



# wwPDB X-ray Structure Validation Summary Report

Jun 10, 2014 – 11:30 AM EDT

PDB ID : 3PQY  
Title : Crystal Structure of 6218 TCR in complex with the H2Db-PA224  
Authors : Gras, S.; Guillonneau, C.; Turner, S.J.; Rossjohn, J.  
Deposited on : 2010-11-28  
Resolution : 3.19 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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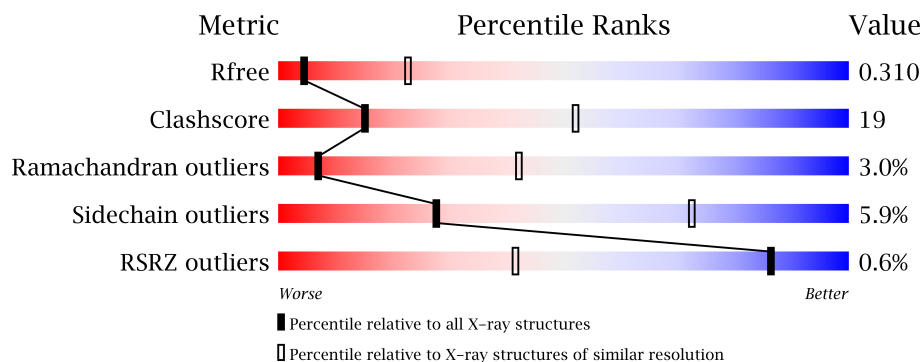
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23161
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 3.19 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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	275	
1	F	275	
1	K	275	
1	P	275	
2	B	99	
2	G	99	
2	L	99	
2	Q	99	
3	C	10	
3	H	10	
3	M	10	
3	R	10	
4	D	195	
4	I	195	

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Mol	Chain	Length	Quality of chain
4	N	195	
4	S	195	
5	E	240	
5	J	240	
5	O	240	
5	T	240	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25956 atoms, of which 0 are hydrogen and 0 are deuterium.

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	275	Total	C	N	O	S	1	0	0
			2260	1428	399	424	9			
1	F	267	Total	C	N	O	S	1	0	0
			2198	1391	389	409	9			
1	K	275	Total	C	N	O	S	0	0	0
			2260	1428	399	424	9			
1	P	273	Total	C	N	O	S	1	0	0
			2244	1418	397	420	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	G	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	L	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	Q	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			

- Molecule 3 is a protein called 10-mer peptide from RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	H	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	M	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	R	10	Total	C	N	O	0	0	0
			84	53	14	17			

- Molecule 4 is a protein called alpha chain of the 6218-TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	189	Total	C	N	O	S	0	0	0
			1464	916	244	295	9			
4	I	188	Total	C	N	O	S	0	0	0
			1464	918	243	294	9			
4	N	174	Total	C	N	O	S	0	0	0
			1350	846	226	269	9			
4	S	174	Total	C	N	O	S	0	0	0
			1348	845	225	269	9			

- Molecule 5 is a protein called beta chain of the 6218-TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	J	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	O	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	T	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	B	2	Total	O	0	0
			2	2		
6	D	1	Total	O	0	0
			1	1		
6	E	2	Total	O	0	0
			2	2		
6	J	1	Total	O	0	0
			1	1		
6	K	1	Total	O	0	0
			1	1		
6	N	1	Total	O	0	0
			1	1		
6	O	2	Total	O	0	0
			2	2		
6	P	2	Total	O	0	0
			2	2		

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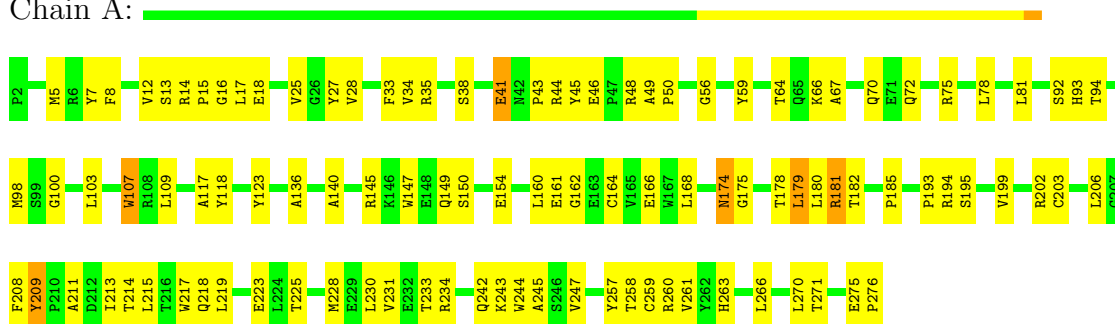
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	1	Total	O	0	0
			1	1		
6	S	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

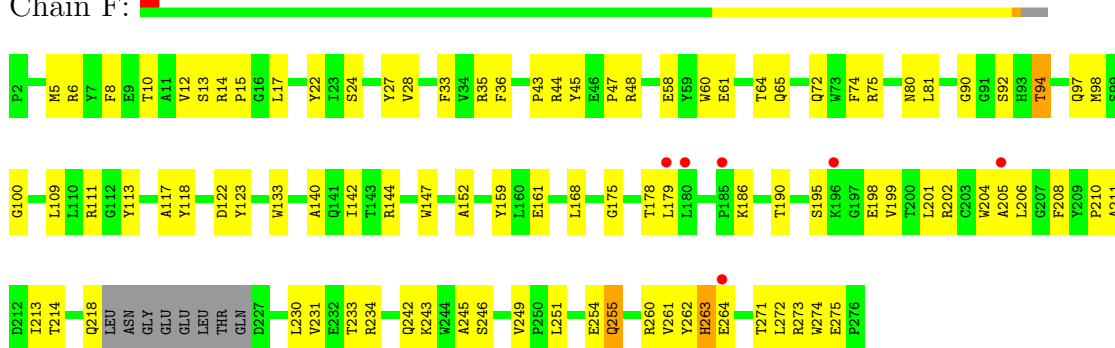
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:



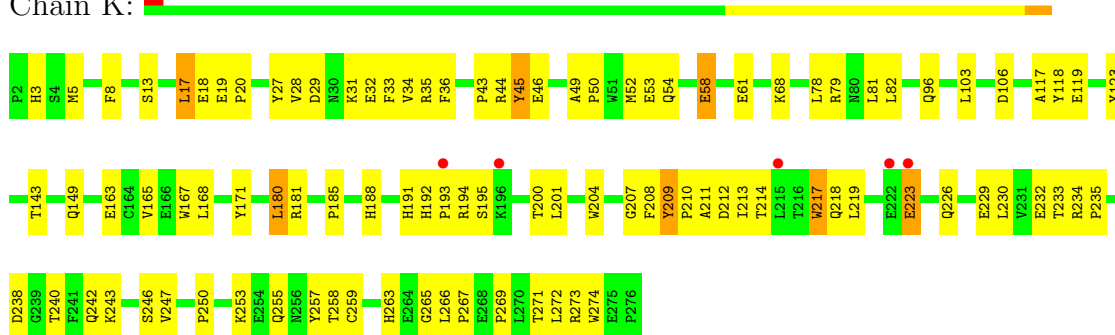
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

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

F241	L109	P2
Q242	L110	M5
K243	R111	R6
W244		Y7
A245	A117	F8
S246	Y118	E9
	W133	
T258	I142	S13
C259	T143	L17
R260	R144	
H263	R145	P20
E264		Y21
G265	L168	Y22
	H169	
P269		V28
L270	K173	
	N176	F33
R273	A177	V34
W274		
GLU	L180	V45
PRO		E46
	S184	P47
	P185	R48
		A49
	H191	P50
	H192	W51
	P193	M52
	R194	S53
	S195	Q54
		F55
		G56
	V199	P57
	T200	E58
	L201	Y59
	R202	W60
	C203	F61
	W204	R62
	A205	
	L206	K66
	G207	A67
	F208	
	Y209	Q72
	P210	
		R75
	Q218	
	G221	L81
	E222	
	E223	N86
	L224	
	T225	S92
		Q97
	L230	
	R234	D102
	P235	D106
	A236	W107
		R109

- |     |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| I1E | Q2 | I7 | Y10 | H13 | P14 | P15 | E16 | N17 | G18 | K19 | P20 | N21 | L22 | L23 | T28 | P32 | P33 | I37 | Q38 | M39 | I46 | M51 | S52 | F56 | M60 | S61 | F62 | S63 | Y63 | I64 | L65 | E69 | F70 | V82 | D85 | E89 | P90 | K91 | R97 | D98 |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| C80 | C81 | D85 | A88 | T92 | V93 | Y94 | W95 | D96 | M99 | I1E | Q2 | P5 | Q6 | I7 | Y10 | S11 | R12 | H13 | P14 | P15 | N21 | I22 | L23 | N24 | V27 | T28 | Q29 | F30 | H31 | P32 | P33 | I37 | Q38 | M39 | L40 | K41 | K45 | I46 | E50 | M51 | S52 | F56 | S57 | K58 | D59 | W60 | S61 | F62 | Y63 | I64 | L65 | A66 | H67 | T68 | E69 | F70 | T75 | Y78 | L79 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- |     |     |     |     |     |     |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| E89 | E90 | K91 | T92 | D96 | M99 |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| I1E | Q2  | K3  | T4  | P5  | Q6  | I7 | Q8 | V9 | Y10 | S11 | R12 | I16 | M17 | G18 | K19 | P20 | M21 | F30 | H31 | P32 | P33 | I37 | Q38 | M39 | L40 | K41 | M42 | K48 | V49 | E50 | D53 | F56 | M60 | S61 | F62 | L65 | A66 | H67 | T68 | E69 | F70 | T71 | P72 | T73 | E74 | I75 | D76 | R81 | V82 |

- |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| L6 | P5 | I7 | V9 | S11 | R12 | H13 | B14 | P15 | V27 | T28 | Q29 | F30 | H31 | P32 | E36 | L40 | K41 | I46 | V49 | F56 | M60 | S61 | F62 | Y63 | H67 | T68 | E69 | F70 | T71 | P72 | Y78 | K83 | S86 | V93 | Y94 | N95 | D96 |
|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- |    |    |    |    |    |    |    |  |     |
|----|----|----|----|----|----|----|--|-----|
| S1 | S2 | L3 | E4 | N5 | F6 | R7 |  | V10 |
|----|----|----|----|----|----|----|--|-----|

- Chain H:
- 

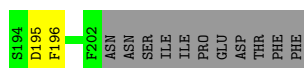
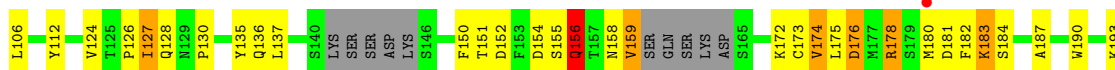
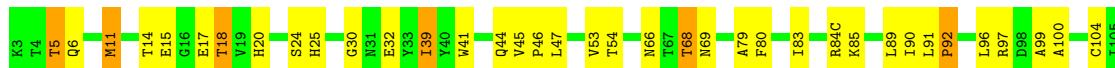






• Molecule 4: alpha chain of the 6218-TCR

Chain S:



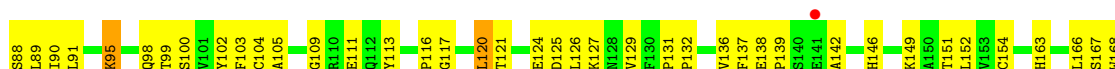
• Molecule 5: beta chain of the 6218-TCR

Chain E:



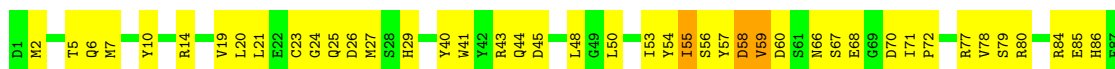
• Molecule 5: beta chain of the 6218-TCR

Chain J:



• Molecule 5: beta chain of the 6218-TCR

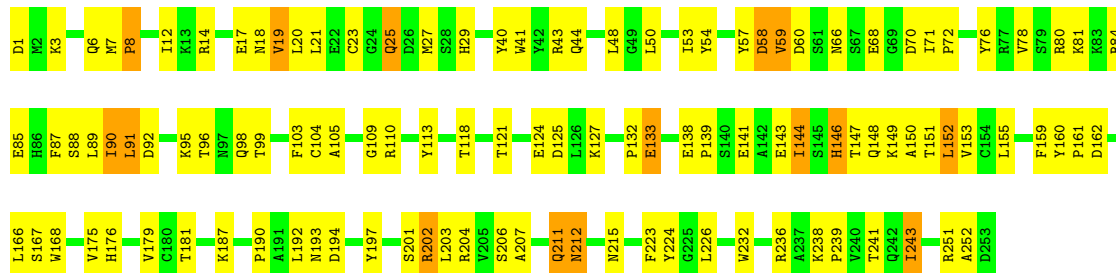
Chain O:





• Molecule 5: beta chain of the 6218-TCR

Chain T:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.89Å 199.06Å 202.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 3.19 49.61 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.61-3.19) 97.4 (49.61-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1.357)	Depositor
R, $R_{free}$	0.246 , 0.316 0.236 , 0.310	Depositor DCC
$R_{free}$ test set	3541 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.3	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 69960 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	25956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.2923e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.21	0/2327	0.37	0/3160
1	F	0.20	0/2264	0.36	0/3073
1	K	0.21	0/2327	0.36	0/3160
1	P	0.20	0/2310	0.37	0/3136
2	B	0.21	0/839	0.40	0/1137
2	G	0.21	0/839	0.38	0/1137
2	L	0.21	0/839	0.40	0/1137
2	Q	0.20	0/839	0.39	0/1137
3	C	0.25	0/85	0.40	0/112
3	H	0.23	0/85	0.34	0/112
3	M	0.23	0/85	0.40	0/112
3	R	0.24	0/85	0.36	0/112
4	D	0.22	0/1495	0.41	0/2032
4	I	0.22	0/1497	0.43	0/2036
4	N	0.22	0/1380	0.42	0/1875
4	S	0.22	0/1377	0.41	0/1873
5	E	0.22	0/1992	0.39	0/2702
5	J	0.22	0/1992	0.39	0/2702
5	O	0.22	0/1992	0.38	0/2702
5	T	0.22	0/1992	0.39	0/2702
All	All	0.21	0/26641	0.39	0/36149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2260	0	2131	73	0
1	F	2198	0	2072	66	0
1	K	2260	0	2133	74	0
1	P	2244	0	2118	66	0
2	B	813	0	782	26	0
2	G	813	0	782	33	0
2	L	813	0	782	35	0
2	Q	813	0	782	21	0
3	C	84	0	80	8	0
3	H	84	0	80	3	0
3	M	84	0	80	2	0
3	R	84	0	80	5	0
4	D	1464	0	1399	73	0
4	I	1464	0	1394	98	0
4	N	1350	0	1294	83	0
4	S	1348	0	1286	64	0
5	E	1941	0	1857	63	0
5	J	1941	0	1857	96	0
5	O	1941	0	1857	71	0
5	T	1941	0	1857	102	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	1	0	0	0	0
6	E	2	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	N	1	0	0	0	0
6	O	2	0	0	0	0
6	P	2	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
All	All	25956	0	24703	956	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 956 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:S:183:LYS:HB2	4:S:184:SER:HB2	1.38	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:S:30:GLY:HA2	4:S:84(C):ARG:HH12	1.22	1.02
5:E:7:MET:HB3	5:E:8:PRO:HD2	1.43	1.00
5:J:59:VAL:HG13	5:J:60:ASP:H	1.30	0.96
5:T:7:MET:HB3	5:T:8:PRO:HD2	1.45	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/275 (99%)	244 (89%)	26 (10%)	3 (1%)	21	72
1	F	263/275 (96%)	222 (84%)	39 (15%)	2 (1%)	27	77
1	K	273/275 (99%)	235 (86%)	30 (11%)	8 (3%)	7	43
1	P	271/275 (98%)	244 (90%)	25 (9%)	2 (1%)	30	80
2	B	96/99 (97%)	87 (91%)	7 (7%)	2 (2%)	11	55
2	G	96/99 (97%)	82 (85%)	11 (12%)	3 (3%)	7	41
2	L	96/99 (97%)	81 (84%)	13 (14%)	2 (2%)	11	55
2	Q	96/99 (97%)	87 (91%)	9 (9%)	0	100	100
3	C	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	1	3
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	M	8/10 (80%)	7 (88%)	0	1 (12%)	1	3
3	R	8/10 (80%)	7 (88%)	0	1 (12%)	1	3
4	D	183/195 (94%)	132 (72%)	37 (20%)	14 (8%)	1	11
4	I	184/195 (94%)	128 (70%)	45 (24%)	11 (6%)	2	20
4	N	170/195 (87%)	119 (70%)	40 (24%)	11 (6%)	2	17
4	S	168/195 (86%)	132 (79%)	31 (18%)	5 (3%)	7	42
5	E	238/240 (99%)	206 (87%)	24 (10%)	8 (3%)	6	38
5	J	238/240 (99%)	200 (84%)	30 (13%)	8 (3%)	6	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	O	238/240 (99%)	207 (87%)	25 (10%)	6 (2%)	9	49
5	T	238/240 (99%)	197 (83%)	34 (14%)	7 (3%)	7	43
All	All	3153/3276 (96%)	2629 (83%)	429 (14%)	95 (3%)	7	42

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	5	ASN
4	D	92	PRO
4	D	179	SER
5	E	8	PRO
5	E	68	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/234 (100%)	225 (96%)	9 (4%)	44	84
1	F	227/234 (97%)	220 (97%)	7 (3%)	52	88
1	K	234/234 (100%)	222 (95%)	12 (5%)	33	77
1	P	232/234 (99%)	222 (96%)	10 (4%)	40	81
2	B	93/94 (99%)	90 (97%)	3 (3%)	51	87
2	G	93/94 (99%)	86 (92%)	7 (8%)	19	61
2	L	93/94 (99%)	88 (95%)	5 (5%)	31	75
2	Q	93/94 (99%)	92 (99%)	1 (1%)	84	96
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	9 (100%)	0	100	100
3	R	9/9 (100%)	9 (100%)	0	100	100
4	D	169/175 (97%)	158 (94%)	11 (6%)	24	68
4	I	168/175 (96%)	150 (89%)	18 (11%)	10	38
4	N	154/175 (88%)	140 (91%)	14 (9%)	14	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	S	154/175 (88%)	140 (91%)	14 (9%)	14	47
5	E	213/213 (100%)	199 (93%)	14 (7%)	24	67
5	J	213/213 (100%)	199 (93%)	14 (7%)	24	67
5	O	213/213 (100%)	202 (95%)	11 (5%)	32	76
5	T	213/213 (100%)	197 (92%)	16 (8%)	19	61
All	All	2832/2900 (98%)	2666 (94%)	166 (6%)	28	72

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	87	PHE
1	K	217	TRP
5	T	54	TYR
5	J	120	LEU
1	K	45	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	146	HIS
2	L	31	HIS
5	T	6	GLN
5	J	171	ASN
1	K	188	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/275 (100%)	0.04	0 100 100	27, 74, 122, 148	1 (0%)
1	F	267/275 (97%)	0.23	6 (2%) 59 14	37, 100, 168, 201	1 (0%)
1	K	275/275 (100%)	0.23	5 (1%) 65 18	29, 95, 177, 194	0
1	P	273/275 (99%)	0.20	3 (1%) 77 27	38, 90, 152, 165	1 (0%)
2	B	98/99 (98%)	-0.09	0 100 100	42, 68, 103, 112	0
2	G	98/99 (98%)	0.14	0 100 100	54, 104, 152, 156	0
2	L	98/99 (98%)	0.12	0 100 100	53, 100, 144, 151	0
2	Q	98/99 (98%)	0.15	1 (1%) 79 29	58, 97, 129, 145	0
3	C	10/10 (100%)	-0.14	0 100 100	31, 38, 66, 70	0
3	H	10/10 (100%)	-0.12	0 100 100	40, 49, 81, 88	0
3	M	10/10 (100%)	-0.05	0 100 100	37, 44, 71, 83	0
3	R	10/10 (100%)	-0.02	0 100 100	42, 49, 80, 86	0
4	D	189/195 (96%)	0.12	2 (1%) 77 27	32, 79, 149, 169	0
4	I	188/195 (96%)	0.06	0 100 100	40, 85, 146, 163	0
4	N	174/195 (89%)	0.16	1 (0%) 86 41	37, 79, 162, 179	0
4	S	174/195 (89%)	0.14	1 (0%) 86 41	40, 85, 150, 197	0
5	E	240/240 (100%)	-0.04	0 100 100	32, 69, 120, 135	0
5	J	240/240 (100%)	-0.02	1 (0%) 90 51	32, 69, 128, 152	0
5	O	240/240 (100%)	-0.00	0 100 100	31, 69, 113, 149	0
5	T	240/240 (100%)	0.09	0 100 100	40, 90, 135, 155	0
All	All	3207/3276 (97%)	0.10	20 (0%) 86 41	27, 82, 152, 201	3 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	222	GLU	3.6
1	K	223	GLU	3.5
1	F	179	LEU	3.0
1	F	180	LEU	3.0
1	K	215	LEU	3.0

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.