	829	0	794	33	0
2	L	829	0	794	12	0
2	Q	829	0	794	12	0
3	C	74	0	80	0	0
3	H	74	0	80	0	0
3	M	74	0	80	0	0
3	R	74	0	80	0	0
4	D	1545	0	1437	7	0
4	I	1545	0	1437	10	0
4	N	1545	0	1437	12	0
4	S	1545	0	1438	11	0
5	E	1942	0	1837	9	0
5	J	1942	0	1837	5	0
5	O	1942	0	1837	8	0
5	T	1942	0	1839	10	0
6	D	5	0	0	0	0
6	I	5	0	0	0	0
6	N	5	0	0	0	0
6	S	5	0	0	0	0
7	A	56	0	0	0	0
7	B	5	0	0	1	0
7	C	4	0	0	0	0
7	D	64	0	0	0	0
7	E	52	0	0	0	0
7	F	89	0	0	0	0
7	G	11	0	0	0	0
7	H	2	0	0	0	0
7	I	33	0	0	0	0
7	J	63	0	0	0	0
7	K	121	0	0	1	0
7	L	19	0	0	0	0
7	M	6	0	0	0	0
7	N	62	0	0	0	0
7	O	106	0	0	0	0
7	P	15	0	0	0	0
7	Q	1	0	0	0	0
7	R	2	0	0	0	0
7	S	40	0	0	0	0
7	T	19	0	0	0	0
All	All	27408	0	25095	225	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.

All (225) 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:17:ASN:ND2	2:B:75:LYS:HB2	1.13	1.46
2:B:17:ASN:ND2	2:B:75:LYS:CB	2.02	1.23
2:B:17:ASN:HD21	2:B:75:LYS:CB	1.55	1.18
1:P:255:GLN:O	1:P:273:ARG:NH1	1.81	1.12
2:B:71:THR:O	2:B:73:THR:HG23	1.49	1.10
2:B:16:GLU:CD	2:B:19:LYS:HD3	1.85	1.01
1:A:82:ARG:HG2	1:A:82:ARG:HH11	1.29	0.94
2:B:17:ASN:HD21	2:B:75:LYS:CG	1.80	0.94
2:B:71:THR:OG1	2:B:73:THR:HG22	1.71	0.91
2:G:17:ASN:CG	2:G:74:GLU:HG3	1.95	0.91
2:G:17:ASN:HB3	2:G:74:GLU:HG3	1.55	0.89
2:B:16:GLU:OE1	2:B:19:LYS:HD3	1.73	0.88
2:G:17:ASN:CB	2:G:74:GLU:HG3	2.05	0.86
1:P:191:HIS:HB2	1:P:275:GLU:C	2.01	0.86
2:G:17:ASN:CG	2:G:74:GLU:CG	2.49	0.85
2:B:16:GLU:HB2	2:B:19:LYS:HD2	1.59	0.84
2:B:17:ASN:HD21	2:B:75:LYS:HB2	1.03	0.84
1:K:49:ALA:HA	1:K:239:ARG:HH12	1.44	0.82
2:B:17:ASN:HD22	2:B:75:LYS:HB2	1.02	0.82
2:B:17:ASN:HD21	2:B:75:LYS:HG3	1.46	0.80
1:A:82:ARG:HG2	1:A:82:ARG:NH1	1.95	0.79
4:N:132:PRO:HB2	4:N:210:ASP:OD1	1.83	0.78
2:B:19:LYS:O	2:B:72:PRO:HG2	1.87	0.73
2:L:77:GLU:OE1	2:L:94:LYS:NZ	2.22	0.72
2:L:4:THR:HA	2:L:86:THR:HG21	1.72	0.71
2:G:19:LYS:O	2:G:72:PRO:HD2	1.92	0.70
4:S:173:CYS:HB2	5:T:183[A]:CYS:SG	2.33	0.69
4:S:173:CYS:HB2	5:T:183[B]:CYS:SG	2.33	0.69
2:B:4:THR:HA	2:B:86:THR:HG21	1.74	0.68
2:Q:4:THR:HA	2:Q:86:THR:HG21	1.74	0.68
1:F:191:HIS:HB2	1:F:274:TRP:CH2	2.29	0.68
1:P:218:GLN:C	1:P:219:ARG:O	2.33	0.67
1:F:202:ARG:NH2	2:G:98:ASP:HB3	2.10	0.67
2:G:20:SER:HA	2:G:71:THR:HA	1.76	0.67
2:B:71:THR:OG1	2:B:73:THR:CG2	2.43	0.66
1:P:218:GLN:HG2	1:P:260:HIS:CE1	2.29	0.66
2:G:4:THR:HA	2:G:86:THR:HG21	1.76	0.66
4:I:175:LEU:HB3	5:J:183[A]:CYS:HB2	1.77	0.66
2:B:76:ASP:N	2:B:76:ASP:OD2	2.30	0.65
2:B:44:GLU:HG2	4:I:179:SER:HB3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TRP:HZ2	2:B:98:ASP:O	1.79	0.65
4:I:175:LEU:HB3	5:J:183[B]:CYS:HB2	1.77	0.65
2:B:74:GLU:HB2	2:B:76:ASP:OD2	1.98	0.63
2:Q:19:LYS:H	2:Q:19:LYS:HD2	1.62	0.63
1:P:272:LEU:HD22	1:P:272:LEU:O	1.99	0.63
2:G:40:LEU:HD23	2:G:43:GLY:HA2	1.81	0.62
1:P:272:LEU:HD13	1:P:272:LEU:N	2.15	0.61
2:B:15:ALA:HB3	2:B:97:ARG:HG3	1.81	0.61
1:P:187:THR:HG21	1:P:261:VAL:HG11	1.81	0.61
1:P:201:LEU:HD11	1:P:254:GLU:HB2	1.82	0.61
1:K:187:THR:HG21	1:K:261:VAL:HG11	1.81	0.61
4:N:175:LEU:HB3	5:O:183[B]:CYS:HB2	1.83	0.61
4:N:175:LEU:HB3	5:O:183[A]:CYS:HB2	1.83	0.60
1:A:98:MET:HE1	2:B:58:LYS:HA	1.84	0.60
1:A:187:THR:HG21	1:A:261:VAL:HG11	1.83	0.60
1:F:187:THR:HB	1:F:272:LEU:HD11	1.82	0.59
2:G:17:ASN:HB3	2:G:74:GLU:CG	2.30	0.59
2:L:15:ALA:HB3	2:L:97:ARG:HG3	1.86	0.58
5:T:132:VAL:HG23	5:T:242:PRO:HG2	1.85	0.58
2:L:17:ASN:OD1	2:L:17:ASN:N	2.37	0.58
1:F:187:THR:HG21	1:F:261:VAL:HG11	1.84	0.58
1:K:249:VAL:HG13	1:K:257:TYR:CE1	2.40	0.57
1:P:218:GLN:HG2	1:P:260:HIS:HE1	1.69	0.57
2:L:15:ALA:HB3	2:L:97:ARG:CG	2.34	0.57
2:Q:42:ASN:OD1	2:Q:76:ASP:HB2	2.03	0.57
2:G:17:ASN:OD1	2:G:74:GLU:CB	2.53	0.56
2:B:71:THR:O	2:B:73:THR:CG2	2.40	0.56
2:G:17:ASN:CB	2:G:74:GLU:CG	2.81	0.56
2:L:17:ASN:O	2:L:72:PRO:O	2.23	0.56
4:N:144:ASP:OD1	4:N:145:LYS:HD3	2.04	0.56
1:P:195:SER:HB3	1:P:197:HIS:CE1	2.41	0.55
2:B:16:GLU:HB2	2:B:19:LYS:CD	2.33	0.55
1:K:35:ARG:HG2	1:K:48:ARG:HD3	1.88	0.55
1:P:195:SER:HB2	1:P:198:GLU:HB2	1.88	0.55
2:G:17:ASN:OD1	2:G:74:GLU:HG3	2.07	0.54
2:G:21:ASN:O	2:G:70:PHE:HB3	2.06	0.54
5:E:195:LEU:HA	5:O:194:ALA:O	2.08	0.54
1:P:273:ARG:O	1:P:273:ARG:HG3	2.07	0.54
1:F:220:ASP:HB3	1:P:273:ARG:HH22	1.73	0.53
5:O:21:LEU:HD22	5:O:121:THR:HG21	1.90	0.53
1:K:50:PRO:HD3	1:K:239:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLU:HG2	4:I:179:SER:CB	2.39	0.53
5:T:21:LEU:HD22	5:T:121:THR:HG21	1.92	0.52
1:P:272:LEU:HD22	1:P:272:LEU:C	2.34	0.52
2:G:17:ASN:OD1	2:G:74:GLU:HB3	2.10	0.52
1:P:5:MET:HB2	1:P:168:LEU:HD13	1.90	0.52
1:F:219:ARG:HH21	1:F:256:ARG:NH2	2.08	0.51
4:S:175:LEU:HB3	5:T:183[A]:CYS:HB2	1.91	0.51
4:S:175:LEU:HB3	5:T:183[B]:CYS:HB2	1.91	0.51
1:A:219:ARG:HH21	1:A:256:ARG:HH22	1.58	0.51
2:B:17:ASN:ND2	2:B:75:LYS:CG	2.57	0.51
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.91	0.51
2:B:44:GLU:HA	4:I:179:SER:O	2.10	0.51
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.91	0.51
1:P:49:ALA:HA	1:P:239:ARG:HH12	1.76	0.51
1:K:50:PRO:HD3	1:K:239:ARG:HH12	1.76	0.51
1:K:12[B]:MET:HE1	1:K:23:ILE:HD12	1.92	0.50
4:D:175:LEU:HB3	5:E:183[A]:CYS:HB2	1.93	0.50
1:P:197:HIS:HA	1:P:251:SER:HB2	1.93	0.50
1:K:49:ALA:HA	1:K:239:ARG:NH1	2.20	0.50
1:P:274:TRP:HE3	1:P:275:GLU:H	1.59	0.50
2:Q:16:GLU:HB3	2:Q:19:LYS:HD3	1.94	0.50
1:A:8:PHE:CE2	1:A:98:MET:HE3	2.47	0.50
1:A:49:ALA:HA	1:A:239:ARG:HH12	1.77	0.49
2:B:44:GLU:HB3	4:I:179:SER:OG	2.12	0.49
1:P:272:LEU:C	1:P:272:LEU:CD2	2.86	0.49
2:B:40:LEU:HD23	2:B:43:GLY:HA2	1.94	0.49
1:K:219:ARG:HH11	1:K:257:TYR:HE1	1.59	0.49
5:J:21:LEU:HD22	5:J:121:THR:HG21	1.94	0.49
2:Q:24:ASN:HB3	2:Q:65:LEU:HD11	1.95	0.49
4:D:175:LEU:HB3	5:E:183[B]:CYS:HB2	1.93	0.48
4:N:133:ALA:HB2	4:N:211:THR:HG22	1.94	0.48
4:N:18:ILE:HG22	4:N:92:GLN:HA	1.95	0.48
1:F:221:GLY:O	1:P:271:THR:HG21	2.14	0.48
1:P:191:HIS:CB	1:P:275:GLU:C	2.82	0.48
1:F:98[B]:MET:HG3	2:G:56:PHE:HE2	1.78	0.48
2:G:70:PHE:HE1	2:G:78:TYR:CZ	2.31	0.48
2:B:73:THR:OG1	2:B:74:GLU:N	2.46	0.48
1:A:219:ARG:HH21	1:A:256:ARG:NH2	2.12	0.48
4:I:18:ILE:HG22	4:I:92:GLN:HA	1.96	0.48
2:G:37:VAL:HG22	2:G:82:VAL:HG22	1.96	0.48
2:G:39:LEU:HB3	2:G:46:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:219:ARG:HD3	1:K:257:TYR:CZ	2.48	0.48
2:L:24:ASN:HB3	2:L:65:LEU:HD11	1.96	0.48
4:D:18:ILE:HG22	4:D:92:GLN:HA	1.95	0.48
2:L:37:VAL:HG22	2:L:82:VAL:HG22	1.95	0.48
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.97	0.47
1:K:141:GLN:O	1:K:145:ARG:HD3	2.15	0.47
2:Q:37:VAL:HG22	2:Q:82:VAL:HG22	1.95	0.47
4:S:18:ILE:HG22	4:S:92:GLN:HA	1.96	0.47
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.95	0.47
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.96	0.47
5:E:21:LEU:HD22	5:E:121:THR:HG21	1.96	0.47
4:N:4:LEU:HD11	4:N:116:GLY:HA3	1.96	0.47
5:O:58:ASN:O	5:O:80:ARG:HD3	2.14	0.47
2:G:17:ASN:CG	2:G:74:GLU:HG2	2.35	0.47
4:N:4:LEU:HD11	4:N:116:GLY:CA	2.45	0.47
1:A:88:SER:HB2	4:S:26:GLN:OE1	2.15	0.47
1:A:204:TRP:CZ2	2:B:98:ASP:O	2.63	0.47
1:K:103:LEU:HD11	1:K:165:VAL:HG13	1.97	0.47
4:D:4:LEU:HD11	4:D:116:GLY:CA	2.46	0.46
4:D:4:LEU:HD11	4:D:116:GLY:HA3	1.96	0.46
1:F:274:TRP:HA	1:F:274:TRP:CE3	2.51	0.46
1:F:249:VAL:HG11	1:F:254:GLU:HG3	1.97	0.46
1:K:224:GLN:HB3	1:K:227:ASP:HB2	1.98	0.46
1:F:10:THR:HG23	1:F:23:ILE:HB	1.98	0.46
1:F:220:ASP:HB3	1:P:273:ARG:NH2	2.30	0.46
1:P:218:GLN:OE1	1:P:221:GLY:HA2	2.16	0.46
2:Q:19:LYS:HD2	2:Q:19:LYS:N	2.30	0.46
2:Q:96:ASP:HB3	2:Q:99:MET:HG2	1.98	0.46
1:K:113:HIS:HD2	7:K:301:HOH:O	1.99	0.46
2:L:96:ASP:HB3	2:L:99:MET:HG2	1.98	0.46
1:F:49:ALA:HA	1:F:239:ARG:HH12	1.81	0.45
4:I:137:LEU:HD22	5:J:142:PRO:HA	1.98	0.45
1:F:103:LEU:HD11	1:F:165:VAL:HG13	1.98	0.45
1:P:275:GLU:C	1:P:275:GLU:CD	2.83	0.45
1:A:8:PHE:HE2	1:A:98:MET:HE3	1.82	0.45
2:B:64:LEU:HD13	2:B:66:TYR:HE1	1.80	0.45
2:B:73:THR:HG21	7:B:104:HOH:O	2.15	0.45
2:G:19:LYS:O	2:G:72:PRO:CD	2.61	0.45
1:K:218:GLN:HA	1:K:222:GLU:O	2.16	0.45
2:G:17:ASN:HD21	2:G:97:ARG:HH12	1.65	0.45
4:I:20:GLN:HB2	4:S:18:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.98	0.44
2:B:96:ASP:HB3	2:B:99:MET:HG2	1.99	0.44
4:D:137:LEU:HD22	5:E:142:PRO:HA	1.98	0.44
5:E:236:THR:HG21	2:G:4:THR:HG21	2.00	0.44
2:G:15:ALA:HB1	2:G:72:PRO:HG2	1.99	0.44
1:F:271:THR:HG21	1:P:221:GLY:O	2.17	0.44
2:G:64:LEU:HD13	2:G:66:TYR:HE1	1.83	0.44
4:N:144:ASP:CG	4:N:145:LYS:HD3	2.43	0.44
2:G:96:ASP:HB3	2:G:99:MET:HG2	2.00	0.44
1:K:189:VAL:HG11	1:K:273:ARG:C	2.42	0.44
5:T:21:LEU:HD12	5:T:89:LEU:HD23	1.99	0.44
1:F:224:GLN:HB3	1:F:227:ASP:HB2	2.00	0.43
2:B:39:LEU:HB3	2:B:46:ILE:HD12	2.00	0.43
5:E:194:ALA:O	5:O:195:LEU:HA	2.18	0.43
2:G:17:ASN:OD1	2:G:74:GLU:CG	2.64	0.43
2:G:20:SER:HA	2:G:72:PRO:HD3	1.99	0.43
5:E:194:ALA:HB1	5:O:195:LEU:HG	1.99	0.43
2:G:17:ASN:CG	2:G:74:GLU:CB	2.91	0.43
1:K:35:ARG:HE	1:K:35:ARG:HB2	1.69	0.43
1:K:12[A]:MET:HE3	1:K:94:ILE:HD11	2.01	0.43
4:S:4:LEU:HD11	4:S:116:GLY:HA3	2.01	0.43
5:T:192:GLN:HE21	5:T:195:LEU:HD13	1.84	0.43
2:Q:64:LEU:HD13	2:Q:66:TYR:HE1	1.83	0.43
1:P:98[B]:MET:HE1	2:Q:58:LYS:HA	2.01	0.42
4:I:45:HIS:CD2	4:I:100:ALA:HB2	2.55	0.42
2:Q:74:GLU:O	2:Q:75:LYS:HD2	2.18	0.42
1:A:103:LEU:HD11	1:A:165:VAL:HG13	2.00	0.42
2:B:71:THR:C	2:B:73:THR:HG23	2.33	0.42
2:G:27:VAL:HG21	2:G:37:VAL:HG21	2.01	0.42
2:L:15:ALA:CB	2:L:97:ARG:HG3	2.49	0.42
4:S:173:CYS:HB2	5:T:183[B]:CYS:HG	1.84	0.42
4:N:207:ILE:O	4:N:210:ASP:OD2	2.37	0.42
5:T:57:GLN:O	5:T:58:ASN:HB2	2.20	0.42
1:P:103:LEU:HD11	1:P:165:VAL:HG13	2.01	0.42
1:P:249:VAL:HG13	1:P:257:TYR:CE1	2.54	0.42
2:B:27:VAL:HG11	2:B:82:VAL:HG21	2.01	0.42
1:K:189:VAL:HG11	1:K:273:ARG:O	2.20	0.41
1:A:202:ARG:HE	1:A:246:ALA:HB2	1.85	0.41
1:K:202:ARG:HD3	1:K:246:ALA:HB2	2.02	0.41
1:K:219:ARG:HD3	1:K:257:TYR:CE1	2.55	0.41
2:B:12:ARG:HB3	2:B:13:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:GLU:H	2:B:77:GLU:HG2	1.39	0.41
1:F:202:ARG:CZ	2:G:98:ASP:O	2.69	0.41
1:P:201:LEU:HD21	1:P:275:GLU:HA	2.01	0.41
1:F:219:ARG:HB2	1:F:257:TYR:CE1	2.55	0.41
2:L:40:LEU:HD23	2:L:43:GLY:HA2	2.03	0.41
4:N:139:ASP:HB2	5:O:140:PHE:CE2	2.55	0.41
2:B:75:LYS:HD3	2:B:75:LYS:O	2.21	0.41
4:N:4:LEU:HD13	4:N:104[A]:CYS:SG	2.61	0.41
5:J:14:LYS:HG3	5:J:128:ASP:HA	2.03	0.40
4:S:4:LEU:HD11	4:S:116:GLY:CA	2.51	0.40
4:D:4:LEU:HD13	4:D:104[A]:CYS:SG	2.61	0.40
2:G:20:SER:HB2	2:G:70:PHE:O	2.20	0.40
2:Q:17:ASN:O	2:Q:72:PRO:O	2.39	0.40
1:F:236:ALA:HB3	1:F:238:ASP:OD1	2.21	0.40
1:A:103:LEU:HD13	1:A:168:LEU:HD23	2.04	0.40
5:E:191:GLU:HB2	5:E:192:GLN:HE21	1.86	0.40
1:F:133:TRP:HB2	1:F:144:GLN:HG3	2.03	0.40
4:S:4:LEU:HD13	4:S:104[A]:CYS:SG	2.62	0.40
2:B:16:GLU:CB	2:B:19:LYS:HD2	2.41	0.40
2:L:42:ASN:C	2:L:44:GLU:H	2.30	0.40
1:P:10:THR:HG22	1:P:96:GLN:HG2	2.02	0.40

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	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
1	F	274/276 (99%)	262 (96%)	12 (4%)	0	100	100
1	K	276/276 (100%)	270 (98%)	6 (2%)	0	100	100
1	P	275/276 (100%)	263 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
2	G	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
2	L	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	Q	97/100 (97%)	91 (94%)	4 (4%)	2 (2%)	5	7
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	M	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	197/197 (100%)	189 (96%)	8 (4%)	0	100	100
4	I	197/197 (100%)	186 (94%)	11 (6%)	0	100	100
4	N	197/197 (100%)	188 (95%)	9 (5%)	0	100	100
4	S	197/197 (100%)	187 (95%)	10 (5%)	0	100	100
5	E	243/242 (100%)	234 (96%)	9 (4%)	0	100	100
5	J	243/242 (100%)	234 (96%)	9 (4%)	0	100	100
5	O	243/242 (100%)	234 (96%)	9 (4%)	0	100	100
5	T	243/242 (100%)	232 (96%)	11 (4%)	0	100	100
All	All	3274/3296 (99%)	3136 (96%)	136 (4%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	72	PRO
2	Q	17	ASN

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	234/234 (100%)	205 (88%)	29 (12%)	4	6
1	F	235/234 (100%)	205 (87%)	30 (13%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	237/234 (101%)	216 (91%)	21 (9%)	9	15
1	P	236/234 (101%)	215 (91%)	21 (9%)	9	15
2	B	94/95 (99%)	79 (84%)	15 (16%)	2	3
2	G	94/95 (99%)	83 (88%)	11 (12%)	5	7
2	L	94/95 (99%)	83 (88%)	11 (12%)	5	7
2	Q	94/95 (99%)	82 (87%)	12 (13%)	4	6
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	1
3	H	9/9 (100%)	7 (78%)	2 (22%)	1	1
3	M	9/9 (100%)	7 (78%)	2 (22%)	1	1
3	R	9/9 (100%)	7 (78%)	2 (22%)	1	1
4	D	173/171 (101%)	163 (94%)	10 (6%)	18	32
4	I	173/171 (101%)	162 (94%)	11 (6%)	16	28
4	N	173/171 (101%)	164 (95%)	9 (5%)	21	36
4	S	173/171 (101%)	161 (93%)	12 (7%)	14	24
5	E	211/208 (101%)	207 (98%)	4 (2%)	50	71
5	J	211/208 (101%)	207 (98%)	4 (2%)	50	71
5	O	211/208 (101%)	204 (97%)	7 (3%)	33	55
5	T	211/208 (101%)	205 (97%)	6 (3%)	38	60
All	All	2890/2868 (101%)	2669 (92%)	221 (8%)	12	21

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	39	ASP
1	A	82	ARG
1	A	89	GLU
1	A	98	MET
1	A	103	LEU
1	A	106	ASP
1	A	131	SER
1	A	141	GLN
1	A	186	LYS
1	A	189	VAL
1	A	196	ASP
1	A	197	HIS

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Mol	Chain	Res	Type
1	A	206	LEU
1	A	220	ASP
1	A	222	GLU
1	A	224	GLN
1	A	225	THR
1	A	227	ASP
1	A	228	THR
1	A	230	LEU
1	A	231	VAL
1	A	247	VAL
1	A	248	VAL
1	A	249	VAL
1	A	256	ARG
1	A	266	LEU
1	A	268	LYS
1	A	272	LEU
2	B	6	LYS
2	B	12	ARG
2	B	19	LYS
2	B	20	SER
2	B	48	LYS
2	B	58	LYS
2	B	64	LEU
2	B	69	GLU
2	B	70	PHE
2	B	71	THR
2	B	73	THR
2	B	75	LYS
2	B	76	ASP
2	B	77	GLU
2	B	99	MET
3	C	6	SER
3	C	8	ILE
4	D	5	GLU
4	D	28	SER
4	D	96	MET
4	D	145	LYS
4	D	163	LYS
4	D	175	LEU
4	D	204	ASN
4	D	206	ILE
4	D	210	ASP

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Mol	Chain	Res	Type
4	D	211	THR
5	E	57	GLN
5	E	92	GLN
5	E	187	GLN
5	E	195	LEU
1	F	10	THR
1	F	35	ARG
1	F	88	SER
1	F	89	GLU
1	F	98[A]	MET
1	F	98[B]	MET
1	F	103	LEU
1	F	106	ASP
1	F	141	GLN
1	F	186	LYS
1	F	191	HIS
1	F	196	ASP
1	F	197	HIS
1	F	200	THR
1	F	202	ARG
1	F	206	LEU
1	F	222	GLU
1	F	224	GLN
1	F	225	THR
1	F	228	THR
1	F	231	VAL
1	F	238	ASP
1	F	242	GLN
1	F	247	VAL
1	F	248	VAL
1	F	249	VAL
1	F	256	ARG
1	F	268	LYS
1	F	272	LEU
1	F	273	ARG
2	G	4	THR
2	G	6	LYS
2	G	16	GLU
2	G	19	LYS
2	G	21	ASN
2	G	27	VAL
2	G	58	LYS

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Mol	Chain	Res	Type
2	G	64	LEU
2	G	69	GLU
2	G	73	THR
2	G	74	GLU
3	H	6	SER
3	H	8	ILE
4	I	5	GLU
4	I	40	SER
4	I	96	MET
4	I	141	LYS
4	I	145	LYS
4	I	163	LYS
4	I	175	LEU
4	I	179	SER
4	I	180	MET
4	I	206	ILE
4	I	210	ASP
5	J	57	GLN
5	J	92	GLN
5	J	187	GLN
5	J	195	LEU
1	K	35	ARG
1	K	88	SER
1	K	89	GLU
1	K	98[A]	MET
1	K	98[B]	MET
1	K	103	LEU
1	K	106	ASP
1	K	186	LYS
1	K	194	VAL
1	K	196	ASP
1	K	206	LEU
1	K	218	GLN
1	K	222	GLU
1	K	225	THR
1	K	228	THR
1	K	231	VAL
1	K	242	GLN
1	K	255	GLN
1	K	268	LYS
1	K	272	LEU
1	K	274	TRP

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Mol	Chain	Res	Type
2	L	6	LYS
2	L	17	ASN
2	L	19	LYS
2	L	27	VAL
2	L	38	ASP
2	L	45	ARG
2	L	47	GLU
2	L	48	LYS
2	L	58	LYS
2	L	69	GLU
2	L	70	PHE
3	M	6	SER
3	M	8	ILE
4	N	5	GLU
4	N	51	THR
4	N	96	MET
4	N	145	LYS
4	N	163	LYS
4	N	175	LEU
4	N	186	SER
4	N	206	ILE
4	N	209	GLU
5	O	57	GLN
5	O	83	GLU
5	O	92	GLN
5	O	132	VAL
5	O	187	GLN
5	O	195	LEU
5	O	217	ARG
1	P	35	ARG
1	P	88	SER
1	P	89	GLU
1	P	98[A]	MET
1	P	98[B]	MET
1	P	103	LEU
1	P	106	ASP
1	P	115	GLN
1	P	116	SER
1	P	141	GLN
1	P	197	HIS
1	P	206	LEU
1	P	226	GLN

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Mol	Chain	Res	Type
1	P	231	VAL
1	P	254	GLU
1	P	255	GLN
1	P	268	LYS
1	P	272	LEU
1	P	273	ARG
1	P	274	TRP
1	P	275	GLU
2	Q	6	LYS
2	Q	12	ARG
2	Q	16	GLU
2	Q	27	VAL
2	Q	38	ASP
2	Q	48	LYS
2	Q	58	LYS
2	Q	64	LEU
2	Q	69	GLU
2	Q	70	PHE
2	Q	73	THR
2	Q	74	GLU
3	R	6	SER
3	R	8	ILE
4	S	5	GLU
4	S	26	GLN
4	S	96	MET
4	S	141	LYS
4	S	145	LYS
4	S	163	LYS
4	S	173	CYS
4	S	193	LYS
4	S	206	ILE
4	S	210	ASP
4	S	211	THR
4	S	212	PHE
5	T	74	ASP
5	T	92	GLN
5	T	143	SER
5	T	187	GLN
5	T	192	GLN
5	T	195	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	86	ASN
1	A	113	HIS
1	A	144	GLN
1	A	180	GLN
1	A	224	GLN
1	A	226	GLN
1	A	262	GLN
2	B	17	ASN
2	B	42	ASN
4	D	20	GLN
5	E	58	ASN
5	E	115	GLN
5	E	179	HIS
5	E	225	GLN
1	F	32	GLN
1	F	72	GLN
1	F	180	GLN
1	F	188	HIS
2	G	13	HIS
4	I	20	GLN
4	I	45	HIS
4	I	126	ASN
4	I	128	GLN
5	J	57	GLN
5	J	58	ASN
5	J	115	GLN
5	J	179	HIS
5	J	225	GLN
1	K	72	GLN
1	K	144	GLN
1	K	218	GLN
1	K	224	GLN
1	K	262	GLN
2	L	13	HIS
2	L	42	ASN
4	N	20	GLN
4	N	126	ASN
4	N	128	GLN
5	O	58	ASN
5	O	96	GLN
5	O	115	GLN
5	O	225	GLN

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Mol	Chain	Res	Type
1	P	32	GLN
1	P	70	ASN
1	P	72	GLN
1	P	197	HIS
1	P	255	GLN
1	P	260	HIS
1	P	262	GLN
2	Q	13	HIS
4	S	20	GLN
4	S	26	GLN
4	S	126	ASN
4	S	128	GLN
5	T	57	GLN
5	T	58	ASN
5	T	96	GLN
5	T	192	GLN
5	T	225	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](#)

4 ligands are modelled in this entry.

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	PO4	N	301	-	4,4,4	2.06	2 (50%)	6,6,6	0.45	0
6	PO4	S	301	-	4,4,4	2.06	3 (75%)	6,6,6	0.43	0
6	PO4	I	301	-	4,4,4	2.55	2 (50%)	6,6,6	0.50	0
6	PO4	D	301	-	4,4,4	2.55	1 (25%)	6,6,6	0.44	0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	301	PO4	P-O1	4.24	1.60	1.50
6	D	301	PO4	P-O1	4.24	1.60	1.50
6	N	301	PO4	P-O1	2.27	1.55	1.50
6	S	301	PO4	P-O1	2.24	1.55	1.50
6	I	301	PO4	P-O2	2.03	1.60	1.54
6	S	301	PO4	P-O3	2.01	1.60	1.54
6	N	301	PO4	P-O2	2.01	1.60	1.54
6	S	301	PO4	P-O4	2.00	1.60	1.54

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/276 (98%)	0.51	20 (7%) 21 17	20, 56, 123, 169	3 (1%)
1	F	273/276 (98%)	0.48	17 (6%) 26 23	18, 55, 120, 169	3 (1%)
1	K	274/276 (99%)	0.20	7 (2%) 57 53	12, 47, 93, 126	5 (1%)
1	P	274/276 (99%)	0.80	22 (8%) 18 15	32, 74, 115, 137	3 (1%)
2	B	99/100 (99%)	1.27	21 (21%) 2 2	37, 88, 132, 168	1 (1%)
2	G	99/100 (99%)	0.71	6 (6%) 27 23	33, 68, 115, 136	1 (1%)
2	L	99/100 (99%)	0.67	6 (6%) 27 23	28, 66, 109, 130	1 (1%)
2	Q	99/100 (99%)	1.01	11 (11%) 10 7	56, 77, 111, 124	1 (1%)
3	C	9/9 (100%)	-0.23	0 100 100	27, 29, 40, 42	0
3	H	9/9 (100%)	-0.10	0 100 100	30, 33, 46, 51	0
3	M	9/9 (100%)	-0.38	0 100 100	18, 23, 36, 37	0
3	R	9/9 (100%)	0.18	0 100 100	46, 52, 62, 62	0
4	D	197/197 (100%)	0.65	20 (10%) 12 9	14, 57, 158, 206	2 (1%)
4	I	197/197 (100%)	0.71	27 (13%) 6 5	18, 67, 168, 225	3 (1%)
4	N	197/197 (100%)	0.57	21 (10%) 11 8	13, 53, 144, 209	2 (1%)
4	S	197/197 (100%)	0.76	31 (15%) 5 4	17, 65, 146, 205	2 (1%)
5	E	242/242 (100%)	0.49	8 (3%) 49 45	17, 66, 123, 166	3 (1%)
5	J	242/242 (100%)	0.39	6 (2%) 58 54	16, 63, 133, 160	3 (1%)
5	O	242/242 (100%)	0.31	16 (6%) 24 20	13, 51, 112, 158	3 (1%)
5	T	242/242 (100%)	0.74	9 (3%) 45 41	29, 73, 115, 167	3 (1%)
All	All	3282/3296 (99%)	0.58	248 (7%) 20 16	12, 65, 133, 225	39 (1%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	199	ALA	5.3
2	Q	1	ILE	5.2
1	F	254	GLU	4.4
1	F	252	GLY	4.4
2	B	22	PHE	4.2
1	A	199	ALA	4.2
4	D	213	PHE	4.0
2	L	73	THR	4.0
1	K	258	THR	3.8
2	Q	58	LYS	3.8
5	O	210	ALA	3.8
2	B	69	GLU	3.8
4	D	134	VAL	3.6
4	S	137	LEU	3.5
4	D	186	SER	3.5
1	P	12	MET	3.4
2	B	39	LEU	3.4
1	A	201	LEU	3.3
2	Q	73	THR	3.3
1	P	274	TRP	3.3
2	Q	54	LEU	3.3
4	S	197	ALA	3.3
5	T	255	ALA	3.3
1	A	107	GLY	3.3
2	G	73	THR	3.3
4	I	202	PHE	3.2
5	E	155	LEU	3.2
4	S	180	MET	3.2
2	G	1	ILE	3.2
1	F	249	VAL	3.2
4	I	207	ILE	3.2
4	S	214	PRO	3.2
4	I	179	SER	3.1
4	S	213	PHE	3.1
4	N	199	ALA	3.1
4	I	134	VAL	3.1
4	S	148	CYS	3.1
4	I	206	ILE	3.1
1	K	270	LEU	3.1
5	T	133	PHE	3.1
4	I	204	ASN	3.1
5	O	255	ALA	3.0
1	P	88	SER	3.0

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Mol	Chain	Res	Type	RSRZ
4	S	140	SER	3.0
4	N	137	LEU	3.0
4	S	202	PHE	3.0
2	B	1	ILE	3.0
4	S	199	ALA	3.0
1	F	203	CYS	3.0
1	P	92	SER	3.0
4	S	179	SER	3.0
1	F	255	GLN	2.9
2	B	20	SER	2.9
2	B	4	THR	2.9
1	F	274	TRP	2.9
2	B	78	TYR	2.9
2	B	70	PHE	2.9
4	I	213	PHE	2.9
5	O	140	PHE	2.9
4	N	179	SER	2.9
2	G	71	THR	2.9
4	D	214	PRO	2.9
2	B	40	LEU	2.9
4	S	161	GLN	2.9
1	A	61[A]	ASP	2.8
4	S	47	GLY	2.8
4	S	160	SER	2.8
1	A	230	LEU	2.8
4	N	198	CYS	2.8
1	P	89	GLU	2.8
5	E	92	GLN	2.8
2	B	18	GLY	2.8
1	A	251	SER	2.8
4	I	187	ALA	2.8
5	J	189	LEU	2.8
4	S	198	CYS	2.8
1	A	254	GLU	2.8
1	F	35	ARG	2.8
1	P	61[A]	ASP	2.8
2	B	43	GLY	2.7
4	N	187	ALA	2.7
1	P	232	GLU	2.7
1	P	221	GLY	2.7
4	N	213	PHE	2.7
4	N	167	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	200	THR	2.7
1	P	98[A]	MET	2.7
5	T	192	GLN	2.7
4	S	157	THR	2.7
5	E	143	SER	2.7
1	F	200	THR	2.7
5	E	201	ALA	2.6
5	O	214	GLN	2.6
1	A	274	TRP	2.6
1	A	192	HIS	2.6
1	P	220	ASP	2.6
2	B	53	ASP	2.6
5	O	209	SER	2.6
1	F	225	THR	2.6
4	I	208	PRO	2.6
2	Q	4	THR	2.6
1	A	193	PRO	2.6
2	B	21	ASN	2.6
4	D	201	ALA	2.6
4	N	146	SER	2.6
2	B	95	TRP	2.5
2	Q	7	ILE	2.5
4	I	205	SER	2.5
5	O	211	THR	2.5
4	S	196	PHE	2.5
5	J	195	LEU	2.5
4	N	148	CYS	2.5
4	D	180	MET	2.5
1	P	270	LEU	2.5
2	Q	64	LEU	2.5
4	N	202	PHE	2.5
4	D	158	ASN	2.5
4	S	147	VAL	2.5
4	S	142	SER	2.5
4	S	211	THR	2.5
4	N	173	CYS	2.4
1	P	257	TYR	2.4
5	E	165	ASP	2.4
2	L	40	LEU	2.4
4	S	158	ASN	2.4
1	A	104	GLY	2.4
4	D	137	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	N	4	LEU	2.4
4	D	202	PHE	2.4
4	I	190	TRP	2.4
4	S	174	VAL	2.4
5	O	232	ASN	2.4
4	S	143	SER	2.4
2	B	75	LYS	2.4
5	J	197	ASP	2.4
1	K	230	LEU	2.4
5	T	46	LEU	2.4
4	S	133	ALA	2.4
1	P	108	ARG	2.4
4	D	159	VAL	2.4
5	T	139	VAL	2.4
5	E	194	ALA	2.4
1	K	274	TRP	2.4
5	O	148	SER	2.3
2	G	40	LEU	2.3
1	A	108	ARG	2.3
4	D	156	GLN	2.3
4	I	46	ASP	2.3
2	Q	75	LYS	2.3
2	Q	44	GLU	2.3
1	P	2	SER	2.3
2	B	19	LYS	2.3
4	I	212	PHE	2.3
1	P	46	GLU	2.3
1	P	203	CYS	2.3
2	B	44	GLU	2.3
4	I	159	VAL	2.3
1	F	41	ALA	2.3
4	I	199	ALA	2.3
4	I	142	SER	2.3
4	D	207	ILE	2.3
2	B	41	LYS	2.3
2	G	72	PRO	2.3
5	O	254	ARG	2.3
1	P	90	ALA	2.2
1	F	66	ILE	2.2
4	D	139	ASP	2.2
1	F	253	GLU	2.2
4	N	214	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
4	N	197	ALA	2.2
5	T	201	ALA	2.2
2	L	71	THR	2.2
5	E	195	LEU	2.2
5	O	46	LEU	2.2
2	Q	69	GLU	2.2
4	D	212	PHE	2.2
1	F	250	PRO	2.2
2	B	9	VAL	2.2
4	D	187	ALA	2.2
4	N	200	ASN	2.2
4	D	188	VAL	2.2
4	I	200	ASN	2.2
4	N	203	ASN	2.2
5	O	192	GLN	2.2
4	S	207	ILE	2.2
5	O	252	TRP	2.2
2	L	17	ASN	2.1
4	D	128	GLN	2.1
4	N	180	MET	2.1
1	P	104	GLY	2.1
1	A	181	ARG	2.1
1	P	181	ARG	2.1
2	G	58	LYS	2.1
4	I	2	GLN	2.1
5	J	192	GLN	2.1
4	I	201	ALA	2.1
4	D	203	ASN	2.1
5	T	9	ARG	2.1
4	I	148	CYS	2.1
1	K	61[A]	ASP	2.1
4	I	28	SER	2.1
4	N	140	SER	2.1
4	N	142	SER	2.1
4	S	155	SER	2.1
4	S	164	ASP	2.1
5	E	209	SER	2.1
1	A	194	VAL	2.1
1	P	261	VAL	2.1
2	L	79	ALA	2.1
4	D	199	ALA	2.1
1	P	16	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
5	O	217	ARG	2.1
4	S	135	TYR	2.1
2	B	58	LYS	2.1
4	I	140	SER	2.1
4	I	143	SER	2.1
4	S	139	ASP	2.1
1	F	98[A]	MET	2.1
4	I	158	ASN	2.1
4	S	203	ASN	2.1
5	O	197	ASP	2.1
4	I	155	SER	2.1
1	K	105	PRO	2.1
1	F	248	VAL	2.0
4	I	153	PHE	2.0
4	N	153	PHE	2.0
4	S	159	VAL	2.0
5	O	208	VAL	2.0
1	A	225	THR	2.0
5	J	252	TRP	2.0
2	L	1	ILE	2.0
1	F	223	ASP	2.0
4	N	205	SER	2.0
5	T	209	SER	2.0
5	J	92	GLN	2.0
2	Q	3	ARG	2.0
4	D	138	ARG	2.0
2	B	23	LEU	2.0
1	A	268	LYS	2.0
1	K	271	THR	2.0
1	P	95	ILE	2.0
4	S	127	ILE	2.0
5	O	213	TRP	2.0
1	A	98	MET	2.0
1	A	105	PRO	2.0
1	A	220	ASP	2.0
4	I	195	ASP	2.0
5	T	135	PRO	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 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
6	PO4	I	301	5/5	0.86	0.10	70,71,75,77	0
6	PO4	S	301	5/5	0.87	0.09	68,74,79,86	0
6	PO4	D	301	5/5	0.89	0.10	56,60,65,75	0
6	PO4	N	301	5/5	0.92	0.08	61,62,65,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.