Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 04:08 AM 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

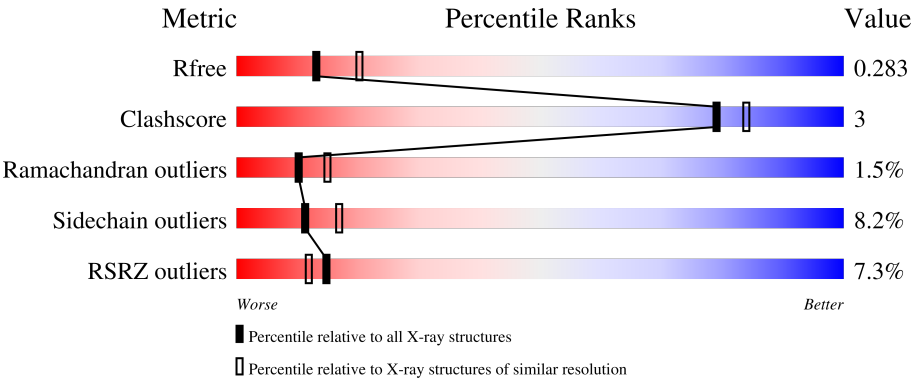
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	2% 86% 12%
1	F	280	8% 82% 16%
1	K	280	8% 84% 14%
1	P	280	14% 72% 12% 15%
2	B	99	% 86% 12%

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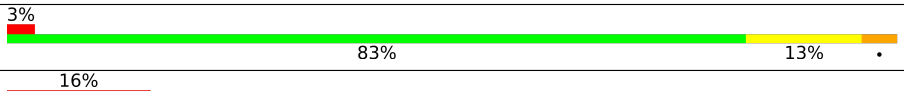
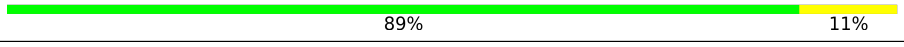
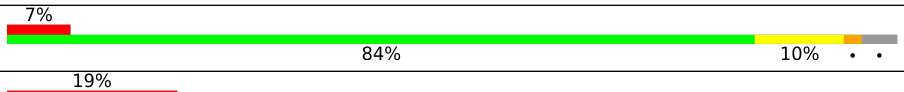
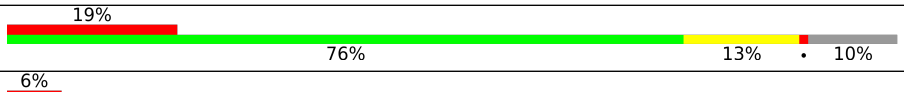
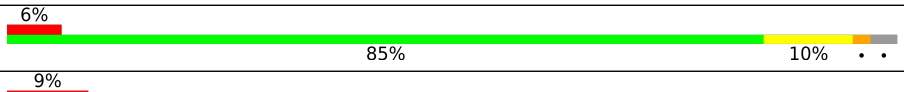
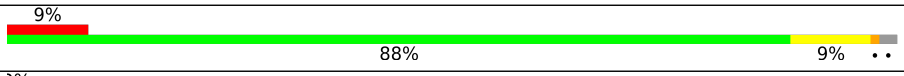
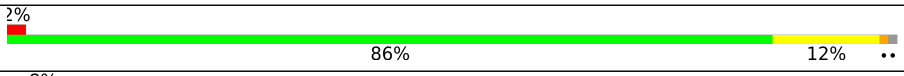
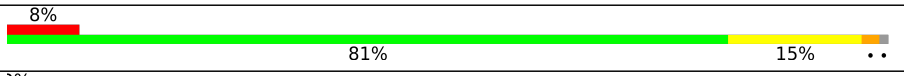
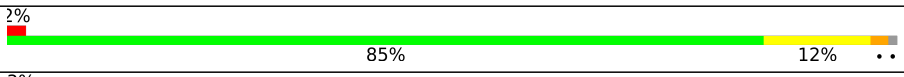
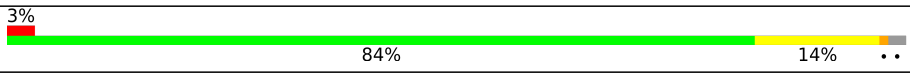
Mol	Chain	Length	Quality of chain
2	G	99	
2	L	99	
2	Q	99	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	207	
4	I	207	
4	N	207	
4	S	207	
5	E	243	
5	J	243	
5	O	243	
5	T	243	

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			

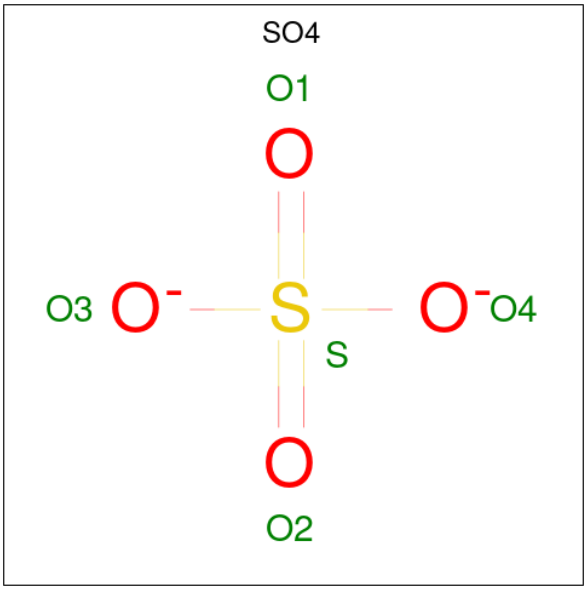
- Molecule 4 is a protein called NP1-B17 TCR alpha chain.

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 (three-letter code: SO4) (formula: O_4S).



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 5 4 1	0	0
6	K	1	Total O S 5 4 1	0	0
6	O	1	Total O S 5 4 1	0	0
6	T	1	Total O S 5 4 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is water.

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

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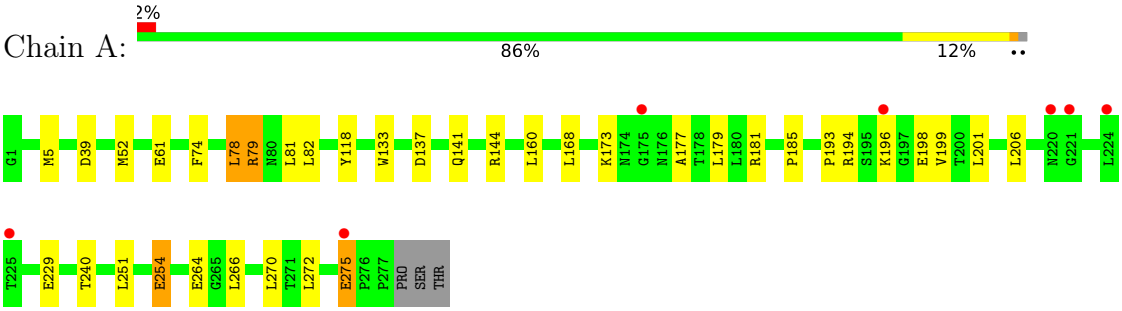
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	23	Total O 23 23	0	0
8	J	33	Total O 33 33	0	0
8	K	40	Total O 40 40	0	0
8	L	19	Total O 19 19	0	0
8	M	1	Total O 1 1	0	0
8	N	32	Total O 32 32	0	0
8	O	57	Total O 57 57	0	0
8	P	40	Total O 40 40	0	0
8	Q	14	Total O 14 14	0	0
8	R	2	Total O 2 2	0	0
8	S	22	Total O 22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

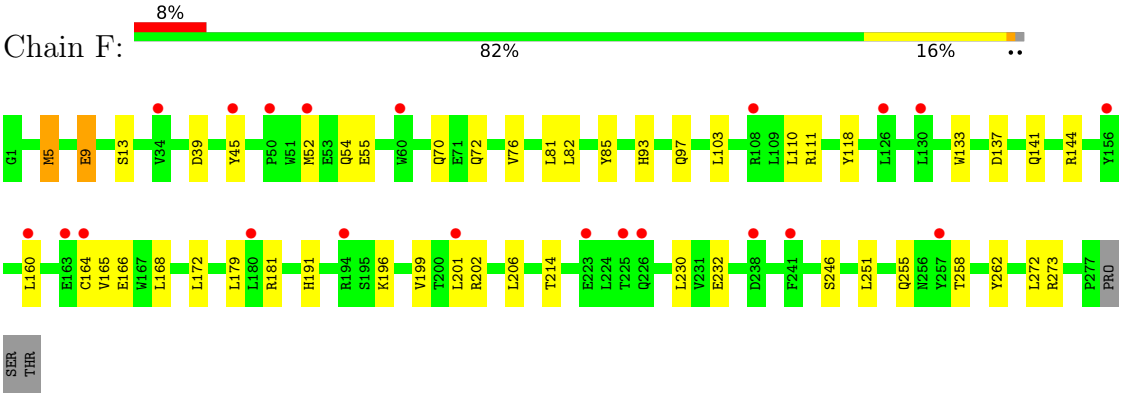
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:



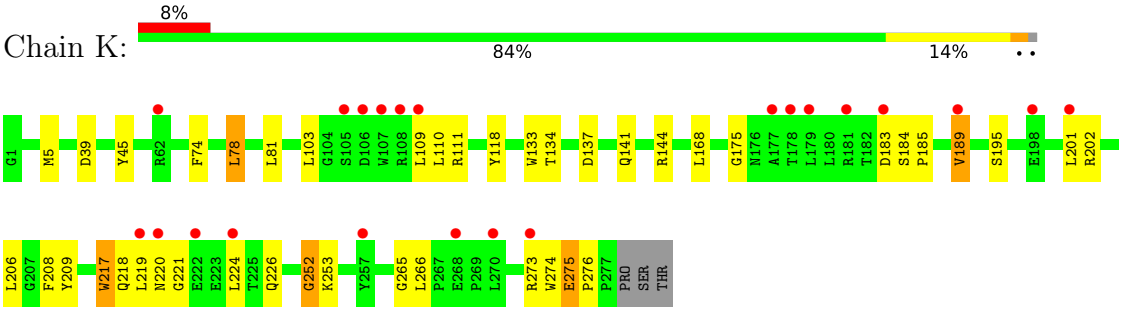
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain F:



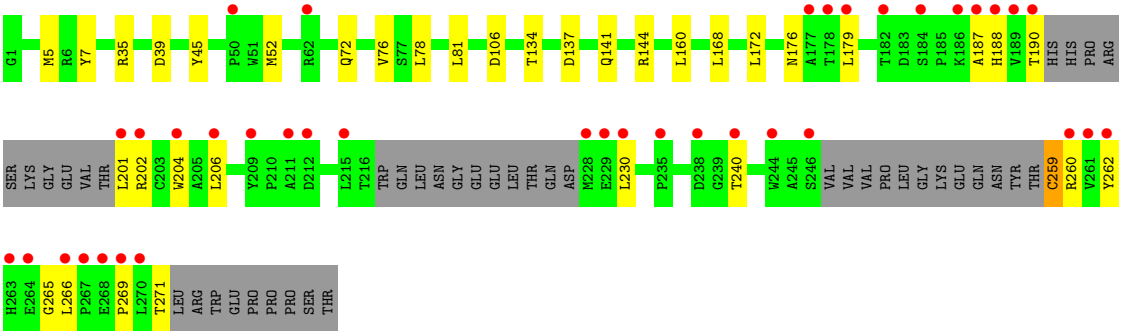
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain K:

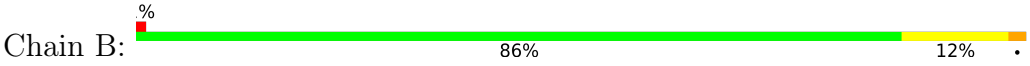


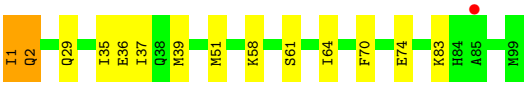
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain P:

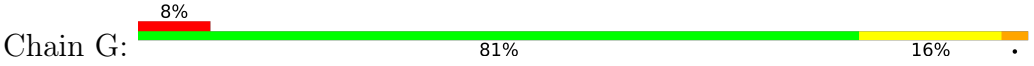


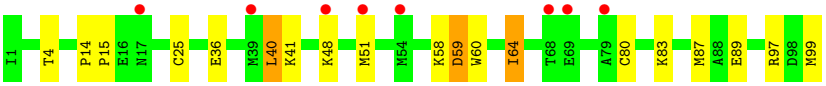
• Molecule 2: Beta-2-microglobulin



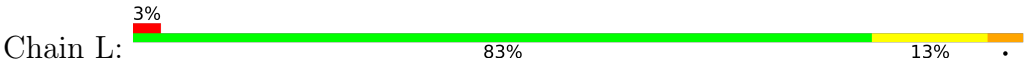


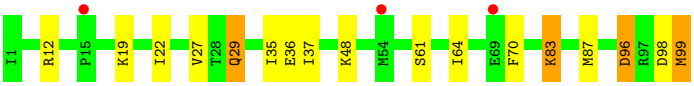
• Molecule 2: Beta-2-microglobulin



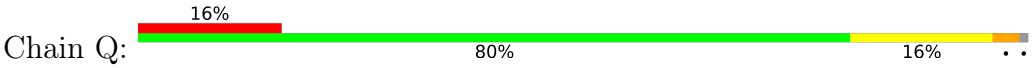


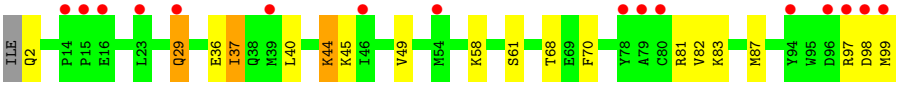
• Molecule 2: Beta-2-microglobulin



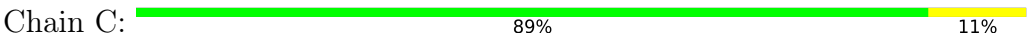


• Molecule 2: Beta-2-microglobulin



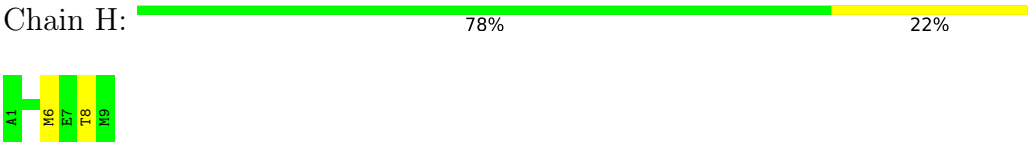


• Molecule 3: influenza NP366 epitope



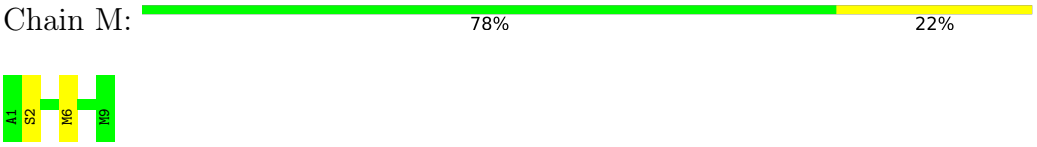
• Molecule 3: influenza NP366 epitope

Chain H:



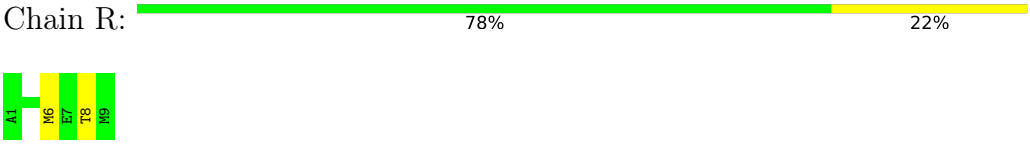
• Molecule 3: influenza NP366 epitope

Chain M:



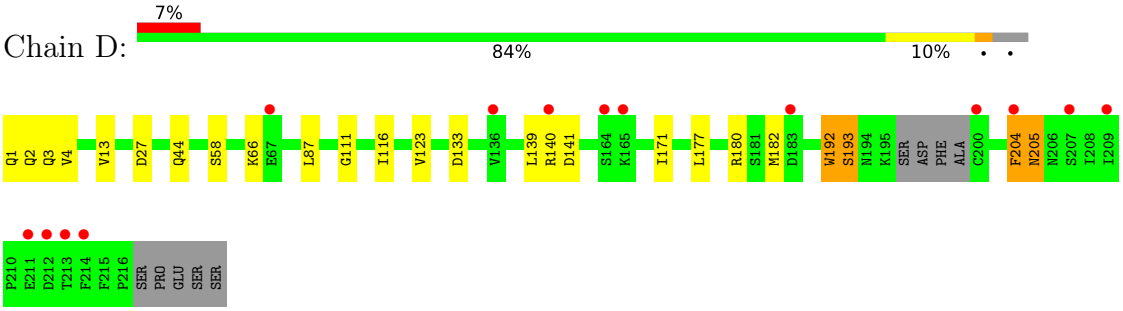
• Molecule 3: influenza NP366 epitope

Chain R:



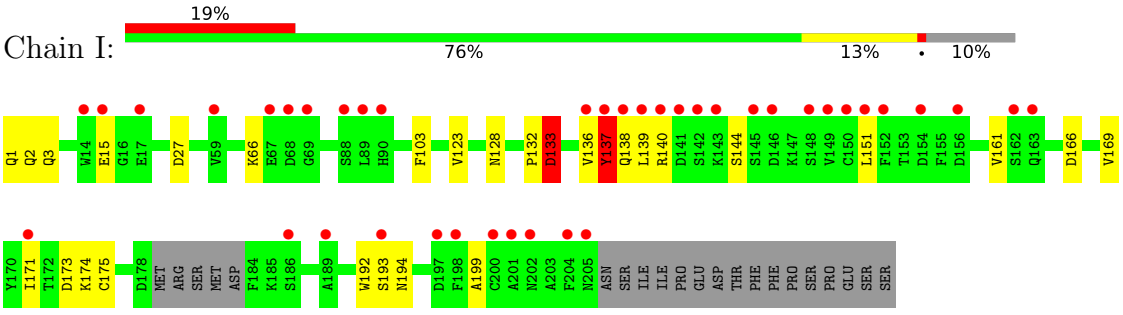
• Molecule 4: NP1-B17 TCR alpha chain

Chain D:



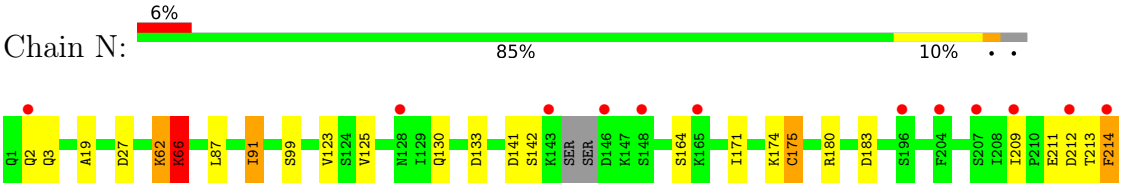
• Molecule 4: NP1-B17 TCR alpha chain

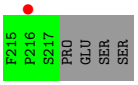
Chain I:



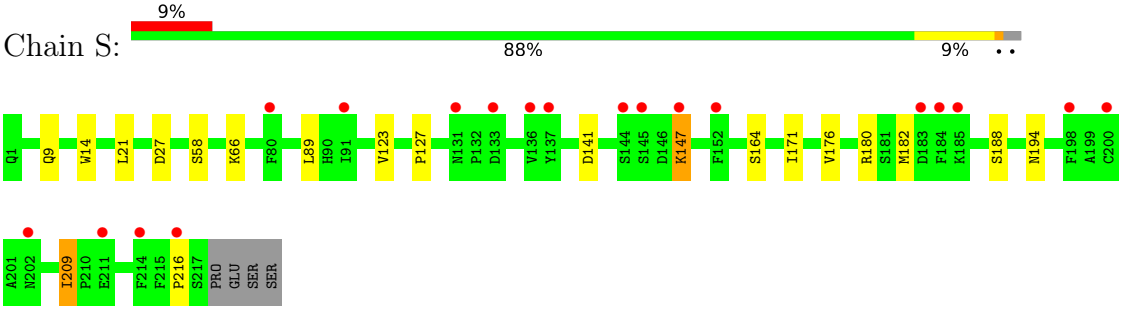
• Molecule 4: NP1-B17 TCR alpha chain

Chain N:

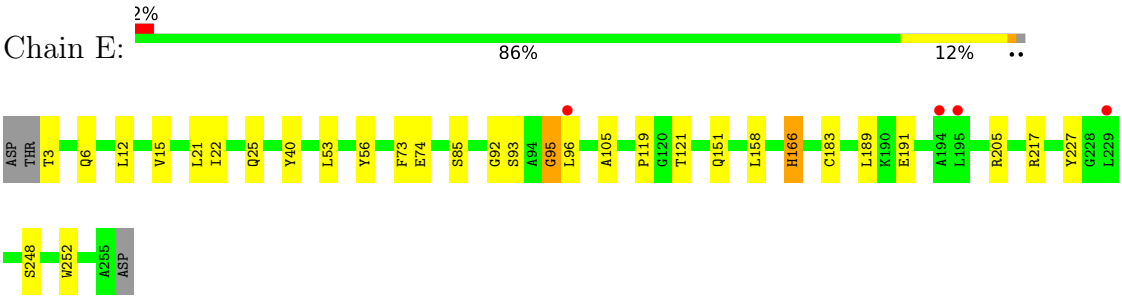




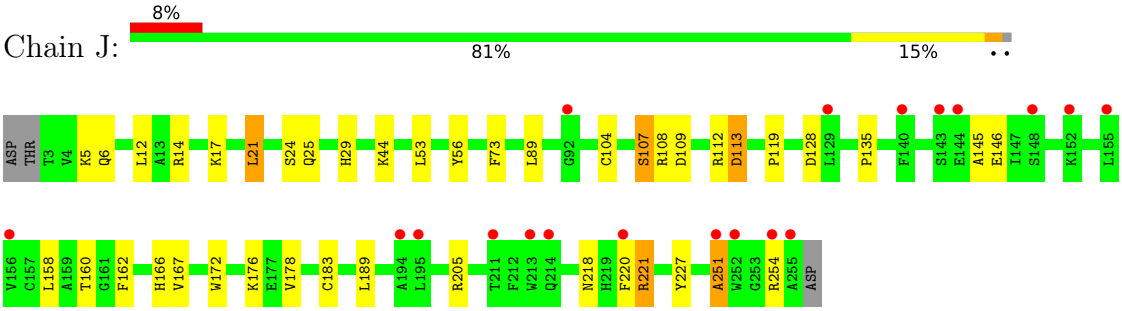
• Molecule 4: NP1-B17 TCR alpha chain



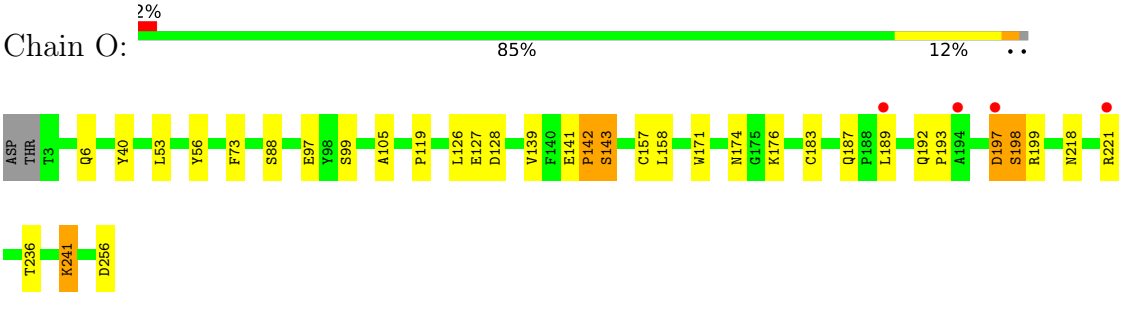
• Molecule 5: NP1-B17 TCR beta chain



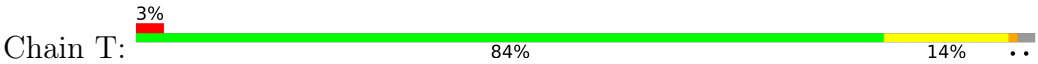
• Molecule 5: NP1-B17 TCR beta chain

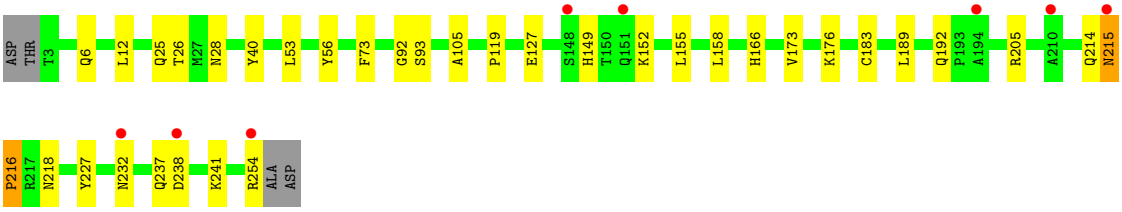


• Molecule 5: NP1-B17 TCR beta chain



• Molecule 5: NP1-B17 TCR beta chain




ASP
THR
T3
Q6
L12
Q25
T26
M27
N28
Y40
L53
Y56
F73
G92
S93
A105
P119
E127
S148
H149
T150
Q151
K152
L155
L158
H166
V173
K176
C183
L189
Q192
P193
A194
R205
A210
Q214
N215
P216
R217
N218
Y227
N232
Q237
D238
K241
R254
ALA
ASP

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.62 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.226 , 0.249 0.259 , 0.283	Depositor DCC
R_{free} test set	6523 reflections (5.12%)	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)	0.28 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.35	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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (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	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

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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

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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: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
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

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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
1:F:76:VAL:HG13	3:H:8:THR:HG21	1.93	0.50
2:G:51:MET:HE1	2:G:64:ILE:HG12	1.94	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

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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: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
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: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
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

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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: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
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%)	11 16
1	F	280/280 (100%)	264 (94%)	15 (5%)	1 (0%)	34 48
1	K	280/280 (100%)	250 (89%)	25 (9%)	5 (2%)	8 12
1	P	234/280 (84%)	221 (94%)	11 (5%)	2 (1%)	17 26
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	15 23
2	G	98/99 (99%)	93 (95%)	5 (5%)	0	100 100

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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%)	7 10
4	I	182/207 (88%)	160 (88%)	18 (10%)	4 (2%)	6 9
4	N	197/207 (95%)	185 (94%)	8 (4%)	4 (2%)	7 10
4	S	201/207 (97%)	178 (89%)	19 (10%)	4 (2%)	7 10
5	E	238/243 (98%)	224 (94%)	11 (5%)	3 (1%)	12 18
5	J	238/243 (98%)	221 (93%)	15 (6%)	2 (1%)	19 29
5	O	240/243 (99%)	221 (92%)	14 (6%)	5 (2%)	7 10
5	T	237/243 (98%)	212 (90%)	20 (8%)	5 (2%)	7 10
All	All	3219/3352 (96%)	2972 (92%)	199 (6%)	48 (2%)	10 15

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

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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 (i)

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%)	14 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	240/238 (101%)	211 (88%)	29 (12%)	5 6
1	K	240/238 (101%)	225 (94%)	15 (6%)	18 28
1	P	203/238 (85%)	182 (90%)	21 (10%)	7 10
2	B	93/93 (100%)	87 (94%)	6 (6%)	17 26
2	G	94/93 (101%)	88 (94%)	6 (6%)	17 27
2	L	94/93 (101%)	84 (89%)	10 (11%)	6 10
2	Q	93/93 (100%)	83 (89%)	10 (11%)	6 9
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
3	R	8/8 (100%)	8 (100%)	0	100 100
4	D	178/188 (95%)	164 (92%)	14 (8%)	12 19
4	I	167/188 (89%)	157 (94%)	10 (6%)	19 30
4	N	182/188 (97%)	166 (91%)	16 (9%)	10 14
4	S	184/188 (98%)	175 (95%)	9 (5%)	25 38
5	E	212/215 (99%)	196 (92%)	16 (8%)	13 21
5	J	212/215 (99%)	192 (91%)	20 (9%)	8 13
5	O	214/215 (100%)	197 (92%)	17 (8%)	12 19
5	T	212/215 (99%)	194 (92%)	18 (8%)	10 15
All	All	2890/2968 (97%)	2655 (92%)	235 (8%)	11 17

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

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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

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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

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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

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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

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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

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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

Sometimes 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 (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 monosaccharides 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	D	301	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	K	301	-	4,4,4	0.15	0	6,6,6	0.04	0
6	SO4	T	301	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	E	301	-	4,4,4	0.13	0	6,6,6	0.06	0
6	SO4	O	301	-	4,4,4	0.14	0	6,6,6	0.06	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, 95^{th} 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%) 57 53	33, 61, 99, 120	7 (2%)
1	F	277/280 (98%)	0.66	21 (7%) 13 11	40, 84, 117, 143	7 (2%)
1	K	277/280 (98%)	0.49	22 (7%) 12 10	34, 67, 109, 123	7 (2%)
1	P	238/280 (85%)	0.81	38 (15%) 1 1	37, 66, 159, 198	5 (2%)
2	B	99/99 (100%)	0.32	1 (1%) 82 81	41, 59, 79, 88	2 (2%)
2	G	99/99 (100%)	0.77	8 (8%) 12 9	54, 75, 103, 111	0
2	L	99/99 (100%)	0.33	3 (3%) 50 47	43, 63, 91, 102	0
2	Q	98/99 (98%)	0.88	16 (16%) 1 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%)	0.07	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%)	0.42	14 (7%) 16 12	39, 64, 115, 129	1 (0%)
4	I	186/207 (89%)	1.15	40 (21%) 0 0	52, 84, 162, 187	1 (0%)
4	N	201/207 (97%)	0.61	13 (6%) 18 16	46, 72, 109, 144	1 (0%)
4	S	203/207 (98%)	0.68	19 (9%) 8 6	43, 79, 122, 140	1 (0%)
5	E	240/243 (98%)	0.18	4 (1%) 70 67	32, 56, 92, 106	1 (0%)
5	J	240/243 (98%)	0.58	19 (7%) 12 10	40, 74, 138, 163	0
5	O	241/243 (99%)	0.22	4 (1%) 70 67	34, 57, 87, 108	2 (0%)
5	T	239/243 (98%)	0.39	8 (3%) 46 43	34, 64, 100, 124	1 (0%)
All	All	3248/3352 (96%)	0.53	237 (7%) 15 12	32, 68, 117, 198	36 (1%)

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	187	ALA	11.1
4	I	138	GLN	10.0
4	I	139	LEU	9.2
4	I	140	ARG	8.6
1	P	268	GLU	8.2
1	P	267	PRO	6.8
5	J	195	LEU	6.7
1	F	225	THR	6.5
1	P	188	HIS	6.5
5	J	143	SER	6.2
4	I	137	TYR	6.2
1	P	262	TYR	6.1
1	K	177	ALA	6.0
1	K	178	THR	5.9
5	J	194	ALA	5.9
4	S	184	PHE	5.8
1	P	228	MET	5.5
1	K	220	ASN	5.5
1	P	269	PRO	5.5
5	J	252	TRP	5.3
2	Q	54[A]	MET	5.3
4	I	202	ASN	5.3
1	P	186	LYS	5.1
1	K	179	LEU	5.1
4	I	201	ALA	5.1
4	S	145	SER	5.0
4	I	146	ASP	5.0
1	P	190	THR	4.8
1	P	189	VAL	4.8
4	I	148	SER	4.8
4	N	146	ASP	4.7
5	T	238	ASP	4.6
4	D	214	PHE	4.5
4	N	2	GLN	4.5
5	J	255	ALA	4.5
2	Q	23	LEU	4.5
2	Q	15	PRO	4.4
1	P	179	LEU	4.4
2	Q	99	MET	4.3
4	S	214	PHE	4.3
4	N	196	SER	4.3
1	P	215	LEU	4.2
4	I	204	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	P	264	GLU	4.1
4	N	209	ILE	4.1
4	N	216	PRO	4.0
1	P	261	VAL	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
2	Q	94	TYR	3.9
5	J	144	GLU	3.8
4	S	183	ASP	3.8
1	P	270	LEU	3.8
2	G	48	LYS	3.8
4	N	214	PHE	3.7
2	Q	14	PRO	3.6
4	I	145	SER	3.6
5	J	220	PHE	3.6
1	P	178	THR	3.6
1	F	223	GLU	3.6
2	Q	97	ARG	3.5
4	D	213	THR	3.5
5	J	251	ALA	3.5
5	J	148	SER	3.5
4	I	69	GLY	3.5
2	G	68	THR	3.5
1	P	246	SER	3.4
1	F	160	LEU	3.4
4	I	152	PHE	3.4
1	K	105	SER	3.4
1	P	202	ARG	3.3
1	P	204	TRP	3.3
1	P	201	LEU	3.3
4	S	202	ASN	3.3
4	I	151	LEU	3.2
2	G	54[A]	MET	3.2
1	F	201	LEU	3.2
4	D	136	VAL	3.2
1	P	211	ALA	3.2
4	N	165	LYS	3.2
1	K	198	GLU	3.1
4	S	185	LYS	3.1
1	K	270	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
4	S	144	SER	3.1
5	O	194	ALA	3.1
1	F	238	ASP	3.1
2	Q	79	ALA	3.1
1	A	196	LYS	3.1
1	K	222	GLU	3.1
4	S	198	PHE	3.0
4	I	142	SER	3.0
1	F	226	GLN	3.0
5	J	214	GLN	3.0
4	I	197	ASP	3.0
5	J	254	ARG	3.0
4	I	150	CYS	3.0
1	P	240	THR	2.9
5	O	197	ASP	2.9
4	I	189	ALA	2.9
2	L	54[A]	MET	2.9
1	K	273	ARG	2.9
2	Q	98	ASP	2.9
4	S	137	TYR	2.9
5	T	151	GLN	2.8
5	T	215	ASN	2.8
1	K	106	ASP	2.8
5	E	194	ALA	2.8
4	S	211	GLU	2.8
1	F	50	PRO	2.8
4	S	200	CYS	2.8
1	K	268	GLU	2.7
4	I	200	CYS	2.7
2	Q	80	CYS	2.7
4	I	193	SER	2.7
2	L	69	GLU	2.7
4	I	141	ASP	2.7
4	I	154	ASP	2.7
2	G	39	MET	2.7
4	I	163	GLN	2.7
2	Q	78	TYR	2.7
1	P	238	ASP	2.7
2	L	15	PRO	2.7
2	Q	96	ASP	2.7
4	N	207	SER	2.7
1	K	108[A]	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	229	GLU	2.7
2	G	17	ASN	2.6
4	I	198	PHE	2.6
5	J	155	LEU	2.6
2	Q	39	MET	2.6
5	J	152	LYS	2.5
4	I	205	ASN	2.5
2	Q	29	GLN	2.5
4	I	67	GLU	2.5
4	D	209	ILE	2.5
1	F	130	LEU	2.5
4	N	212	ASP	2.5
4	D	200	CYS	2.5
1	K	201	LEU	2.5
1	A	275	GLU	2.5
1	F	52	MET	2.5
4	I	149	VAL	2.5
4	D	204	PHE	2.5
4	N	143	LYS	2.5
2	Q	46	ILE	2.4
5	O	189	LEU	2.4
1	K	107	TRP	2.4
1	A	175	GLY	2.4
4	D	140	ARG	2.4
4	I	162	SER	2.4
4	D	67	GLU	2.4
4	S	147	LYS	2.4
1	F	34	VAL	2.4
5	T	232	ASN	2.4
1	F	257	TYR	2.4
4	D	165	LYS	2.4
5	E	96	LEU	2.4
5	T	194	ALA	2.4
5	J	140	PHE	2.4
1	K	62[A]	ARG	2.4
1	P	244	TRP	2.3
1	P	212	ASP	2.3
1	A	221	GLY	2.3
5	J	211	THR	2.3
5	J	213	TRP	2.3
4	S	133	ASP	2.3
1	F	163	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	50	PRO	2.3
2	Q	16	GLU	2.3
4	D	183	ASP	2.3
1	F	45	TYR	2.3
1	A	225	THR	2.3
5	T	254	ARG	2.3
1	F	126	LEU	2.3
1	P	182	THR	2.3
2	B	85	ALA	2.3
1	F	60	TRP	2.3
1	A	220	ASN	2.3
4	S	131	ASN	2.3
1	F	194	ARG	2.3
4	I	59	VAL	2.3
1	K	183	ASP	2.2
1	K	189	VAL	2.2
4	S	216	PRO	2.2
5	T	148	SER	2.2
4	I	186	SER	2.2
2	G	51	MET	2.2
1	P	209	TYR	2.2
5	J	156	VAL	2.2
5	J	129	LEU	2.2
1	P	177	ALA	2.2
1	F	156	TYR	2.2
4	I	143	LYS	2.2
1	F	108[A]	ARG	2.2
4	S	80	PHE	2.2
4	I	88	SER	2.2
1	F	164	CYS	2.2
4	I	15	GLU	2.1
4	S	136	VAL	2.1
1	K	109	LEU	2.1
2	G	79	ALA	2.1
2	G	69	GLU	2.1
4	N	204	PHE	2.1
1	K	257	TYR	2.1
4	I	136	VAL	2.1
1	F	180	LEU	2.1
1	K	224	LEU	2.1
4	D	212	ASP	2.1
1	P	260	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	207	SER	2.1
1	K	219	LEU	2.1
4	I	68	ASP	2.1
4	I	156	ASP	2.1
4	I	90	HIS	2.1
4	I	171	ILE	2.1
4	N	128	ASN	2.1
1	P	62[A]	ARG	2.1
4	N	148	SER	2.1
1	F	241	PHE	2.1
1	P	184[A]	SER	2.1
4	I	89	LEU	2.1
4	S	152	PHE	2.1
5	E	195	LEU	2.0
1	P	235	PRO	2.0
5	O	221[A]	ARG	2.0
4	S	91	ILE	2.0
4	I	17	GLU	2.0
5	T	210	ALA	2.0
5	J	92	GLY	2.0
4	I	14	TRP	2.0
1	A	224	LEU	2.0
5	E	229	LEU	2.0
1	K	181	ARG	2.0
1	P	206	LEU	2.0
1	P	263	HIS	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 monosaccharides 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, 95^{th} 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	D	301	5/5	0.72	0.25	118,118,119,119	0
6	SO4	T	301	5/5	0.73	0.35	115,115,115,115	0
6	SO4	E	301	5/5	0.79	0.17	115,116,116,116	0
7	NA	E	302	1/1	0.85	0.17	50,50,50,50	0
7	NA	J	301	1/1	0.86	0.16	38,38,38,38	0
6	SO4	K	301	5/5	0.88	0.12	114,114,114,115	0
7	NA	T	303	1/1	0.88	0.10	49,49,49,49	0
7	NA	T	302	1/1	0.91	0.11	42,42,42,42	0
7	NA	I	301	1/1	0.92	0.23	48,48,48,48	0
6	SO4	O	301	5/5	0.92	0.13	102,102,102,102	0
7	NA	K	302	1/1	0.95	0.07	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.