



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:01 PM UTC

PDB ID : 5SWZ / pdb_00005swz
Title : Crystal Structure of NP1-B17 TCR-H2Db-NP complex
Authors : Gras, S.; Del Campo, C.M.; Farenc, C.; Josephs, T.M.; Rossjohn, J.
Deposited on : 2016-08-09
Resolution : 2.65 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

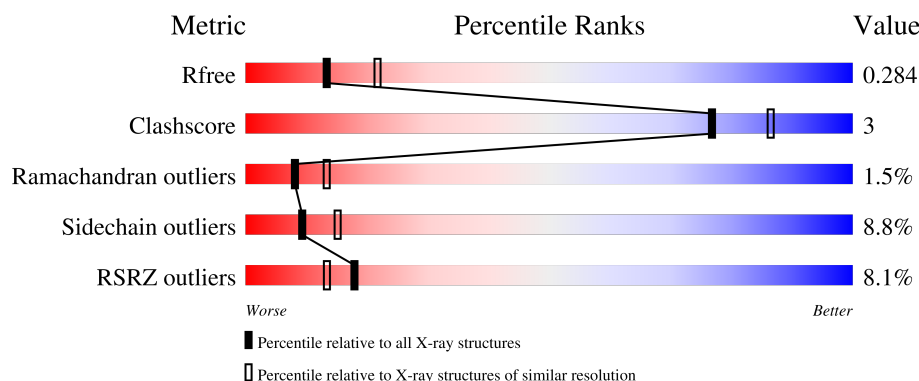
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	280	4% 85% 12% ..
1	F	280	11% 81% 17% ..
1	K	280	8% 81% 14% ..
1	P	280	8% 71% 13% 15%
2	B	99	5% 89% 8% .

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Mol	Chain	Length	Quality of chain
2	G	99	
2	L	99	
2	Q	99	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	207	
4	I	207	
4	N	207	
4	S	207	
5	E	243	
5	J	243	
5	O	243	
5	T	243	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 27034 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	5	0
			2317	1460	415	433	9			
1	F	277	Total	C	N	O	S	0	5	0
			2317	1460	415	433	9			
1	K	277	Total	C	N	O	S	0	5	0
			2317	1460	415	433	9			
1	P	238	Total	C	N	O	S	0	4	0
			1983	1250	353	371	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	0	0
			818	523	138	150	7			
2	G	99	Total	C	N	O	S	0	1	0
			826	528	139	151	8			
2	L	99	Total	C	N	O	S	0	1	0
			826	528	139	151	8			
2	Q	98	Total	C	N	O	S	0	1	0
			818	522	138	150	8			

- Molecule 3 is a protein called influenza NP366 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			68	38	10	18	2			
3	H	9	Total	C	N	O	S	0	0	0
			68	38	10	18	2			
3	M	9	Total	C	N	O	S	0	0	0
			68	38	10	18	2			
3	R	9	Total	C	N	O	S	0	0	0
			68	38	10	18	2			

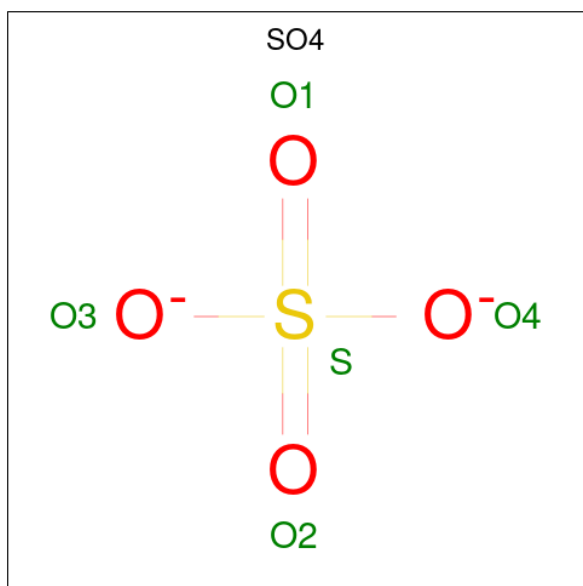
- Molecule 4 is a protein called NP1-B17 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1557	977	256	318	6			
4	I	186	Total	C	N	O	S	0	0	0
			1461	916	241	299	5			
4	N	201	Total	C	N	O	S	0	0	0
			1586	996	260	323	7			
4	S	203	Total	C	N	O	S	0	0	0
			1598	1002	262	327	7			

- Molecule 5 is a protein called NP1-B17 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1940	1231	338	362	9			
5	J	240	Total	C	N	O	S	0	0	0
			1940	1231	338	362	9			
5	O	241	Total	C	N	O	S	0	1	0
			1960	1241	343	367	9			
5	T	239	Total	C	N	O	S	0	0	0
			1935	1228	337	361	9			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	O	1	Total	O	S	0	0
			5	4	1		
6	T	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Na	0	0
			1	1		
7	I	1	Total	Na	0	0
			1	1		
7	J	1	Total	Na	0	0
			1	1		
7	K	1	Total	Na	0	0
			1	1		
7	T	2	Total	Na	0	0
			2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	55	Total	O	0	0
			55	55		
8	B	15	Total	O	0	0
			15	15		
8	C	4	Total	O	0	0
			4	4		
8	D	30	Total	O	0	0
			30	30		
8	E	50	Total	O	0	0
			50	50		
8	F	31	Total	O	0	0
			31	31		
8	G	18	Total	O	0	0
			18	18		
8	H	2	Total	O	0	0
			2	2		

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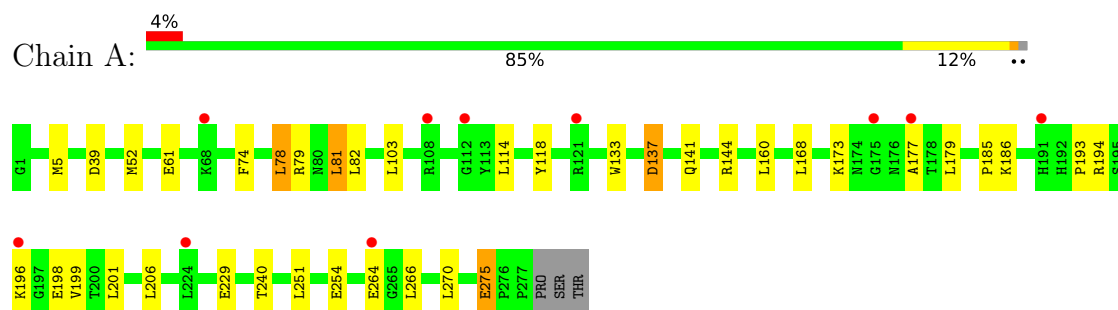
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	23	Total 23	O 23	0	0
8	J	33	Total 33	O 33	0	0
8	K	40	Total 40	O 40	0	0
8	L	19	Total 19	O 19	0	0
8	M	1	Total 1	O 1	0	0
8	N	32	Total 32	O 32	0	0
8	O	57	Total 57	O 57	0	0
8	P	40	Total 40	O 40	0	0
8	Q	14	Total 14	O 14	0	0
8	R	2	Total 2	O 2	0	0
8	S	22	Total 22	O 22	0	0
8	T	44	Total 44	O 44	0	0

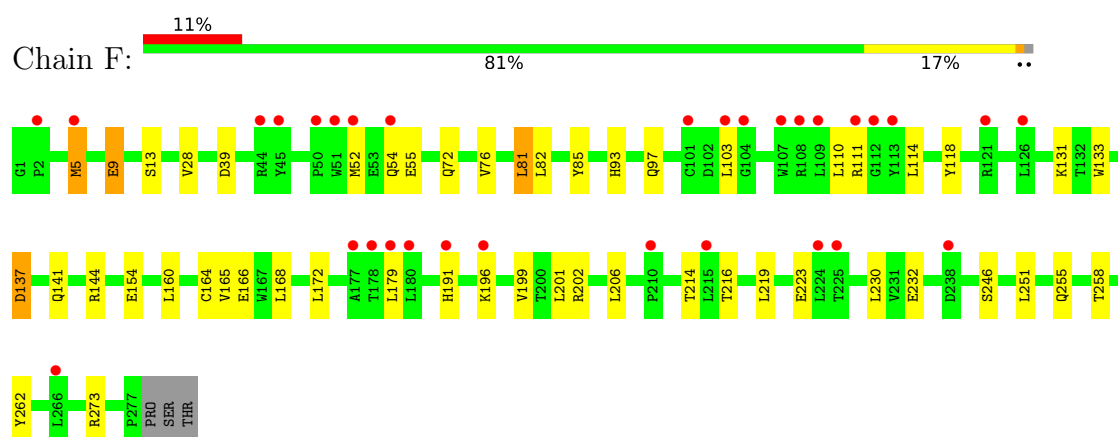
3 Residue-property plots [i](#)

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.

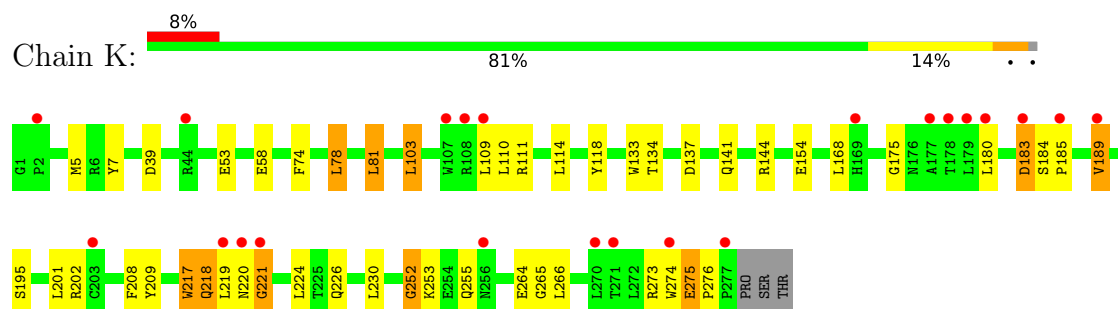
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



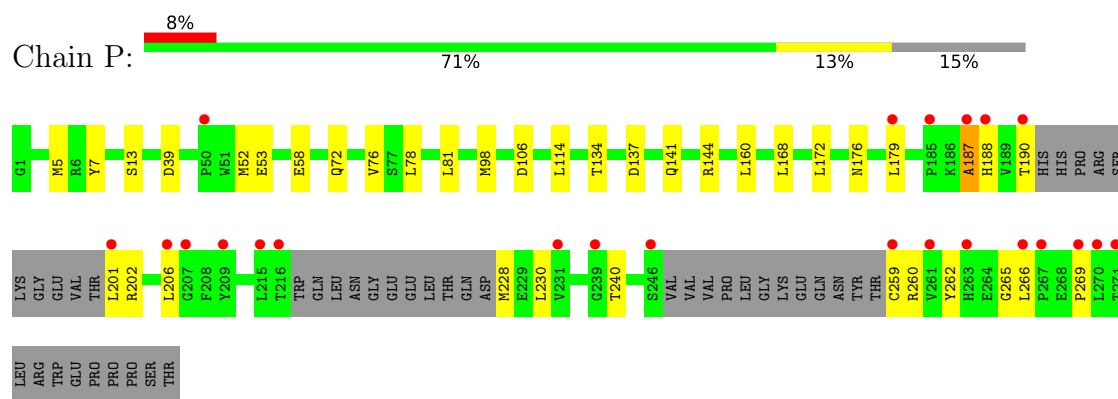
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



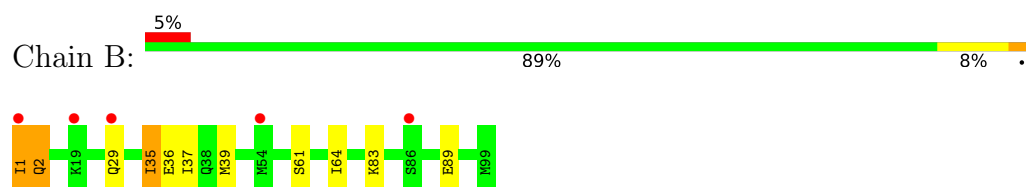
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



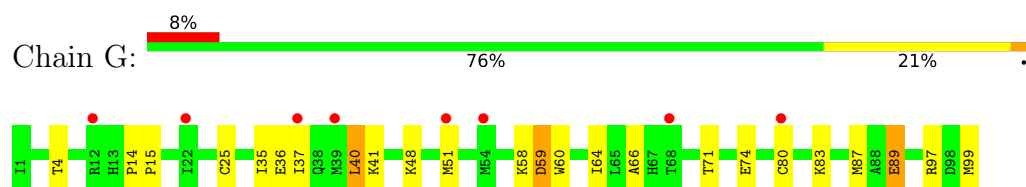
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



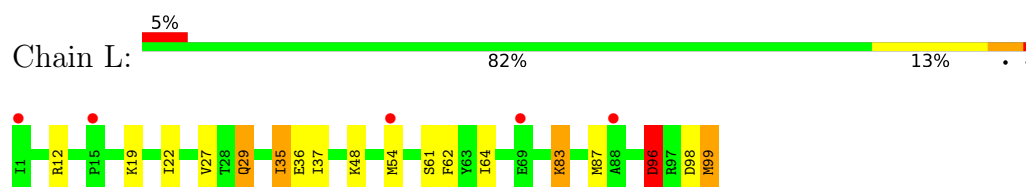
- Molecule 2: Beta-2-microglobulin



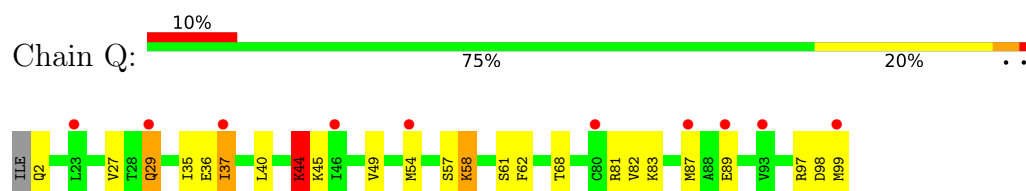
- Molecule 2: Beta-2-microglobulin



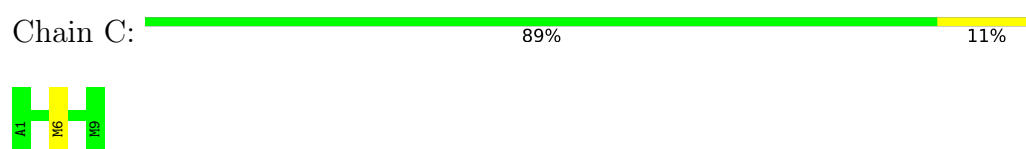
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: influenza NP366 epitope



- Molecule 3: influenza NP366 epitope

Chain H:  78% 22%



- Molecule 3: influenza NP366 epitope

Chain M:  78% 22%



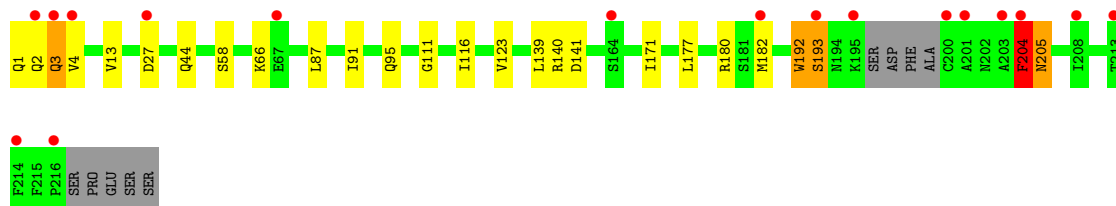
- Molecule 3: influenza NP366 epitope

Chain R:  78% 22%



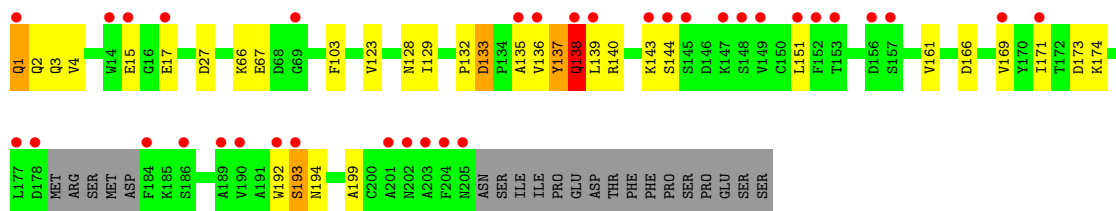
- Molecule 4: NP1-B17 TCR alpha chain

Chain D:  8% 83% 10% . .



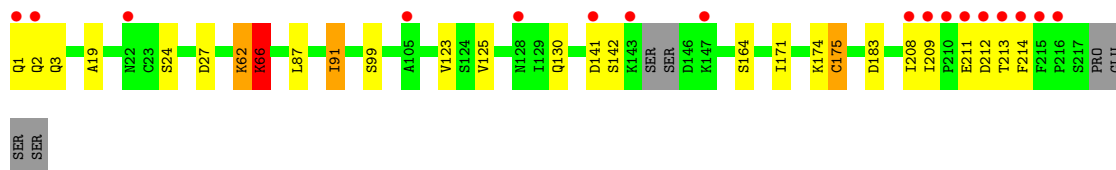
- Molecule 4: NP1-B17 TCR alpha chain

Chain I:  17% 73% 14% . 10%

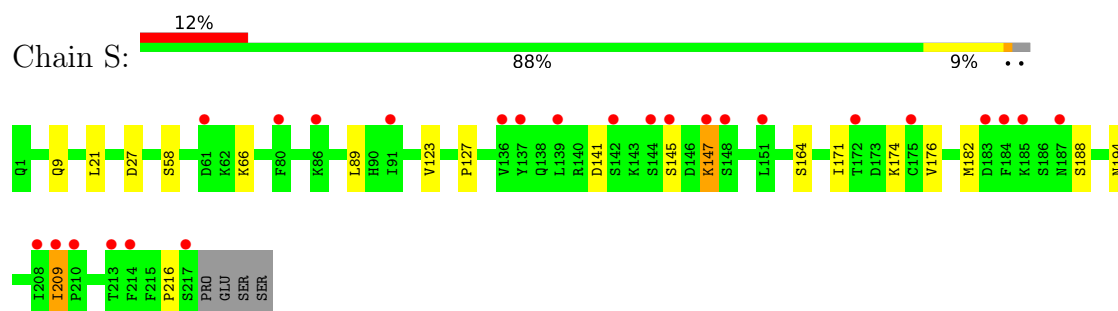


- Molecule 4: NP1-B17 TCR alpha chain

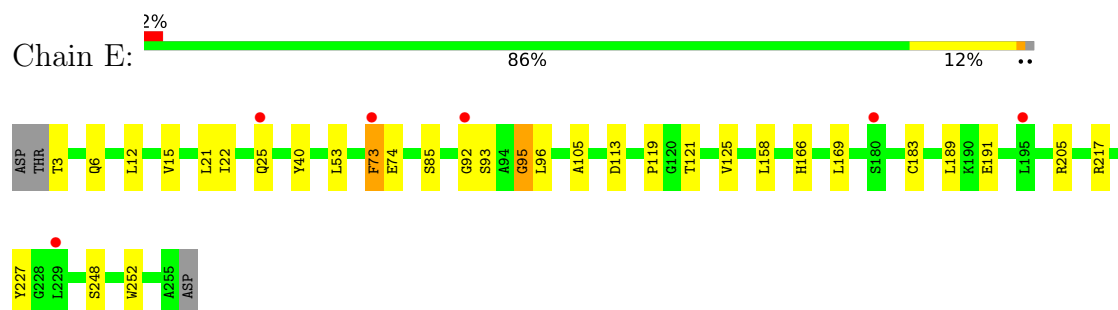
Chain N:  8% 84% 11% . .



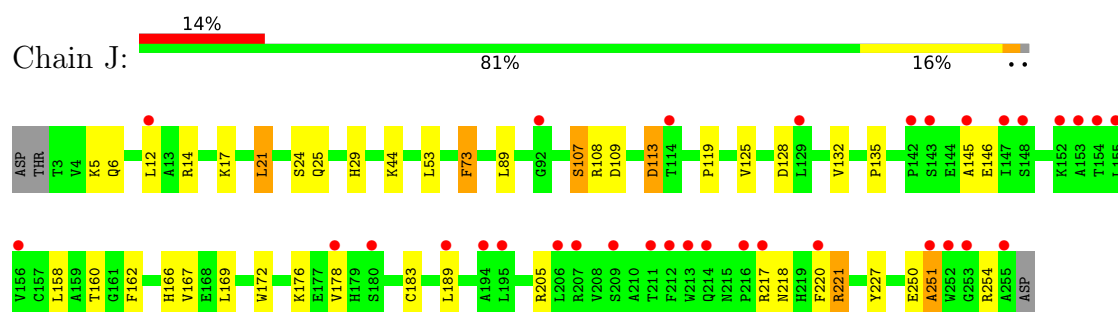
- Molecule 4: NP1-B17 TCR alpha chain



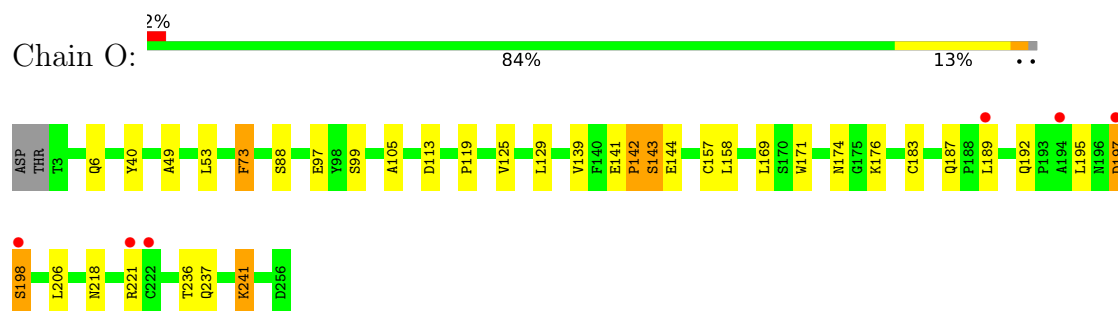
- Molecule 5: NP1-B17 TCR beta chain



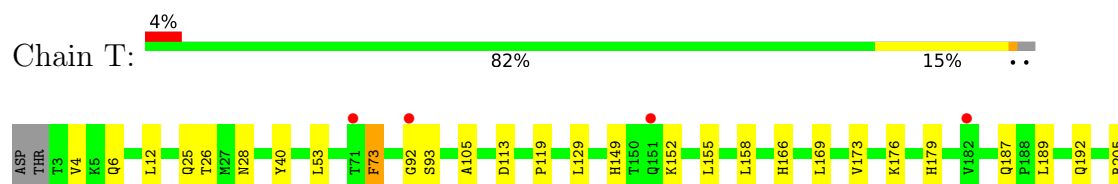
- Molecule 5: NP1-B17 TCR beta chain

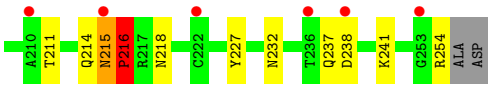


- Molecule 5: NP1-B17 TCR beta chain



- Molecule 5: NP1-B17 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	92.23Å 100.19Å 469.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.80 – 2.65 38.80 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.80-2.65) 99.9 (38.80-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.226 , 0.249 0.260 , 0.284	Depositor DCC
R_{free} test set	6523 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27034	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: SO4, NA

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	0.65	0/2385	1.16	1/3240 (0.0%)
1	F	0.69	0/2385	1.19	5/3240 (0.2%)
1	K	0.69	0/2385	1.23	12/3240 (0.4%)
1	P	0.65	0/2037	1.16	4/2759 (0.1%)
2	B	0.73	0/844	1.12	2/1144 (0.2%)
2	G	0.74	0/852	1.20	5/1154 (0.4%)
2	L	0.74	0/852	1.15	2/1154 (0.2%)
2	Q	0.75	0/844	1.20	4/1143 (0.3%)
3	C	0.57	0/67	1.00	0/86
3	H	0.59	0/67	0.98	0/86
3	M	0.58	0/67	0.97	0/86
3	R	0.57	0/67	1.00	0/86
4	D	0.72	0/1594	1.13	8/2164 (0.4%)
4	I	0.76	0/1495	1.16	9/2028 (0.4%)
4	N	0.70	0/1624	1.09	2/2203 (0.1%)
4	S	0.70	0/1637	1.10	2/2222 (0.1%)
5	E	0.66	0/1994	1.12	4/2711 (0.1%)
5	J	0.68	0/1994	1.13	4/2711 (0.1%)
5	O	0.67	0/2014	1.19	11/2736 (0.4%)
5	T	0.65	0/1989	1.14	8/2704 (0.3%)
All	All	0.69	0/27193	1.16	83/36897 (0.2%)

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	217	ARG	N-CA-C	-9.10	102.69	113.88
5	O	142	PRO	CA-C-N	8.89	137.70	121.70
5	O	142	PRO	C-N-CA	8.89	137.70	121.70
5	O	197	ASP	CA-C-N	8.33	136.69	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	197	ASP	C-N-CA	8.33	136.69	121.70
1	F	164	CYS	CA-C-N	8.23	136.51	121.70
1	F	164	CYS	C-N-CA	8.23	136.51	121.70
2	G	40	LEU	CA-C-N	7.85	135.83	121.70
2	G	40	LEU	C-N-CA	7.85	135.83	121.70
4	D	192	TRP	CA-C-N	7.83	135.78	121.70
4	D	192	TRP	C-N-CA	7.83	135.78	121.70
4	I	192	TRP	CA-C-N	7.38	134.99	121.70
4	I	192	TRP	C-N-CA	7.38	134.99	121.70
1	F	85	TYR	CA-C-N	7.38	134.98	121.70
1	F	85	TYR	C-N-CA	7.38	134.98	121.70
2	B	1	ILE	CA-C-N	7.35	134.93	121.70
2	B	1	ILE	C-N-CA	7.35	134.93	121.70
1	K	217	TRP	CA-C-N	7.35	134.93	121.70
1	K	217	TRP	C-N-CA	7.35	134.93	121.70
2	G	59	ASP	CA-C-N	7.20	134.67	121.70
2	G	59	ASP	C-N-CA	7.20	134.67	121.70
5	O	221[A]	ARG	CA-C-N	7.11	134.50	121.70
5	O	221[A]	ARG	C-N-CA	7.11	134.50	121.70
5	O	221[B]	ARG	CA-C-N	7.11	134.50	121.70
5	O	221[B]	ARG	C-N-CA	7.11	134.50	121.70
1	K	252	GLY	CA-C-N	6.99	134.29	121.70
1	K	252	GLY	C-N-CA	6.99	134.29	121.70
5	T	211	THR	N-CA-C	-6.77	104.18	113.18
1	K	183	ASP	CA-C-N	6.76	133.87	121.70
1	K	183	ASP	C-N-CA	6.76	133.87	121.70
2	L	96	ASP	CA-C-N	6.75	133.85	121.70
2	L	96	ASP	C-N-CA	6.75	133.85	121.70
5	T	179	HIS	CA-C-N	6.68	130.83	120.82
5	T	179	HIS	C-N-CA	6.68	130.83	120.82
4	N	1	GLN	CA-C-N	6.52	133.44	121.70
4	N	1	GLN	C-N-CA	6.52	133.44	121.70
5	T	73	PHE	CA-CB-CG	6.51	120.31	113.80
1	K	218	GLN	CA-C-N	6.50	133.40	121.70
1	K	218	GLN	C-N-CA	6.50	133.40	121.70
4	D	204	PHE	CA-C-N	6.45	133.31	121.70
4	D	204	PHE	C-N-CA	6.45	133.31	121.70
4	I	17	GLU	CB-CG-CD	6.30	123.31	112.60
4	I	135	ALA	N-CA-C	6.16	123.91	110.80
2	G	71	THR	CB-CA-C	6.08	116.53	110.33
4	I	138	GLN	N-CA-C	6.05	118.98	108.76
5	T	216	PRO	CA-C-N	6.05	132.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	216	PRO	C-N-CA	6.05	132.59	121.70
5	O	113	ASP	CA-C-N	6.00	130.24	121.31
5	O	113	ASP	C-N-CA	6.00	130.24	121.31
5	E	113	ASP	CA-C-N	5.96	130.19	121.31
5	E	113	ASP	C-N-CA	5.96	130.19	121.31
5	T	113	ASP	CA-C-N	5.96	130.19	121.31
5	T	113	ASP	C-N-CA	5.96	130.19	121.31
5	E	73	PHE	CA-C-N	5.88	132.77	121.54
5	E	73	PHE	C-N-CA	5.88	132.77	121.54
4	I	1	GLN	CA-C-N	5.85	132.23	121.70
4	I	1	GLN	C-N-CA	5.85	132.23	121.70
1	A	137	ASP	CA-CB-CG	5.76	118.36	112.60
2	Q	57	SER	CA-C-N	5.75	127.99	120.28
2	Q	57	SER	C-N-CA	5.75	127.99	120.28
1	F	137	ASP	CA-CB-CG	5.65	118.25	112.60
4	I	193	SER	CA-C-N	5.57	131.72	121.70
4	I	193	SER	C-N-CA	5.57	131.72	121.70
1	P	187	ALA	CA-C-N	5.46	131.52	121.70
1	P	187	ALA	C-N-CA	5.46	131.52	121.70
2	Q	44	LYS	CA-C-N	5.39	128.89	120.75
2	Q	44	LYS	C-N-CA	5.39	128.89	120.75
1	K	221	GLY	CA-C-N	5.37	127.47	120.28
1	K	221	GLY	C-N-CA	5.37	127.47	120.28
5	J	250	GLU	CA-C-N	5.31	131.68	121.54
5	J	250	GLU	C-N-CA	5.31	131.68	121.54
4	S	145	SER	CA-C-N	5.28	131.20	121.70
4	S	145	SER	C-N-CA	5.28	131.20	121.70
5	O	73	PHE	CA-CB-CG	5.14	118.94	113.80
1	P	228	MET	CA-C-N	5.12	130.91	121.70
1	P	228	MET	C-N-CA	5.12	130.91	121.70
4	D	3	GLN	CA-C-N	5.08	130.84	121.70
4	D	3	GLN	C-N-CA	5.08	130.84	121.70
1	K	53	GLU	CA-C-N	5.07	127.07	120.28
1	K	53	GLU	C-N-CA	5.07	127.07	120.28
4	D	91	ILE	CA-C-N	5.05	128.39	120.82
4	D	91	ILE	C-N-CA	5.05	128.39	120.82
5	J	73	PHE	CA-CB-CG	5.04	118.84	113.80

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	2317	0	2193	11	0
1	F	2317	0	2193	11	0
1	K	2317	0	2193	18	0
1	P	1983	0	1872	10	0
2	B	818	0	797	5	0
2	G	826	0	807	11	0
2	L	826	0	805	7	0
2	Q	818	0	793	8	0
3	C	68	0	54	0	0
3	H	68	0	54	1	0
3	M	68	0	54	0	0
3	R	68	0	54	2	0
4	D	1557	0	1458	7	0
4	I	1461	0	1373	11	0
4	N	1586	0	1491	8	0
4	S	1598	0	1502	5	0
5	E	1940	0	1867	7	0
5	J	1940	0	1869	14	0
5	O	1960	0	1885	11	0
5	T	1935	0	1863	9	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
6	K	5	0	0	0	0
6	O	5	0	0	0	0
6	T	5	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	T	2	0	0	0	0
8	A	55	0	0	0	0
8	B	15	0	0	0	0
8	C	4	0	0	0	0
8	D	30	0	0	0	0
8	E	50	0	0	0	0
8	F	31	0	0	0	0
8	G	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2	0	0	0	0
8	I	23	0	0	0	0
8	J	33	0	0	0	0
8	K	40	0	0	0	0
8	L	19	0	0	0	0
8	M	1	0	0	0	0
8	N	32	0	0	0	0
8	O	57	0	0	0	0
8	P	40	0	0	0	0
8	Q	14	0	0	0	0
8	R	2	0	0	0	0
8	S	22	0	0	0	0
8	T	44	0	0	0	0
All	All	27034	0	25177	147	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 (147) 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:G:25:CYS:HG	2:G:80:CYS:HG	1.05	0.99
5:J:109:ASP:OD2	5:J:113:ASP:HB2	1.67	0.94
5:J:108:ARG:NH2	5:J:113:ASP:OD1	2.06	0.85
5:J:145:ALA:HB1	5:J:146:GLU:HA	1.57	0.84
4:D:3:GLN:H	4:D:4:VAL:HA	1.44	0.83
2:Q:29:GLN:HA	2:Q:61:SER:HB3	1.67	0.75
1:K:185:PRO:HB3	1:K:208:PHE:HB3	1.72	0.70
1:K:252:GLY:HA3	1:K:253:LYS:HB2	1.73	0.70
2:L:36:GLU:HB2	2:L:83:LYS:HB3	1.75	0.69
1:P:187:ALA:HB1	1:P:188:HIS:HB3	1.75	0.69
5:T:237:GLN:H	5:T:238:ASP:HA	1.57	0.69
4:I:133:ASP:N	4:I:133:ASP:OD1	2.25	0.67
4:I:136:VAL:O	4:I:137:TYR:HB2	1.94	0.66
2:L:35:ILE:HG12	2:L:37:ILE:HD11	1.78	0.65
1:P:98:MET:HE1	2:Q:58:LYS:HG3	1.79	0.64
4:N:175:CYS:HB3	5:O:183:CYS:SG	2.37	0.63
5:E:25:GLN:HB3	5:E:85:SER:HA	1.81	0.63
5:T:215:ASN:HB2	5:T:216:PRO:O	1.99	0.63
2:B:1:ILE:HA	2:B:2:GLN:CB	2.29	0.63
1:P:76:VAL:HG13	3:R:8:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:6:GLN:HB2	5:T:119:PRO:HD2	1.83	0.59
5:O:174:ASN:HD21	5:O:218:ASN:HA	1.67	0.59
5:T:166:HIS:HB3	5:T:227:TYR:HB2	1.85	0.59
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.85	0.57
2:G:37:ILE:HD13	2:G:51:MET:HE1	1.86	0.57
1:K:275:GLU:HB2	1:K:276:PRO:HA	1.85	0.57
5:E:40:TYR:HB2	5:E:105:ALA:HB3	1.87	0.57
1:P:5:MET:HB2	1:P:168:LEU:HD13	1.86	0.57
5:T:40:TYR:HB2	5:T:105:ALA:HB3	1.87	0.57
5:E:15:VAL:HG12	5:E:95:GLY:HA2	1.87	0.57
2:G:51:MET:HE3	2:G:66:ALA:HB2	1.87	0.56
5:O:40:TYR:HB2	5:O:105:ALA:HB3	1.86	0.56
2:L:29:GLN:HA	2:L:61:SER:HB3	1.89	0.55
4:D:192:TRP:HA	4:D:193:SER:HB3	1.89	0.54
4:S:21:LEU:HB2	4:S:89:LEU:HB3	1.88	0.54
5:T:216:PRO:HB2	5:T:218:ASN:H	1.72	0.54
4:D:140:ARG:HB2	4:D:141:ASP:HB2	1.90	0.54
4:N:209:ILE:HG23	4:N:212:ASP:HB2	1.89	0.53
1:K:252:GLY:CA	1:K:253:LYS:HB2	2.38	0.53
1:A:194:ARG:HB3	1:A:198:GLU:HG3	1.89	0.53
1:P:5:MET:HE2	1:P:7:TYR:HE1	1.74	0.53
4:N:19:ALA:HB3	4:N:91:ILE:HG23	1.90	0.53
4:D:204:PHE:HA	4:D:205:ASN:O	2.08	0.53
1:K:220:ASN:HD21	1:K:273:ARG:HH22	1.57	0.52
5:O:6:GLN:HB2	5:O:119:PRO:HD2	1.91	0.52
2:B:1:ILE:HA	2:B:2:GLN:HB2	1.90	0.52
2:G:59:ASP:H	2:G:60:TRP:HA	1.74	0.52
4:S:127:PRO:HG2	4:S:176:VAL:HG11	1.91	0.52
5:J:166:HIS:HB3	5:J:227:TYR:HB2	1.91	0.52
5:J:220:PHE:HB2	5:J:251:ALA:HB2	1.92	0.51
2:L:27:VAL:HG21	2:L:37:ILE:HD12	1.92	0.51
1:F:214:THR:HB	1:F:262:TYR:HB2	1.92	0.51
1:K:183:ASP:HA	1:K:184[B]:SER:HB2	1.93	0.50
5:O:197:ASP:HA	5:O:198:SER:CB	2.41	0.50
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.94	0.50
5:O:197:ASP:HA	5:O:198:SER:HB3	1.93	0.50
1:F:202:ARG:HH12	2:G:99:MET:HA	1.76	0.50
5:J:172:TRP:HB2	5:J:221:ARG:HG2	1.93	0.50
4:N:211:GLU:HB2	4:N:212:ASP:HA	1.94	0.50
1:F:76:VAL:HG13	3:H:8:THR:HG21	1.93	0.50
1:K:217:TRP:HA	1:K:218:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:ASP:HB2	1:K:209:TYR:H	1.77	0.49
4:I:1:GLN:HB2	4:I:3:GLN:HB2	1.94	0.49
4:I:132:PRO:C	4:I:133:ASP:OD1	2.56	0.49
1:K:81:LEU:HD23	1:K:118:TYR:CD1	2.47	0.49
2:Q:44:LYS:HD2	2:Q:45:LYS:H	1.78	0.49
5:J:5:LYS:HB3	5:J:24:SER:HB2	1.95	0.49
4:D:4:VAL:HG23	4:D:116:ILE:HG22	1.95	0.48
5:E:6:GLN:HB2	5:E:119:PRO:HD2	1.94	0.48
2:B:29:GLN:HA	2:B:61:SER:HB2	1.95	0.48
5:J:6:GLN:HB2	5:J:119:PRO:HD2	1.94	0.48
2:L:96:ASP:HB3	2:L:99:MET:HB2	1.95	0.48
1:A:133:TRP:HB2	1:A:144:ARG:HG3	1.96	0.48
1:A:201:LEU:HD11	1:A:254:GLU:HB2	1.95	0.48
1:K:133:TRP:HB2	1:K:144:ARG:HG3	1.96	0.48
1:K:5:MET:HE2	1:K:7:TYR:HE1	1.79	0.47
1:K:183:ASP:HA	1:K:184[A]:SER:HB3	1.97	0.47
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.49	0.47
4:D:2:GLN:HB2	4:D:3:GLN:HA	1.97	0.47
4:I:15:GLU:HB3	4:I:128:ASN:HB2	1.97	0.47
1:K:218:GLN:HA	1:K:219:LEU:C	2.39	0.47
1:P:52:MET:HA	1:P:52:MET:HE2	1.97	0.47
4:D:192:TRP:HA	4:D:193:SER:CB	2.45	0.47
1:F:133:TRP:HB2	1:F:144:ARG:HG3	1.96	0.46
5:T:216:PRO:HB2	5:T:218:ASN:N	2.29	0.46
5:J:21:LEU:HD23	5:J:89:LEU:HD23	1.97	0.46
5:E:92:GLY:HA2	5:E:93:SER:HA	1.79	0.46
2:G:59:ASP:N	2:G:60:TRP:HA	2.31	0.46
4:N:211:GLU:OE1	4:N:213:THR:OG1	2.33	0.46
1:A:52:MET:HA	1:A:52:MET:HE2	1.97	0.46
1:F:72:GLN:O	1:F:76:VAL:HG12	2.16	0.45
2:L:54[B]:MET:HE2	2:L:62:PHE:HB3	1.99	0.45
1:P:72:GLN:O	1:P:76:VAL:HG12	2.15	0.45
1:F:81:LEU:HD23	1:F:118:TYR:CD1	2.51	0.45
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.98	0.45
4:I:138:GLN:O	4:I:139:LEU:HG	2.15	0.45
4:N:164:SER:HB2	4:N:171:ILE:HD12	1.98	0.45
1:F:5:MET:HB2	1:F:168:LEU:HD22	1.98	0.45
1:F:202:ARG:HD3	1:F:246:SER:HB3	1.99	0.45
2:G:36:GLU:HB2	2:G:83:LYS:HB3	1.99	0.45
5:J:145:ALA:CB	5:J:146:GLU:HA	2.39	0.45
1:F:103:LEU:HD11	1:F:165:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:PRO:HG2	2:G:97:ARG:HB2	1.98	0.44
2:G:40:LEU:HB3	2:G:41:LYS:O	2.17	0.44
1:K:220:ASN:HA	1:K:221:GLY:HA2	1.78	0.44
2:G:89:GLU:CD	5:O:49:ALA:H	2.26	0.44
1:F:9:GLU:HG2	1:F:97:GLN:HB3	1.99	0.44
5:E:166:HIS:HB3	5:E:227:TYR:HB2	2.00	0.44
2:Q:36:GLU:HB2	2:Q:83:LYS:HB3	2.00	0.44
1:P:141:GLN:HA	1:P:144:ARG:HG2	2.00	0.43
5:O:142:PRO:HA	5:O:143:SER:CB	2.47	0.43
2:Q:37:ILE:HG12	2:Q:82:VAL:HG22	2.00	0.43
1:P:190:THR:HG23	1:P:202:ARG:HE	1.84	0.43
5:T:92:GLY:HA2	5:T:93:SER:HA	1.79	0.43
1:P:76:VAL:CG1	3:R:8:THR:HG21	2.47	0.43
2:Q:54[B]:MET:HE2	2:Q:62:PHE:HB3	2.00	0.43
4:S:147:LYS:HE2	4:S:194:ASN:HA	2.01	0.43
4:I:161:VAL:HG21	4:I:173:ASP:HA	2.01	0.42
2:B:36:GLU:HB2	2:B:83:LYS:HB3	2.00	0.42
2:Q:49:VAL:HG23	2:Q:68:THR:HB	2.00	0.42
5:J:14:ARG:HB3	5:J:17:LYS:HG3	2.01	0.42
5:O:157:CYS:HB2	5:O:171:TRP:CZ2	2.54	0.42
2:B:35:ILE:HG23	2:B:37:ILE:HD11	2.01	0.42
5:J:29:HIS:HB3	5:J:107:SER:O	2.19	0.42
4:I:1:GLN:HA	4:I:2:GLN:HB2	2.02	0.42
4:I:166:ASP:HB3	4:I:169:VAL:HG22	2.01	0.42
1:A:266:LEU:HD21	1:A:270:LEU:HG	2.01	0.42
4:I:103:PHE:CZ	5:J:44:LYS:HE2	2.55	0.42
4:N:62:LYS:HG2	4:N:66:LYS:N	2.35	0.42
4:I:138:GLN:OE1	4:I:199:ALA:HB2	2.20	0.42
1:K:103:LEU:HD13	1:K:168:LEU:HD23	2.01	0.42
1:K:74:PHE:O	1:K:78:LEU:HB2	2.20	0.41
5:O:241:LYS:H	5:O:241:LYS:HG2	1.64	0.41
2:Q:40:LEU:HD11	2:Q:81:ARG:HB2	2.02	0.41
1:A:74:PHE:O	1:A:78:LEU:HB2	2.21	0.41
2:G:14:PRO:HA	2:G:15:PRO:HD3	1.96	0.41
5:J:135:PRO:HB3	5:J:162:PHE:HB3	2.03	0.41
1:A:79:ARG:HA	1:A:82:LEU:HD12	2.03	0.41
1:A:193:PRO:HA	1:A:199:VAL:HG23	2.03	0.41
2:L:12:ARG:HH21	2:L:22:ILE:HD13	1.85	0.41
5:E:21:LEU:HD22	5:E:121:THR:HG21	2.03	0.41
1:K:189:VAL:HG21	1:K:274:TRP:H	1.86	0.41
4:N:141:ASP:HB2	5:O:141:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:209:ILE:H	4:S:209:ILE:HD13	1.85	0.41
5:T:214:GLN:O	5:T:215:ASN:HB2	2.20	0.40
1:F:13:SER:HB3	1:F:93:HIS:H	1.86	0.40
4:S:164:SER:HB3	4:S:171:ILE:HD12	2.03	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	280/280 (100%)	262 (94%)	14 (5%)	4 (1%)	9	14
1	F	280/280 (100%)	264 (94%)	15 (5%)	1 (0%)	30	45
1	K	280/280 (100%)	250 (89%)	25 (9%)	5 (2%)	6	11
1	P	234/280 (84%)	221 (94%)	11 (5%)	2 (1%)	14	24
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	12	20
2	G	98/99 (99%)	93 (95%)	5 (5%)	0	100	100
2	L	98/99 (99%)	94 (96%)	4 (4%)	0	100	100
2	Q	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	H	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	M	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	R	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
4	D	194/207 (94%)	175 (90%)	15 (8%)	4 (2%)	5	9
4	I	182/207 (88%)	160 (88%)	18 (10%)	4 (2%)	5	9
4	N	197/207 (95%)	185 (94%)	8 (4%)	4 (2%)	6	10
4	S	201/207 (97%)	178 (89%)	19 (10%)	4 (2%)	6	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	238/243 (98%)	224 (94%)	11 (5%)	3 (1%)	9	16
5	J	238/243 (98%)	221 (93%)	15 (6%)	2 (1%)	16	27
5	O	240/243 (99%)	221 (92%)	14 (6%)	5 (2%)	5	9
5	T	237/243 (98%)	212 (90%)	20 (8%)	5 (2%)	5	9
All	All	3219/3352 (96%)	2972 (92%)	199 (6%)	48 (2%)	8	13

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	196	LYS
4	I	137	TYR
4	I	140	ARG
1	K	195	SER
1	K	275	GLU
4	N	214	PHE
5	O	143	SER
5	O	198	SER
5	T	215	ASN
5	T	216	PRO
1	A	196	LYS
2	B	2	GLN
5	E	74	GLU
5	E	96	LEU
4	I	144	SER
5	J	73	PHE
5	J	251	ALA
1	K	226	GLN
5	O	73	PHE
1	P	269	PRO
5	T	173	VAL
4	D	193	SER
4	D	205	ASN
4	S	147	LYS
3	C	6	MET
3	H	6	MET
3	M	6	MET
4	N	66	LYS
3	R	6	MET
4	S	66	LYS
4	S	141	ASP
5	T	73	PHE

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Mol	Chain	Res	Type
5	T	149	HIS
1	A	177	ALA
4	D	66	LYS
4	I	66	LYS
1	A	229	GLU
1	A	275	GLU
1	K	175	GLY
4	N	99	SER
4	N	142	SER
5	O	99	SER
4	S	216	PRO
1	P	265	GLY
4	D	111	GLY
1	K	265	GLY
5	E	95	GLY
5	O	192	GLN

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	240/238 (101%)	223 (93%)	17 (7%)	13	23
1	F	240/238 (101%)	207 (86%)	33 (14%)	3	5
1	K	240/238 (101%)	218 (91%)	22 (9%)	8	14
1	P	203/238 (85%)	181 (89%)	22 (11%)	6	9
2	B	93/93 (100%)	89 (96%)	4 (4%)	26	44
2	G	94/93 (101%)	86 (92%)	8 (8%)	10	17
2	L	94/93 (101%)	84 (89%)	10 (11%)	6	10
2	Q	93/93 (100%)	81 (87%)	12 (13%)	4	6
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
3	M	8/8 (100%)	7 (88%)	1 (12%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	8/8 (100%)	8 (100%)	0	100	100
4	D	178/188 (95%)	164 (92%)	14 (8%)	11	19
4	I	167/188 (89%)	154 (92%)	13 (8%)	11	20
4	N	182/188 (97%)	167 (92%)	15 (8%)	10	18
4	S	184/188 (98%)	176 (96%)	8 (4%)	26	44
5	E	212/215 (99%)	197 (93%)	15 (7%)	13	23
5	J	212/215 (99%)	191 (90%)	21 (10%)	7	11
5	O	214/215 (100%)	197 (92%)	17 (8%)	11	19
5	T	212/215 (99%)	193 (91%)	19 (9%)	9	14
All	All	2890/2968 (97%)	2639 (91%)	251 (9%)	9	16

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	61	GLU
1	A	78	LEU
1	A	81	LEU
1	A	103	LEU
1	A	114	LEU
1	A	137	ASP
1	A	141	GLN
1	A	160	LEU
1	A	173	LYS
1	A	179	LEU
1	A	186	LYS
1	A	206	LEU
1	A	240	THR
1	A	251	LEU
1	A	264	GLU
1	A	275	GLU
2	B	35	ILE
2	B	39	MET
2	B	64	ILE
2	B	89	GLU
4	D	1	GLN
4	D	13	VAL
4	D	27	ASP
4	D	44	GLN

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Mol	Chain	Res	Type
4	D	58	SER
4	D	87	LEU
4	D	95	GLN
4	D	123	VAL
4	D	139	LEU
4	D	171	ILE
4	D	177	LEU
4	D	180	ARG
4	D	182	MET
4	D	204	PHE
5	E	3	THR
5	E	12	LEU
5	E	22	ILE
5	E	53	LEU
5	E	73	PHE
5	E	125	VAL
5	E	158	LEU
5	E	169	LEU
5	E	183	CYS
5	E	189	LEU
5	E	191	GLU
5	E	205	ARG
5	E	217	ARG
5	E	248	SER
5	E	252	TRP
1	F	5	MET
1	F	9	GLU
1	F	28	VAL
1	F	39	ASP
1	F	52	MET
1	F	54	GLN
1	F	55	GLU
1	F	81	LEU
1	F	82	LEU
1	F	110	LEU
1	F	111	ARG
1	F	114	LEU
1	F	131	LYS
1	F	137	ASP
1	F	141	GLN
1	F	154	GLU
1	F	160	LEU

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Mol	Chain	Res	Type
1	F	166	GLU
1	F	172	LEU
1	F	179	LEU
1	F	191	HIS
1	F	199	VAL
1	F	201	LEU
1	F	206	LEU
1	F	216	THR
1	F	219	LEU
1	F	223	GLU
1	F	230	LEU
1	F	232	GLU
1	F	251	LEU
1	F	255	GLN
1	F	258	THR
1	F	273	ARG
2	G	4	THR
2	G	35	ILE
2	G	48	LYS
2	G	58	LYS
2	G	64	ILE
2	G	74	GLU
2	G	87	MET
2	G	89	GLU
4	I	4	VAL
4	I	27	ASP
4	I	67	GLU
4	I	123	VAL
4	I	129	ILE
4	I	133	ASP
4	I	138	GLN
4	I	143	LYS
4	I	151	LEU
4	I	171	ILE
4	I	174	LYS
4	I	193	SER
4	I	194	ASN
5	J	12	LEU
5	J	21	LEU
5	J	25	GLN
5	J	53	LEU
5	J	107	SER

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Mol	Chain	Res	Type
5	J	113	ASP
5	J	125	VAL
5	J	128	ASP
5	J	132	VAL
5	J	158	LEU
5	J	160	THR
5	J	167	VAL
5	J	169	LEU
5	J	176	LYS
5	J	178	VAL
5	J	183	CYS
5	J	189	LEU
5	J	205	ARG
5	J	218	ASN
5	J	221	ARG
5	J	254	ARG
1	K	39	ASP
1	K	58	GLU
1	K	78	LEU
1	K	81	LEU
1	K	103	LEU
1	K	109	LEU
1	K	110	LEU
1	K	111	ARG
1	K	114	LEU
1	K	134	THR
1	K	137	ASP
1	K	141	GLN
1	K	154	GLU
1	K	180	LEU
1	K	189	VAL
1	K	201	LEU
1	K	202	ARG
1	K	224	LEU
1	K	230	LEU
1	K	255	GLN
1	K	264	GLU
1	K	266	LEU
2	L	19	LYS
2	L	29	GLN
2	L	35	ILE
2	L	48	LYS

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Mol	Chain	Res	Type
2	L	64	ILE
2	L	83	LYS
2	L	87	MET
2	L	96	ASP
2	L	98	ASP
2	L	99	MET
3	M	2	SER
4	N	2	GLN
4	N	3	GLN
4	N	24	SER
4	N	27	ASP
4	N	62	LYS
4	N	66	LYS
4	N	87	LEU
4	N	91	ILE
4	N	123	VAL
4	N	125	VAL
4	N	130	GLN
4	N	174	LYS
4	N	175	CYS
4	N	183	ASP
4	N	208	ILE
5	O	53	LEU
5	O	88	SER
5	O	97	GLU
5	O	125	VAL
5	O	129	LEU
5	O	139	VAL
5	O	144	GLU
5	O	158	LEU
5	O	169	LEU
5	O	176	LYS
5	O	187	GLN
5	O	189	LEU
5	O	195	LEU
5	O	206	LEU
5	O	236	THR
5	O	237	GLN
5	O	241	LYS
1	P	13	SER
1	P	39	ASP
1	P	53	GLU

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Mol	Chain	Res	Type
1	P	58	GLU
1	P	78	LEU
1	P	81	LEU
1	P	106	ASP
1	P	114	LEU
1	P	134	THR
1	P	137	ASP
1	P	160	LEU
1	P	172	LEU
1	P	176	ASN
1	P	179	LEU
1	P	201	LEU
1	P	206	LEU
1	P	230	LEU
1	P	240	THR
1	P	259	CYS
1	P	260	ARG
1	P	262	TYR
1	P	266	LEU
2	Q	2	GLN
2	Q	27	VAL
2	Q	29	GLN
2	Q	35	ILE
2	Q	37	ILE
2	Q	44	LYS
2	Q	58	LYS
2	Q	87	MET
2	Q	89	GLU
2	Q	97	ARG
2	Q	98	ASP
2	Q	99	MET
4	S	9	GLN
4	S	27	ASP
4	S	58	SER
4	S	123	VAL
4	S	174	LYS
4	S	182	MET
4	S	188	SER
4	S	209	ILE
5	T	4	VAL
5	T	12	LEU
5	T	25	GLN

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Mol	Chain	Res	Type
5	T	26	THR
5	T	28	ASN
5	T	53	LEU
5	T	129	LEU
5	T	152	LYS
5	T	155	LEU
5	T	158	LEU
5	T	169	LEU
5	T	176	LYS
5	T	187	GLN
5	T	189	LEU
5	T	192	GLN
5	T	205	ARG
5	T	232	ASN
5	T	241	LYS
5	T	254	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	127	ASN
1	A	218	GLN
2	B	6	GLN
2	B	8	GLN
2	B	67	HIS
3	C	5	ASN
4	D	43	GLN
4	D	114	GLN
4	D	158	GLN
4	D	160	ASN
4	D	163	GLN
4	D	194	ASN
5	E	20	ASN
5	E	48	GLN
5	E	131	ASN
5	E	214	GLN
5	E	232	ASN
5	E	237	GLN
1	F	3	HIS
1	F	54	GLN

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Mol	Chain	Res	Type
1	F	127	ASN
1	F	220	ASN
1	F	255	GLN
1	F	256	ASN
2	G	6	GLN
2	G	13	HIS
4	I	22	ASN
4	I	205	ASN
5	J	6	GLN
5	J	7	ASN
5	J	43	GLN
5	J	48	GLN
5	J	82	ASN
5	J	83	ASN
5	J	131	ASN
5	J	218	ASN
5	J	219	HIS
5	J	225	GLN
5	J	232	ASN
5	J	245	GLN
1	K	97	GLN
1	K	174	ASN
1	K	188	HIS
1	K	220	ASN
2	L	6	GLN
2	L	29	GLN
3	M	5	ASN
4	N	1	GLN
4	N	90	HIS
4	N	128	ASN
4	N	138	GLN
4	N	202	ASN
5	O	20	ASN
5	O	43	GLN
5	O	48	GLN
5	O	131	ASN
5	O	218	ASN
5	O	232	ASN
5	O	245	GLN
1	P	30	ASN
1	P	42	ASN
1	P	97	GLN

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Mol	Chain	Res	Type
1	P	141	GLN
1	P	176	ASN
1	P	263	HIS
2	Q	2	GLN
2	Q	6	GLN
2	Q	13	HIS
2	Q	17	ASN
2	Q	29	GLN
3	R	5	ASN
4	S	9	GLN
4	S	43	GLN
4	S	131	ASN
4	S	202	ASN
5	T	7	ASN
5	T	20	ASN
5	T	83	ASN
5	T	131	ASN
5	T	149	HIS
5	T	214	GLN
5	T	245	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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	SO4	K	301	-	4,4,4	0.26	0	6,6,6	0.07	0
6	SO4	E	301	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	T	301	-	4,4,4	0.25	0	6,6,6	0.09	0
6	SO4	O	301	-	4,4,4	0.25	0	6,6,6	0.09	0
6	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.08	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	277/280 (98%)	0.45	10 (3%) 46 38	19, 61, 98, 120	12 (4%)
1	F	277/280 (98%)	0.99	31 (11%) 10 8	24, 83, 117, 143	12 (4%)
1	K	277/280 (98%)	0.63	22 (7%) 18 14	21, 66, 109, 123	12 (4%)
1	P	238/280 (85%)	0.67	23 (9%) 13 10	19, 65, 159, 198	9 (3%)
2	B	99/99 (100%)	0.40	5 (5%) 33 26	37, 58, 79, 88	2 (2%)
2	G	99/99 (100%)	0.92	8 (8%) 18 13	35, 75, 103, 111	1 (1%)
2	L	99/99 (100%)	0.65	5 (5%) 33 26	27, 62, 91, 102	1 (1%)
2	Q	98/99 (98%)	0.97	10 (10%) 12 9	31, 85, 108, 115	1 (1%)
3	C	9/9 (100%)	-0.15	0 100 100	40, 42, 48, 51	0
3	H	9/9 (100%)	0.58	0 100 100	50, 60, 68, 72	0
3	M	9/9 (100%)	0.16	0 100 100	42, 49, 59, 60	0
3	R	9/9 (100%)	0.19	0 100 100	41, 49, 56, 59	0
4	D	198/207 (95%)	0.65	17 (8%) 16 12	39, 64, 115, 129	1 (0%)
4	I	186/207 (89%)	1.22	35 (18%) 3 2	52, 84, 162, 187	1 (0%)
4	N	201/207 (97%)	0.89	17 (8%) 16 12	46, 72, 109, 144	1 (0%)
4	S	203/207 (98%)	0.92	25 (12%) 8 7	43, 79, 122, 140	1 (0%)
5	E	240/243 (98%)	0.35	6 (2%) 58 52	32, 56, 92, 106	1 (0%)
5	J	240/243 (98%)	0.91	33 (13%) 6 5	40, 74, 138, 163	0
5	O	241/243 (99%)	0.40	6 (2%) 58 52	31, 56, 87, 108	3 (1%)
5	T	239/243 (98%)	0.63	10 (4%) 40 32	34, 64, 100, 124	1 (0%)
All	All	3248/3352 (96%)	0.71	263 (8%) 18 13	19, 67, 117, 198	59 (1%)

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	139	LEU	4.9
5	T	215	ASN	4.9
1	A	108[A]	ARG	4.8
4	D	200	CYS	4.7
4	S	184	PHE	4.4
4	I	151	LEU	4.2
1	P	271	THR	4.1
5	J	211	THR	4.1
4	N	143	LYS	4.1
4	N	2	GLN	4.1
1	P	201	LEU	4.1
4	S	185	LYS	4.0
5	O	197	ASP	3.9
2	Q	54[A]	MET	3.8
5	J	255	ALA	3.8
5	J	252	TRP	3.8
5	O	194	ALA	3.8
1	A	175	GLY	3.8
2	Q	46	ILE	3.8
4	N	147	LYS	3.8
5	E	92	GLY	3.7
4	I	149	VAL	3.7
1	F	108[A]	ARG	3.7
4	D	204	PHE	3.7
5	T	92	GLY	3.6
2	G	54[A]	MET	3.6
2	Q	80	CYS	3.6
4	N	214	PHE	3.6
5	J	143	SER	3.6
4	D	164	SER	3.6
1	K	177	ALA	3.5
1	P	261	VAL	3.5
5	O	221[A]	ARG	3.5
5	J	251	ALA	3.5
4	I	135	ALA	3.4
5	J	194	ALA	3.4
1	F	225	THR	3.4
1	K	220	ASN	3.3
1	K	178	THR	3.3
5	J	216	PRO	3.3
5	J	213	TRP	3.2
1	F	50	PRO	3.2
1	K	109	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
4	N	213	THR	3.2
1	F	180	LEU	3.2
5	E	25	GLN	3.2
1	P	215	LEU	3.2
4	S	214	PHE	3.2
1	K	256	ASN	3.1
5	T	182	VAL	3.1
5	J	253	GLY	3.1
1	P	187	ALA	3.1
4	N	208	ILE	3.1
5	J	145	ALA	3.1
4	S	183	ASP	3.1
5	J	142	PRO	3.1
1	K	271	THR	3.0
4	I	143	LYS	3.0
4	I	201	ALA	3.0
4	I	152	PHE	3.0
5	O	222	CYS	3.0
1	K	270	LEU	3.0
1	K	185	PRO	3.0
5	T	210	ALA	3.0
2	L	1	ILE	3.0
4	I	189	ALA	3.0
5	J	212	PHE	3.0
4	S	80	PHE	3.0
5	T	151	GLN	2.9
1	A	121	ARG	2.9
4	D	4	VAL	2.9
4	N	210	PRO	2.9
4	I	138	GLN	2.9
1	F	238	ASP	2.9
1	K	183	ASP	2.9
4	S	208	ILE	2.9
2	B	86	SER	2.9
5	E	73	PHE	2.9
4	S	145	SER	2.8
2	B	1	ILE	2.8
4	I	184	PHE	2.8
1	F	5	MET	2.8
1	P	267	PRO	2.8
4	S	209	ILE	2.8
4	I	178	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	I	190	VAL	2.8
5	J	178	VAL	2.8
1	F	121	ARG	2.8
4	I	156	ASP	2.8
1	P	190	THR	2.8
4	I	17	GLU	2.8
1	P	259	CYS	2.8
1	P	246	SER	2.8
4	S	217	SER	2.8
1	P	188	HIS	2.8
1	F	178	THR	2.8
1	K	179	LEU	2.7
1	A	196	LYS	2.7
4	S	86	LYS	2.7
1	K	189	VAL	2.7
1	A	112	GLY	2.7
4	D	216	PRO	2.7
1	K	108[A]	ARG	2.7
1	F	107	TRP	2.7
4	I	204	PHE	2.7
4	S	213	THR	2.7
1	P	50	PRO	2.7
2	G	51	MET	2.6
1	K	219	LEU	2.6
4	N	128	ASN	2.6
4	S	144	SER	2.6
1	K	274	TRP	2.6
1	P	270	LEU	2.6
4	I	177	LEU	2.6
4	I	136	VAL	2.6
5	J	220	PHE	2.6
5	E	229	LEU	2.6
1	K	44	ARG	2.6
5	J	217	ARG	2.6
5	J	92	GLY	2.6
4	D	3	GLN	2.6
5	J	148	SER	2.5
5	J	129	LEU	2.5
5	J	114	THR	2.5
4	I	145	SER	2.5
1	K	107	TRP	2.5
1	F	109	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	224	LEU	2.5
1	P	206	LEU	2.5
4	S	139	LEU	2.5
4	S	147	LYS	2.5
4	I	148	SER	2.5
4	D	195	LYS	2.5
4	I	147	LYS	2.5
1	P	179	LEU	2.5
2	Q	23	LEU	2.5
5	T	222	CYS	2.5
1	A	224	LEU	2.5
2	G	22	ILE	2.5
4	I	192	TRP	2.5
1	F	45	TYR	2.5
4	D	201	ALA	2.5
4	I	144	SER	2.4
4	I	15	GLU	2.4
1	K	277	PRO	2.4
4	I	171	ILE	2.4
4	D	193	SER	2.4
5	J	180	SER	2.4
1	F	101	CYS	2.4
4	I	1	GLN	2.4
1	F	177	ALA	2.4
4	D	214	PHE	2.4
1	P	263	HIS	2.4
5	J	214	GLN	2.4
5	J	156	VAL	2.4
5	J	12	LEU	2.4
5	J	195	LEU	2.4
4	S	175	CYS	2.4
1	F	2	PRO	2.4
5	J	207	ARG	2.4
4	S	148	SER	2.3
5	T	238	ASP	2.3
4	I	14	TRP	2.3
2	Q	29	GLN	2.3
4	N	105	ALA	2.3
4	S	91	ILE	2.3
1	A	191	HIS	2.3
5	J	154	THR	2.3
5	J	209	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	2	PRO	2.3
1	P	239	GLY	2.3
2	G	80	CYS	2.3
4	S	136	VAL	2.3
5	E	195	LEU	2.3
2	B	19	LYS	2.3
2	L	54[A]	MET	2.3
2	Q	99	MET	2.3
1	P	269	PRO	2.3
2	Q	93	VAL	2.3
1	P	266	LEU	2.3
4	I	203	ALA	2.3
1	F	52	MET	2.3
4	I	153	THR	2.3
5	J	152	LYS	2.3
1	F	113	TYR	2.3
1	A	264	GLU	2.3
1	F	210	PRO	2.3
4	N	1	GLN	2.3
5	T	253	GLY	2.3
1	F	126	LEU	2.3
1	F	191	HIS	2.2
1	P	216	THR	2.2
2	G	68	THR	2.2
4	D	67	GLU	2.2
4	N	211	GLU	2.2
1	F	44	ARG	2.2
2	G	12	ARG	2.2
4	S	142	SER	2.2
5	O	198	SER	2.2
1	K	180	LEU	2.2
4	S	151	LEU	2.2
5	O	189	LEU	2.2
2	Q	89	GLU	2.2
5	T	71	THR	2.2
4	D	208	ILE	2.2
1	A	177	ALA	2.2
5	J	153	ALA	2.2
2	L	69	GLU	2.2
4	I	205	ASN	2.2
2	B	29	GLN	2.2
4	I	69	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	203	ALA	2.1
1	K	203	CYS	2.1
1	A	68	LYS	2.1
4	I	202	ASN	2.1
1	F	103	LEU	2.1
1	F	266	LEU	2.1
2	G	39	MET	2.1
4	D	182	MET	2.1
4	I	157	SER	2.1
4	N	209	ILE	2.1
1	F	51	TRP	2.1
4	D	213	THR	2.1
4	D	2	GLN	2.1
1	F	179	LEU	2.1
1	P	209	TYR	2.1
5	J	155	LEU	2.1
1	P	231	VAL	2.1
1	P	185	PRO	2.1
2	L	15	PRO	2.1
4	S	210	PRO	2.1
5	J	206	LEU	2.1
4	N	22	ASN	2.1
1	K	169	HIS	2.1
1	K	221	GLY	2.1
4	N	141	ASP	2.1
4	I	193	SER	2.1
4	S	172	THR	2.1
2	B	54	MET	2.1
2	Q	87	MET	2.1
1	P	207	GLY	2.1
2	Q	37	ILE	2.1
2	L	88	ALA	2.0
5	T	236	THR	2.0
4	N	216	PRO	2.0
5	J	189	LEU	2.0
4	S	187	ASN	2.0
1	F	104	GLY	2.0
2	G	37	ILE	2.0
5	J	147	ILE	2.0
4	I	169	VAL	2.0
1	F	111	ARG	2.0
4	N	215	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	27	ASP	2.0
4	N	212	ASP	2.0
4	S	61	ASP	2.0
1	F	196	LYS	2.0
4	I	186	SER	2.0
5	E	180	SER	2.0
1	F	54	GLN	2.0
1	F	215	LEU	2.0
1	F	112	GLY	2.0
4	S	137	TYR	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(Å ²)	Q<0.9
6	SO4	K	301	5/5	0.68	0.12	114,114,114,115	0
6	SO4	T	301	5/5	0.69	0.16	115,115,115,115	0
6	SO4	E	301	5/5	0.75	0.17	115,116,116,116	0
6	SO4	D	301	5/5	0.76	0.17	118,118,119,119	0
7	NA	J	301	1/1	0.79	0.09	38,38,38,38	0
7	NA	E	302	1/1	0.86	0.17	50,50,50,50	0
6	SO4	O	301	5/5	0.89	0.12	102,102,102,102	0
7	NA	K	302	1/1	0.90	0.13	79,79,79,79	0
7	NA	T	302	1/1	0.90	0.11	42,42,42,42	0
7	NA	T	303	1/1	0.91	0.22	49,49,49,49	0
7	NA	I	301	1/1	0.94	0.17	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.