



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2016 – 05:57 PM EDT

PDB ID : 5SWZ
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

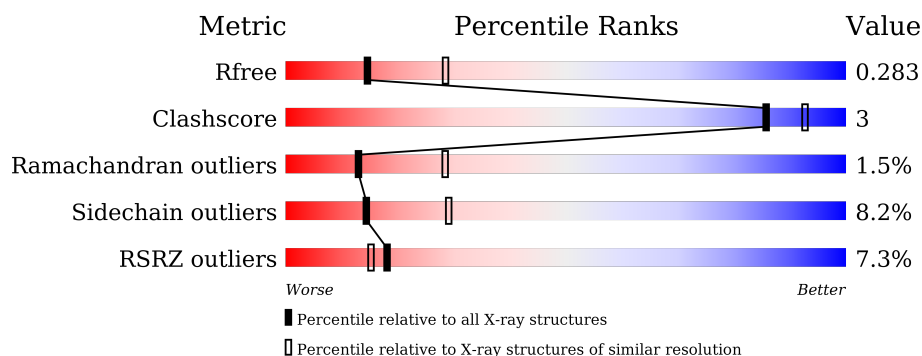
1 Overall quality at a glance i

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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	<div> <div>3%</div> <div>86%12%..</div> </div>
1	F	280	<div> <div>8%</div> <div>82%16%..</div> </div>
1	K	280	<div> <div>8%</div> <div>84%14%..</div> </div>
1	P	280	<div> <div>13%</div> <div>72%13%15%</div> </div>
2	B	99	<div> <div>%</div> <div>86%12%. .</div> </div>
2	G	99	<div> <div>8%</div> <div>81%16%. .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	D	301	-	-	-	X

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			

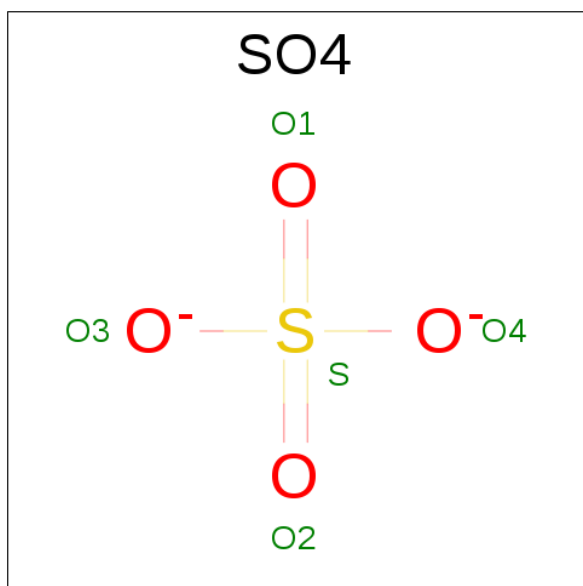
- Molecule 4 is a protein called NP1-B17 TCR alpha chain.

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 (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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 (three-letter code: NA) (formula: Na).

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

- 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		

Continued on next page...

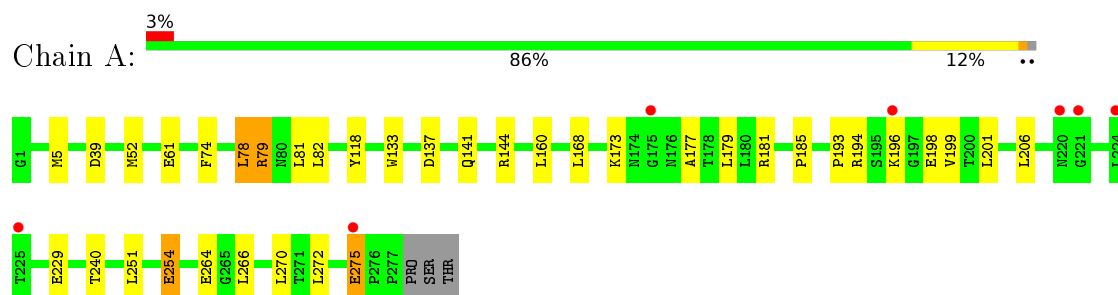
Continued from previous page...

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

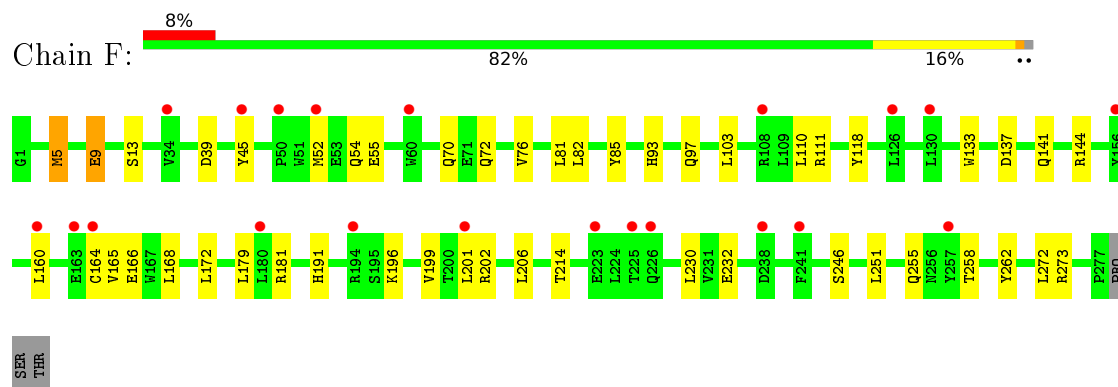
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

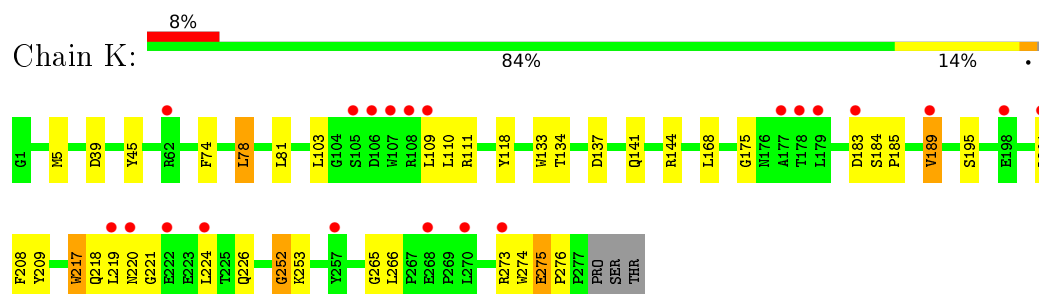
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



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

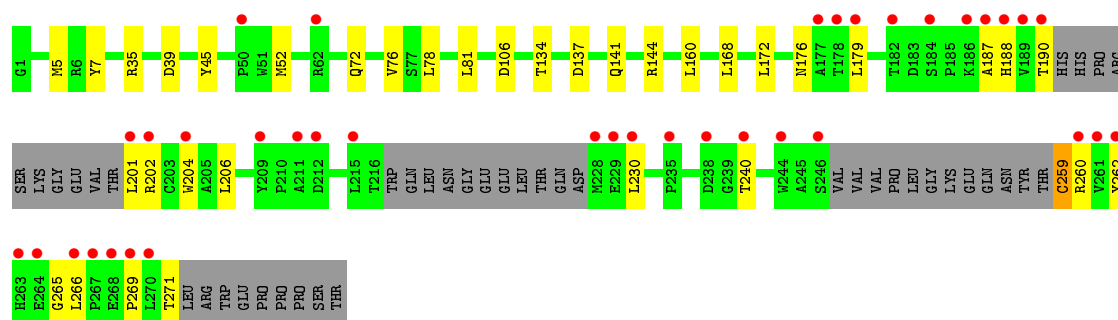


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

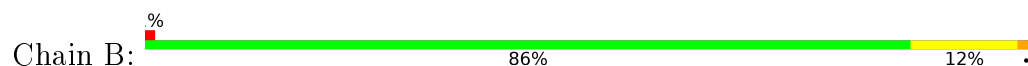


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

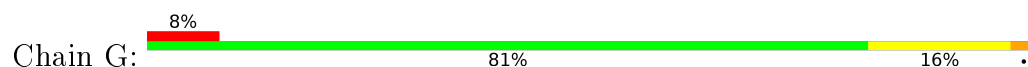




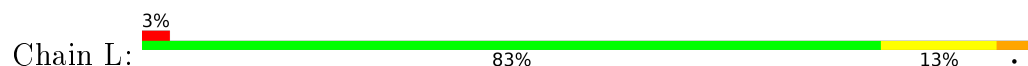
- Molecule 2: Beta-2-microglobulin



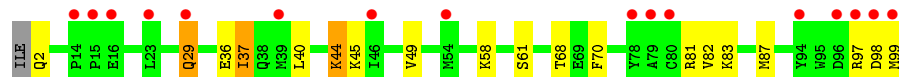
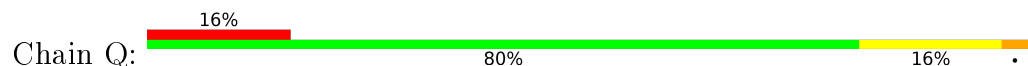
- Molecule 2: Beta-2-microglobulin



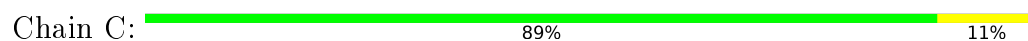
- Molecule 2: Beta-2-microglobulin



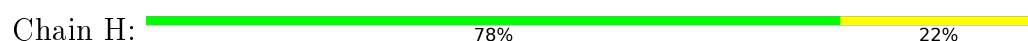
- Molecule 2: Beta-2-microglobulin



- Molecule 3: influenza NP366 epitope



- Molecule 3: influenza NP366 epitope





- Molecule 3: influenza NP366 epitope

Chain M: 78% 22%



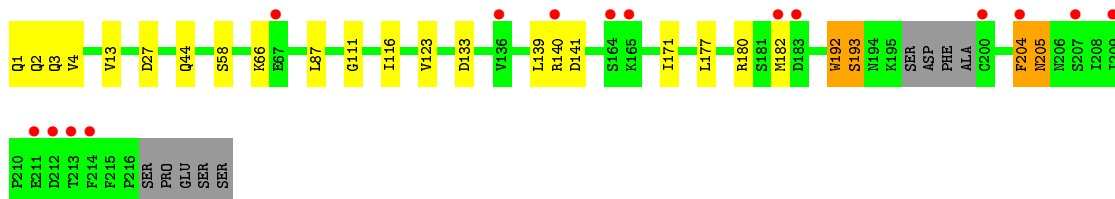
- Molecule 3: influenza NP366 epitope

Chain R: 78% 22%



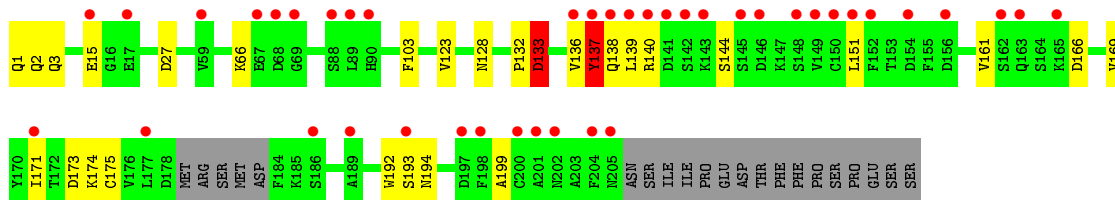
- Molecule 4: NP1-B17 TCR alpha chain

Chain D: 7% 84% 10%



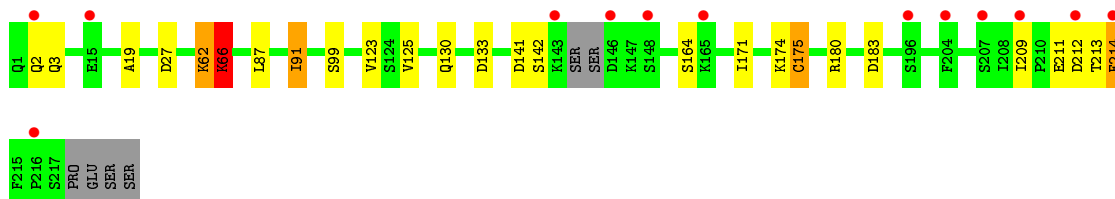
- Molecule 4: NP1-B17 TCR alpha chain

Chain I: 20% 76% 13% 10%



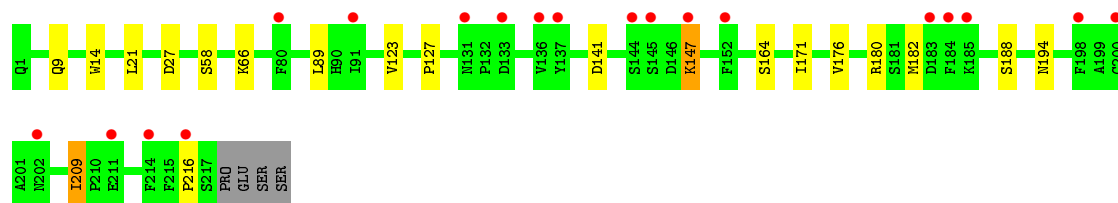
- Molecule 4: NP1-B17 TCR alpha chain

Chain N: 6% 85% 10%



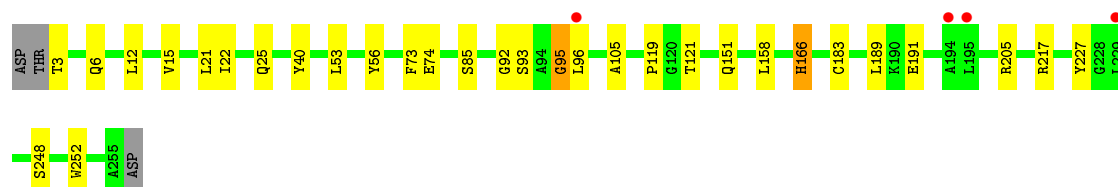
- Molecule 4: NP1-B17 TCR alpha chain

Chain S: 9% 88% 9% ..



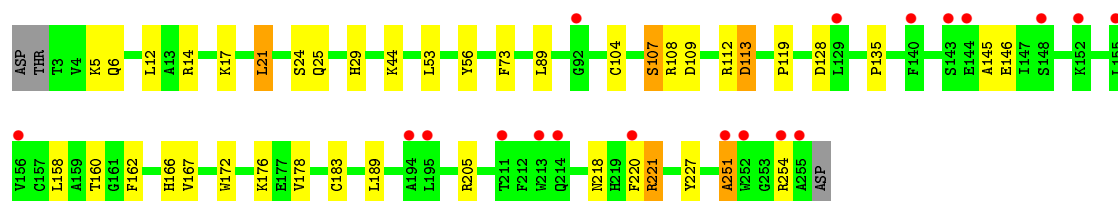
• Molecule 5: NP1-B17 TCR beta chain

Chain E: 2% 86% 12% ..



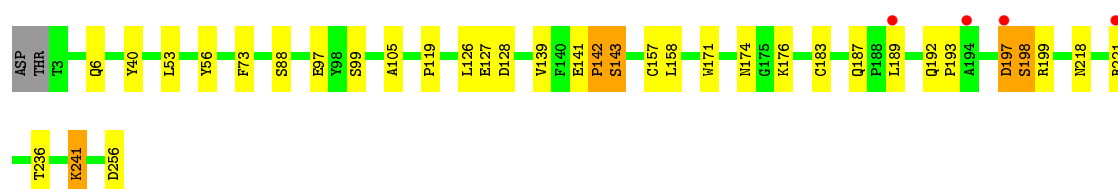
• Molecule 5: NP1-B17 TCR beta chain

Chain J: 8% 81% 15% ..



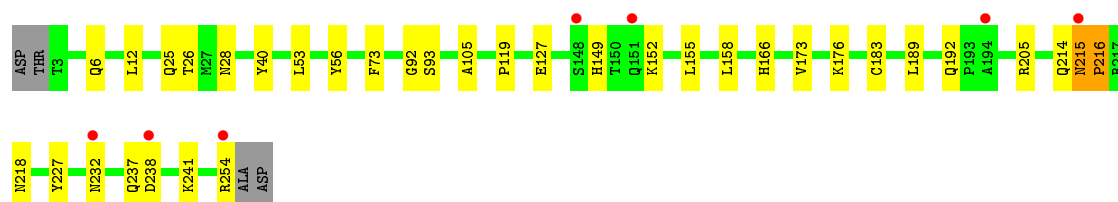
• Molecule 5: NP1-B17 TCR beta chain

Chain O: 2% 85% 12% ..



• Molecule 5: NP1-B17 TCR beta chain

Chain T: 3% 84% 14% ..



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 47.71 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.80-2.65) 100.0 (47.71-2.65)	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 0.258 , 0.283	Depositor DCC
R_{free} test set	6526 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.4	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	0.90	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: NA, SO4

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	0.35	0/2385	0.56	0/3240
1	F	0.37	0/2385	0.59	2/3240 (0.1%)
1	K	0.38	0/2385	0.60	2/3240 (0.1%)
1	P	0.36	0/2037	0.56	0/2759
2	B	0.39	0/844	0.61	1/1144 (0.1%)
2	G	0.39	0/852	0.64	2/1154 (0.2%)
2	L	0.38	0/852	0.61	0/1154
2	Q	0.39	0/844	0.60	0/1143
3	C	0.29	0/67	0.48	0/86
3	H	0.30	0/67	0.48	0/86
3	M	0.30	0/67	0.47	0/86
3	R	0.30	0/67	0.50	0/86
4	D	0.38	0/1594	0.61	1/2164 (0.0%)
4	I	0.42	0/1495	0.66	2/2028 (0.1%)
4	N	0.36	0/1624	0.56	0/2203
4	S	0.37	0/1637	0.56	0/2222
5	E	0.34	0/1994	0.58	0/2711
5	J	0.37	0/1994	0.63	1/2711 (0.0%)
5	O	0.35	0/2014	0.65	4/2736 (0.1%)
5	T	0.35	0/1989	0.62	0/2704
All	All	0.37	0/27193	0.60	15/36897 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	142	PRO	C-N-CA	6.40	137.70	121.70
5	O	197	ASP	C-N-CA	6.00	136.69	121.70
1	F	164	CYS	C-N-CA	5.93	136.51	121.70
5	J	104	CYS	CA-CB-SG	5.74	124.33	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	40	LEU	C-N-CA	5.65	135.83	121.70
4	D	192	TRP	C-N-CA	5.63	135.78	121.70
4	I	133	ASP	C-N-CD	5.58	140.13	128.40
4	I	192	TRP	C-N-CA	5.32	134.99	121.70
1	F	85	TYR	C-N-CA	5.31	134.98	121.70
2	B	1	ILE	C-N-CA	5.29	134.93	121.70
1	K	217	TRP	C-N-CA	5.29	134.93	121.70
2	G	59	ASP	C-N-CA	5.19	134.67	121.70
5	O	221[A]	ARG	C-N-CA	5.14	134.54	121.70
5	O	221[B]	ARG	C-N-CA	5.14	134.54	121.70
1	K	252	GLY	C-N-CA	5.04	134.29	121.70

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	17	0
1	P	1983	0	1872	10	0
2	B	818	0	797	5	0
2	G	826	0	807	9	0
2	L	826	0	805	6	0
2	Q	818	0	793	6	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	1960	0	1885	10	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
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	142	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 (142) 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	1.03	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	4:I:133:ASP:N	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
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:259:CYS:N	1:P:271:THR:HG1	1.99	0.61
1:P:76:VAL:HG13	3:R:8:THR:HG21	1.82	0.60
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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:52:MET:HA	1:A:52:MET:HE2	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:P:52:MET:HA	1:P:52:MET:HE2	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
2:G:51:MET:HE1	2:G:64:ILE:HG12	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
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
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:72:GLN:O	1:F:76:VAL:HG12	2.16	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
2:G:40:LEU:HB3	2:G:41:LYS:O	2.17	0.44
2:G:15:PRO:HG2	2:G:97:ARG:HB2	1.98	0.44
1:K:220:ASN:HA	1:K:221:GLY:HA2	1.78	0.44
4:I:132:PRO:C	4:I:133:ASP:OD1	2.56	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
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:166:ASP:HB3	4:I:169:VAL:HG22	2.01	0.42
4:I:1:GLN:HA	4:I:2:GLN:HB2	2.02	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
1:K:218:GLN:HA	1:K:219:LEU:C	2.39	0.42
4:I:138:GLN:OE1	4:I:199:ALA:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:5:MET:HE2	1:P:7:TYR:HE1	1.85	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:193:PRO:HA	1:A:199:VAL:HG23	2.03	0.41
1:A:79:ARG:HA	1:A:82:LEU:HD12	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:S:209:ILE:HD13	4:S:209:ILE:H	1.85	0.41
4:N:141:ASP:HB2	5:O:141:GLU:HG2	2.01	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%)	14	31
1	F	280/280 (100%)	264 (94%)	15 (5%)	1 (0%)	39	65
1	K	280/280 (100%)	250 (89%)	25 (9%)	5 (2%)	11	23
1	P	234/280 (84%)	221 (94%)	11 (5%)	2 (1%)	21	44
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	19	41
2	G	98/99 (99%)	93 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	9	20
4	I	182/207 (88%)	160 (88%)	18 (10%)	4 (2%)	8	19
4	N	197/207 (95%)	185 (94%)	8 (4%)	4 (2%)	9	21
4	S	201/207 (97%)	178 (89%)	19 (10%)	4 (2%)	9	21
5	E	238/243 (98%)	224 (94%)	11 (5%)	3 (1%)	15	33
5	J	238/243 (98%)	221 (93%)	15 (6%)	2 (1%)	24	47
5	O	240/243 (99%)	221 (92%)	14 (6%)	5 (2%)	9	20
5	T	237/243 (98%)	212 (90%)	20 (8%)	5 (2%)	9	20
All	All	3219/3352 (96%)	2972 (92%)	199 (6%)	48 (2%)	13	28

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	18 38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	240/238 (101%)	211 (88%)	29 (12%)	6	12
1	K	240/238 (101%)	225 (94%)	15 (6%)	22	44
1	P	203/238 (85%)	182 (90%)	21 (10%)	9	18
2	B	93/93 (100%)	87 (94%)	6 (6%)	21	43
2	G	94/93 (101%)	88 (94%)	6 (6%)	22	43
2	L	94/93 (101%)	84 (89%)	10 (11%)	8	17
2	Q	93/93 (100%)	83 (89%)	10 (11%)	8	16
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%)	6	11
3	R	8/8 (100%)	8 (100%)	0	100	100
4	D	178/188 (95%)	164 (92%)	14 (8%)	15	32
4	I	167/188 (89%)	157 (94%)	10 (6%)	24	47
4	N	182/188 (97%)	166 (91%)	16 (9%)	12	25
4	S	184/188 (98%)	175 (95%)	9 (5%)	31	58
5	E	212/215 (99%)	196 (92%)	16 (8%)	17	35
5	J	212/215 (99%)	192 (91%)	20 (9%)	11	22
5	O	214/215 (100%)	197 (92%)	17 (8%)	15	32
5	T	212/215 (99%)	194 (92%)	18 (8%)	13	27
All	All	2890/2968 (97%)	2655 (92%)	235 (8%)	14	30

All (235) 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	79	ARG
1	A	137	ASP
1	A	141	GLN
1	A	160	LEU
1	A	173	LYS
1	A	179	LEU
1	A	181	ARG
1	A	206	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	240	THR
1	A	251	LEU
1	A	254	GLU
1	A	264	GLU
1	A	272	LEU
1	A	275	GLU
2	B	39	MET
2	B	51	MET
2	B	58	LYS
2	B	64	ILE
2	B	70	PHE
2	B	74	GLU
4	D	1	GLN
4	D	13	VAL
4	D	27	ASP
4	D	44	GLN
4	D	58	SER
4	D	87	LEU
4	D	123	VAL
4	D	133	ASP
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	56	TYR
5	E	73	PHE
5	E	151	GLN
5	E	158	LEU
5	E	166	HIS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	5	MET
1	F	9	GLU
1	F	39	ASP
1	F	45	TYR
1	F	52	MET
1	F	54	GLN
1	F	55	GLU
1	F	70	GLN
1	F	82	LEU
1	F	110	LEU
1	F	111	ARG
1	F	137	ASP
1	F	141	GLN
1	F	160	LEU
1	F	166	GLU
1	F	172	LEU
1	F	179	LEU
1	F	181	ARG
1	F	191	HIS
1	F	199	VAL
1	F	201	LEU
1	F	206	LEU
1	F	230	LEU
1	F	232	GLU
1	F	251	LEU
1	F	255	GLN
1	F	258	THR
1	F	272	LEU
1	F	273	ARG
2	G	4	THR
2	G	48	LYS
2	G	58	LYS
2	G	64	ILE
2	G	87	MET
2	G	89	GLU
4	I	27	ASP
4	I	123	VAL
4	I	133	ASP
4	I	137	TYR
4	I	151	LEU
4	I	171	ILE
4	I	174	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	175	CYS
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	56	TYR
5	J	107	SER
5	J	112	ARG
5	J	113	ASP
5	J	128	ASP
5	J	158	LEU
5	J	160	THR
5	J	167	VAL
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	45	TYR
1	K	78	LEU
1	K	109	LEU
1	K	110	LEU
1	K	111	ARG
1	K	134	THR
1	K	137	ASP
1	K	141	GLN
1	K	189	VAL
1	K	201	LEU
1	K	202	ARG
1	K	206	LEU
1	K	224	LEU
1	K	266	LEU
2	L	19	LYS
2	L	29	GLN
2	L	48	LYS
2	L	64	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	70	PHE
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	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	133	ASP
4	N	174	LYS
4	N	175	CYS
4	N	180	ARG
4	N	183	ASP
4	N	214	PHE
5	O	53	LEU
5	O	56	TYR
5	O	88	SER
5	O	97	GLU
5	O	126	LEU
5	O	127	GLU
5	O	128	ASP
5	O	139	VAL
5	O	158	LEU
5	O	176	LYS
5	O	187	GLN
5	O	189	LEU
5	O	193	PRO
5	O	199	ARG
5	O	236	THR
5	O	241	LYS
5	O	256	ASP
1	P	35	ARG
1	P	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	45	TYR
1	P	78	LEU
1	P	81	LEU
1	P	106	ASP
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	204	TRP
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	29	GLN
2	Q	37	ILE
2	Q	44	LYS
2	Q	58	LYS
2	Q	70	PHE
2	Q	87	MET
2	Q	97	ARG
2	Q	98	ASP
2	Q	99	MET
4	S	9	GLN
4	S	14	TRP
4	S	27	ASP
4	S	58	SER
4	S	123	VAL
4	S	180	ARG
4	S	182	MET
4	S	188	SER
4	S	209	ILE
5	T	12	LEU
5	T	25	GLN
5	T	26	THR
5	T	28	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	T	53	LEU
5	T	56	TYR
5	T	127	GLU
5	T	152	LYS
5	T	155	LEU
5	T	158	LEU
5	T	176	LYS
5	T	183	CYS
5	T	189	LEU
5	T	192	GLN
5	T	205	ARG
5	T	232	ASN
5	T	241	LYS
5	T	254	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	131	ASN
5	E	219	HIS
1	F	54	GLN
5	J	7	ASN
5	J	82	ASN
5	J	83	ASN
5	O	174	ASN
4	S	202	ASN
5	T	7	ASN
5	T	83	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	D	301	-	4,4,4	0.19	0	6,6,6	0.08	0
6	SO4	E	301	-	4,4,4	0.17	0	6,6,6	0.07	0
6	SO4	K	301	-	4,4,4	0.18	0	6,6,6	0.06	0
6	SO4	O	301	-	4,4,4	0.17	0	6,6,6	0.08	0
6	SO4	T	301	-	4,4,4	0.19	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	D	301	-	-	0/0/0/0	0/0/0/0
6	SO4	E	301	-	-	0/0/0/0	0/0/0/0
6	SO4	K	301	-	-	0/0/0/0	0/0/0/0
6	SO4	O	301	-	-	0/0/0/0	0/0/0/0
6	SO4	T	301	-	-	0/0/0/0	0/0/0/0

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

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	277/280 (98%)	0.30	7 (2%) 61 59	33, 61, 99, 120	7 (2%)
1	F	277/280 (98%)	0.66	21 (7%) 17 14	40, 84, 117, 143	7 (2%)
1	K	277/280 (98%)	0.49	21 (7%) 17 14	34, 67, 109, 123	7 (2%)
1	P	238/280 (85%)	0.81	37 (15%) 3 2	37, 66, 159, 198	5 (2%)
2	B	99/99 (100%)	0.32	1 (1%) 84 84	41, 59, 79, 88	2 (2%)
2	G	99/99 (100%)	0.78	8 (8%) 15 12	54, 75, 103, 111	0
2	L	99/99 (100%)	0.33	3 (3%) 54 52	43, 63, 91, 102	0
2	Q	98/99 (98%)	0.88	16 (16%) 2 1	48, 85, 108, 115	0
3	C	9/9 (100%)	-0.05	0 100 100	40, 42, 48, 51	0
3	H	9/9 (100%)	0.06	0 100 100	50, 60, 68, 72	0
3	M	9/9 (100%)	-0.17	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%)	0.43	15 (7%) 17 14	39, 64, 115, 129	1 (0%)
4	I	186/207 (89%)	1.14	41 (22%) 1 1	52, 84, 162, 187	1 (0%)
4	N	201/207 (97%)	0.61	13 (6%) 22 20	46, 72, 109, 144	1 (0%)
4	S	203/207 (98%)	0.69	19 (9%) 11 8	43, 79, 122, 140	1 (0%)
5	E	240/243 (98%)	0.18	4 (1%) 73 72	32, 56, 92, 106	1 (0%)
5	J	240/243 (98%)	0.58	19 (7%) 15 13	40, 74, 138, 163	0
5	O	241/243 (99%)	0.23	4 (1%) 73 72	34, 57, 87, 108	2 (0%)
5	T	239/243 (98%)	0.39	7 (2%) 55 53	34, 64, 100, 124	1 (0%)
All	All	3248/3352 (96%)	0.53	236 (7%) 18 15	32, 68, 117, 198	36 (1%)

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	187	ALA	11.2
4	I	138	GLN	10.0
4	I	139	LEU	9.1
4	I	140	ARG	8.9
1	P	268	GLU	8.4
1	P	267	PRO	6.9
1	F	225	THR	6.7
5	J	195	LEU	6.7
1	P	188	HIS	6.5
5	J	143	SER	6.3
1	P	262	TYR	6.2
1	K	177	ALA	6.0
1	K	178	THR	6.0
5	J	194	ALA	5.9
4	I	137	TYR	5.9
4	S	184	PHE	5.8
1	K	220	ASN	5.5
1	P	228	MET	5.5
1	P	269	PRO	5.4
2	Q	54[A]	MET	5.4
5	J	252	TRP	5.3
1	P	186	LYS	5.2
4	I	202	ASN	5.2
1	K	179	LEU	5.2
4	S	145	SER	5.0
4	I	201	ALA	4.9
4	I	146	ASP	4.9
1	P	190	THR	4.8
1	P	189	VAL	4.8
4	N	146	ASP	4.7
5	T	238	ASP	4.7
4	I	148	SER	4.7
4	N	2	GLN	4.6
2	Q	15	PRO	4.6
4	D	214	PHE	4.6
2	Q	23	LEU	4.5
5	J	255	ALA	4.5
1	P	179	LEU	4.4
2	Q	99	MET	4.4
4	S	214	PHE	4.3
4	N	196	SER	4.3
1	P	215	LEU	4.2
4	I	204	PHE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	N	216	PRO	4.1
1	P	261	VAL	4.1
4	N	209	ILE	4.0
1	P	264	GLU	4.0
1	P	266	LEU	4.0
1	P	230	LEU	3.9
4	D	211	GLU	3.9
4	D	164	SER	3.9
5	J	144	GLU	3.9
2	Q	94	TYR	3.9
2	Q	14	PRO	3.8
2	G	48	LYS	3.8
4	S	183	ASP	3.8
4	N	214	PHE	3.7
1	P	178	THR	3.7
1	P	270	LEU	3.7
4	D	213	THR	3.6
4	I	145	SER	3.6
5	J	220	PHE	3.5
1	F	223	GLU	3.5
5	J	251	ALA	3.5
1	P	246	SER	3.5
4	I	69	GLY	3.5
2	G	68	THR	3.5
2	Q	97	ARG	3.5
4	I	152	PHE	3.4
1	F	160	LEU	3.4
1	K	105	SER	3.4
5	J	148	SER	3.3
1	P	202	ARG	3.3
1	P	204	TRP	3.3
1	P	201	LEU	3.3
4	D	136	VAL	3.3
4	S	202	ASN	3.3
4	I	151	LEU	3.3
2	G	54[A]	MET	3.2
1	P	211	ALA	3.2
5	O	194	ALA	3.1
1	K	270	LEU	3.1
1	F	201	LEU	3.1
4	N	165	LYS	3.1
4	S	185	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	198	GLU	3.1
4	S	144	SER	3.1
1	F	238	ASP	3.1
1	A	196	LYS	3.1
4	S	198	PHE	3.0
2	Q	79	ALA	3.0
4	I	142	SER	3.0
1	P	240	THR	3.0
1	K	222	GLU	3.0
1	F	226	GLN	3.0
4	I	197	ASP	3.0
5	J	214	GLN	2.9
5	O	197	ASP	2.9
4	I	150	CYS	2.9
5	J	254	ARG	2.9
2	Q	98	ASP	2.9
4	S	211	GLU	2.9
4	I	189	ALA	2.9
5	T	215	ASN	2.9
2	L	54[A]	MET	2.9
1	K	106	ASP	2.8
1	K	273	ARG	2.8
4	S	137	TYR	2.8
4	I	141	ASP	2.8
5	T	151	GLN	2.8
4	S	200	CYS	2.8
2	Q	96	ASP	2.8
5	E	194	ALA	2.8
2	Q	80	CYS	2.8
2	L	69	GLU	2.7
4	I	193	SER	2.7
1	K	268	GLU	2.7
1	P	229	GLU	2.7
4	I	200	CYS	2.7
1	P	238	ASP	2.7
4	I	154	ASP	2.7
1	F	50	PRO	2.7
2	L	15	PRO	2.7
1	K	108[A]	ARG	2.7
4	I	163	GLN	2.7
2	G	39	MET	2.7
2	Q	78	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	N	207	SER	2.7
5	J	155	LEU	2.6
4	I	198	PHE	2.6
2	G	17	ASN	2.6
2	Q	39	MET	2.6
2	Q	29	GLN	2.6
1	F	52	MET	2.6
4	D	209	ILE	2.5
4	D	200	CYS	2.5
4	N	212	ASP	2.5
1	A	275	GLU	2.5
2	Q	46	ILE	2.5
1	F	130	LEU	2.5
4	I	67	GLU	2.5
4	I	205	ASN	2.5
5	J	152	LYS	2.5
4	D	204	PHE	2.5
4	D	140	ARG	2.5
1	K	201	LEU	2.5
4	N	143	LYS	2.5
4	I	149	VAL	2.5
5	T	232	ASN	2.5
5	T	194	ALA	2.4
5	O	189	LEU	2.4
5	J	140	PHE	2.4
1	F	257	TYR	2.4
1	A	175	GLY	2.4
1	F	34	VAL	2.4
4	D	67	GLU	2.4
4	S	147	LYS	2.4
5	E	96	LEU	2.4
1	K	107	TRP	2.4
4	D	165	LYS	2.4
5	J	211	THR	2.4
5	J	213	TRP	2.4
4	S	133	ASP	2.4
1	F	163	GLU	2.4
4	S	131	ASN	2.3
1	K	62[A]	ARG	2.3
1	A	225	THR	2.3
1	A	220	ASN	2.3
1	P	244	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	S	216	PRO	2.3
1	F	45	TYR	2.3
1	F	126	LEU	2.3
2	B	85	ALA	2.3
4	D	183	ASP	2.3
4	I	162	SER	2.3
2	Q	16	GLU	2.3
1	F	194	ARG	2.3
1	P	212	ASP	2.3
1	P	50	PRO	2.3
4	I	186	SER	2.3
5	J	129	LEU	2.3
1	K	189	VAL	2.3
4	I	59	VAL	2.3
1	A	221	GLY	2.2
1	P	182	THR	2.2
5	T	254	ARG	2.2
1	F	60	TRP	2.2
2	G	51	MET	2.2
1	P	209	TYR	2.2
5	J	156	VAL	2.2
1	F	108[A]	ARG	2.2
1	K	183	ASP	2.2
1	F	156	TYR	2.2
4	D	212	ASP	2.2
5	T	148	SER	2.2
1	K	219	LEU	2.2
2	G	69	GLU	2.2
4	N	204	PHE	2.2
4	I	136	VAL	2.2
1	K	109	LEU	2.2
1	K	224	LEU	2.2
1	P	260	ARG	2.2
4	S	80	PHE	2.2
4	I	88	SER	2.1
4	I	15	GLU	2.1
4	S	136	VAL	2.1
4	I	68	ASP	2.1
1	P	177	ALA	2.1
2	G	79	ALA	2.1
4	I	143	LYS	2.1
1	F	180	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	164	CYS	2.1
1	F	241	PHE	2.1
4	I	171	ILE	2.1
1	K	257	TYR	2.1
1	P	62[A]	ARG	2.1
4	D	207	SER	2.1
4	I	90	HIS	2.1
5	E	195	LEU	2.1
4	S	152	PHE	2.1
4	I	89	LEU	2.1
4	S	91	ILE	2.1
1	P	184[A]	SER	2.1
4	I	17	GLU	2.1
4	I	156	ASP	2.0
4	N	148	SER	2.0
5	O	221[A]	ARG	2.0
5	J	92	GLY	2.0
4	D	182	MET	2.0
1	A	224	LEU	2.0
4	I	177	LEU	2.0
1	P	263	HIS	2.0
4	N	15	GLU	2.0
5	E	229	LEU	2.0
1	P	235	PRO	2.0
4	I	165	LYS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
6	SO4	D	301	5/5	0.71	0.25	3.58	118,118,119,119	0
6	SO4	T	301	5/5	0.73	0.35	1.37	115,115,115,115	0
7	NA	E	302	1/1	0.85	0.17	0.43	50,50,50,50	0
7	NA	I	301	1/1	0.92	0.23	0.23	48,48,48,48	0
6	SO4	E	301	5/5	0.80	0.17	-0.15	115,116,116,116	0
7	NA	J	301	1/1	0.85	0.16	-0.55	38,38,38,38	0
7	NA	T	302	1/1	0.91	0.11	-1.63	42,42,42,42	0
6	SO4	O	301	5/5	0.92	0.13	-1.76	102,102,102,102	0
7	NA	T	303	1/1	0.88	0.10	-1.94	49,49,49,49	0
6	SO4	K	301	5/5	0.88	0.12	-	114,114,114,115	0
7	NA	K	302	1/1	0.95	0.06	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.