



# Full wwPDB X-ray Structure Validation Report i

Sep 2, 2023 – 05:48 PM EDT

PDB ID : 3RDT  
Title : Crystal Structure of 809.B5 TCR complexed with MHC Class II I-Ab/3k peptide  
Authors : Trenh, P.; Huseby, E.S.; Stern, L.J.  
Deposited on : 2011-04-01  
Resolution : 2.70 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](mailto: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>.

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The following versions of software and data (see references ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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

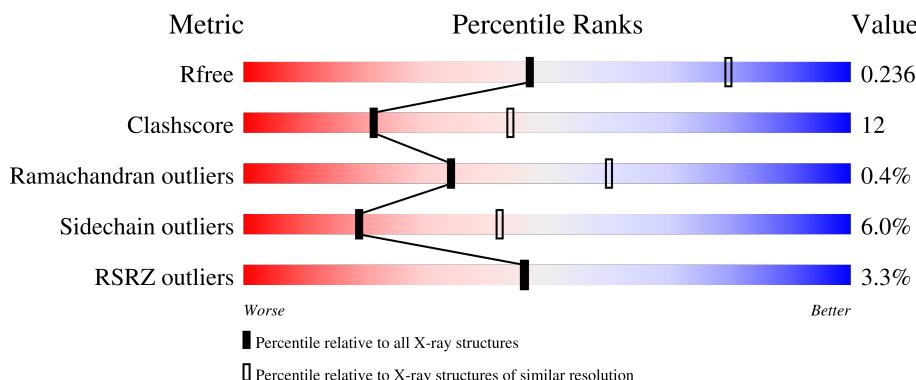
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

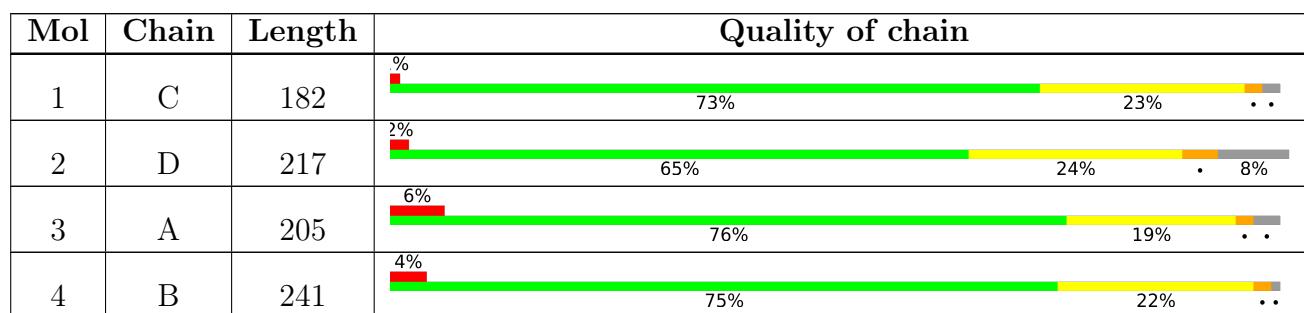
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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.



## 2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 6399 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 II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	179	1409	913	220	273	3	0	0	0

- Molecule 2 is a protein called 3K peptide, linker and MHC H-2 class II I-Ab beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	199	1625	1021	290	307	7	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	linker	UNP P14483
D	-11	GLY	-	linker	UNP P14483
D	-10	GLY	-	linker	UNP P14483
D	-9	GLY	-	linker	UNP P14483
D	-8	SER	-	linker	UNP P14483
D	-7	LEU	-	linker	UNP P14483
D	-6	VAL	-	linker	UNP P14483
D	-5	PRO	-	linker	UNP P14483
D	-4	ARG	-	linker	UNP P14483
D	-3	GLY	-	linker	UNP P14483
D	-2	SER	-	linker	UNP P14483
D	-1	GLY	-	linker	UNP P14483
D	0	GLY	-	linker	UNP P14483
D	1	GLY	-	linker	UNP P14483
D	2	GLY	-	linker	UNP P14483

- Molecule 3 is a protein called TCR 809.B5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	199	Total	C	N	O	S	0	0	0

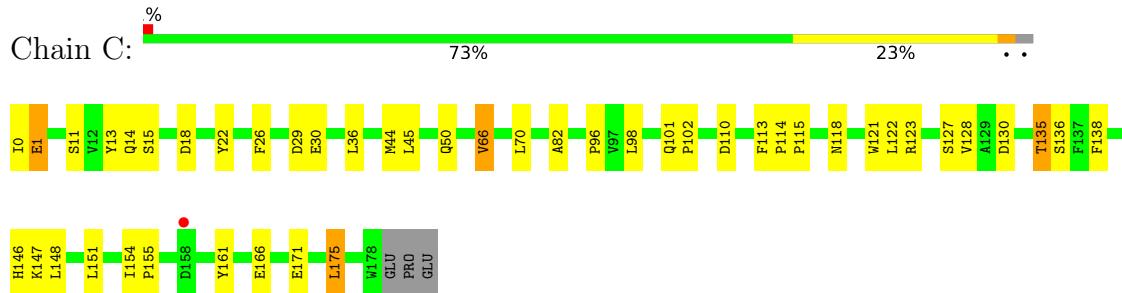
- Molecule 4 is a protein called TCR 809.B5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	238	Total	C	N	O	S	0	0	0

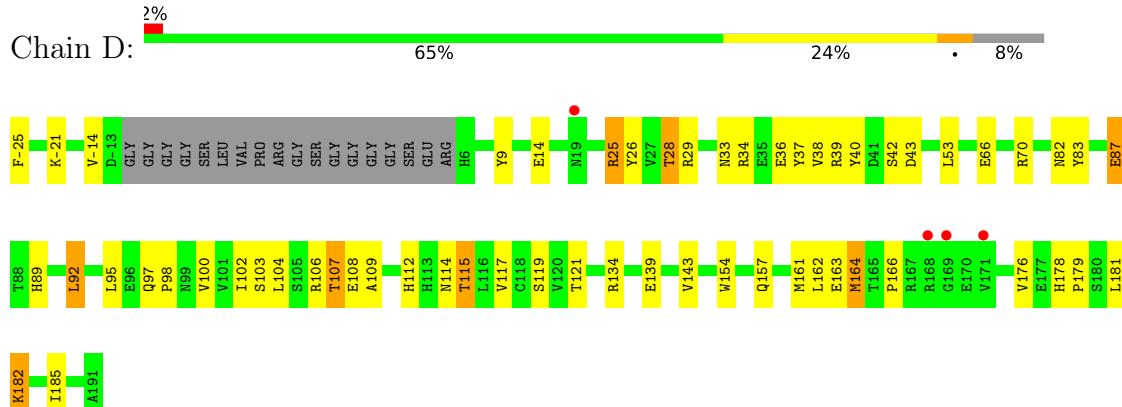
### 3 Residue-property plots [\(i\)](#)

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.

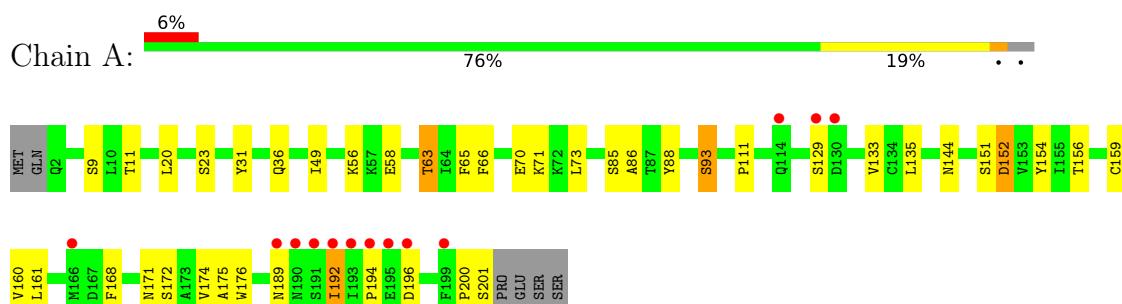
- Molecule 1: H-2 class II histocompatibility antigen, A-B alpha chain



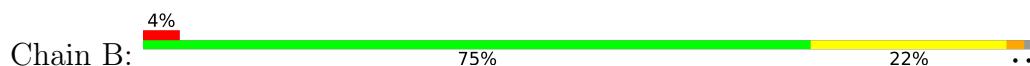
- Molecule 2: 3K peptide, linker and MHC H-2 class II I-Ab beta chain

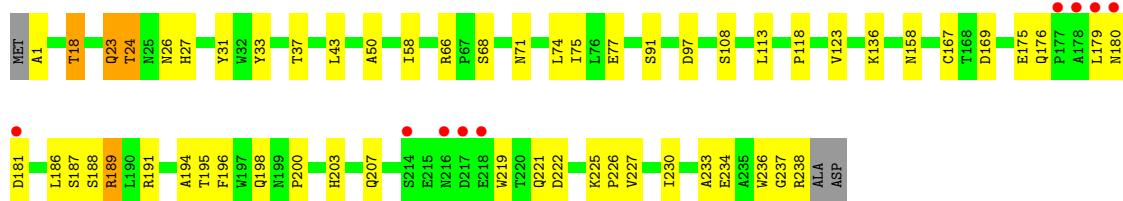


- Molecule 3: TCR 809.B5 alpha chain



- Molecule 4: TCB 809 B5 beta chain





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.85 Å    73.02 Å    65.67 Å 90.00°    90.71°    90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.98 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.70) 98.3 (29.98-2.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle^1$	3.32 (at 2.72 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
$R$ , $R_{free}$	0.206 , 0.241 0.199 , 0.236	Depositor DCC
$R_{free}$ test set	1531 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.8	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

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	C	0.46	0/1453	0.58	0/1991
2	D	0.46	0/1665	0.61	0/2262
3	A	0.40	0/1550	0.54	0/2111
4	B	0.42	0/1906	0.54	0/2603
All	All	0.43	0/6574	0.57	0/8967

There are no bond length outliers.

There are no bond angle outliers.

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	C	1409	0	1310	39	0
2	D	1625	0	1538	51	0
3	A	1512	0	1380	30	0
4	B	1853	0	1725	45	0
All	All	6399	0	5953	148	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 12.

All (148) 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)
3:A:144:ASN:H	3:A:192:ILE:HD11	1.35	0.90
2:D:114:ASN:HB3	2:D:164:MET:CE	2.05	0.87
2:D:115:THR:HB	2:D:163:GLU:OE1	1.77	0.83
1:C:70:LEU:HD13	2:D:9:TYR:HB2	1.60	0.82
1:C:175:LEU:HD12	1:C:175:LEU:N	1.94	0.81
1:C:175:LEU:HD12	1:C:175:LEU:H	1.45	0.81
3:A:66:PHE:HD1	3:A:73:LEU:HD13	1.45	0.80
1:C:1:GLU:H	1:C:1:GLU:CD	1.89	0.76
2:D:117:VAL:HG22	2:D:161:MET:HG2	1.68	0.76
2:D:114:ASN:HB3	2:D:164:MET:HE1	1.66	0.75
2:D:-25:PHE:CE2	2:D:89:HIS:HD2	2.05	0.74
4:B:221:GLN:HG3	4:B:222:ASP:H	1.54	0.73
4:B:1:ALA:N	4:B:24:THR:HG22	2.05	0.71
4:B:221:GLN:CG	4:B:222:ASP:H	2.04	0.71
2:D:106:ARG:NH1	2:D:107:THR:HG23	2.06	0.70
4:B:179:LEU:HB3	4:B:181:ASP:OD1	1.91	0.69
2:D:182:LYS:HD2	2:D:182:LYS:H	1.56	0.69
4:B:1:ALA:H3	4:B:24:THR:HG22	1.58	0.68
3:A:151:SER:O	3:A:152:ASP:HB2	1.93	0.68
2:D:121:THR:HG22	2:D:157:GLN:HG3	1.75	0.68
4:B:203:HIS:HB3	4:B:236:TRP:CZ3	2.29	0.67
1:C:135:THR:CG2	1:C:148:LEU:H	2.07	0.67
4:B:189:ARG:N	4:B:189:ARG:HD3	2.08	0.67
3:A:168:PHE:CD2	4:B:136:LYS:HE2	2.30	0.66
4:B:203:HIS:HB3	4:B:236:TRP:CE3	2.31	0.66
2:D:87:GLU:HA	2:D:87:GLU:OE1	1.96	0.65
1:C:118:ASN:HB2	1:C:166:GLU:HB2	1.78	0.65
1:C:13:TYR:HB2	1:C:66:VAL:CG1	2.28	0.64
2:D:114:ASN:HB3	2:D:164:MET:HE3	1.78	0.64
4:B:23:GLN:HG3	4:B:91:SER:CB	2.28	0.64
2:D:182:LYS:H	2:D:182:LYS:CD	2.11	0.64
1:C:135:THR:HG23	1:C:136:SER:O	1.98	0.63
4:B:158:ASN:HA	4:B:203:HIS:CE1	2.33	0.63
4:B:221:GLN:HG3	4:B:222:ASP:N	2.13	0.62
2:D:-25:PHE:CZ	2:D:89:HIS:CD2	2.88	0.62
1:C:135:THR:HG22	1:C:148:LEU:H	1.65	0.61
3:A:36:GLN:HG3	3:A:88:TYR:CE1	2.36	0.61
4:B:169:ASP:HB2	4:B:186:LEU:HD12	1.81	0.61
2:D:178:HIS:CG	2:D:179:PRO:HD2	2.36	0.60
2:D:37:TYR:CD2	2:D:38:VAL:HG23	2.36	0.59
4:B:18:THR:HB	4:B:75:ILE:HD12	1.85	0.58
1:C:30:GLU:HB3	1:C:44:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PHE:CG	2:D:34:ARG:HD2	2.39	0.58
3:A:159:CYS:HB2	4:B:189:ARG:NH2	2.19	0.58
2:D:178:HIS:CD2	2:D:179:PRO:HD2	2.38	0.58
3:A:194:PRO:HB2	3:A:196:ASP:OD1	2.04	0.58
3:A:135:LEU:HD11	3:A:172:SER:HB2	1.84	0.57
1:C:113:PHE:CZ	2:D:34:ARG:HG3	2.39	0.57
3:A:58:GLU:HG3	3:A:63:THR:HG22	1.87	0.57
2:D:28:THR:O	2:D:39:ARG:HB2	2.06	0.56
1:C:123:ARG:HB3	1:C:128:VAL:HG21	1.87	0.56
1:C:175:LEU:N	1:C:175:LEU:CD1	2.67	0.56
1:C:0:ILE:HD12	1:C:0:ILE:N	2.21	0.56
2:D:83:TYR:CZ	2:D:92:LEU:HD21	2.41	0.56
4:B:58:ILE:HG13	4:B:58:ILE:O	2.07	0.55
2:D:36:GLU:OE1	2:D:39:ARG:HD3	2.07	0.54
1:C:121:TRP:CG	1:C:151:LEU:HD22	2.43	0.54
2:D:182:LYS:HD2	2:D:182:LYS:N	2.22	0.54
2:D:28:THR:HB	2:D:40:TYR:HB3	1.89	0.54
2:D:104:LEU:HD21	2:D:108:GLU:HB2	1.88	0.54
2:D:-25:PHE:CE2	2:D:89:HIS:CD2	2.91	0.53
2:D:66:GLU:HG3	4:B:97:ASP:OD2	2.09	0.52
4:B:74:LEU:C	4:B:75:ILE:HD13	2.30	0.52
3:A:111:PRO:CG	3:A:160:VAL:HG21	2.40	0.52
4:B:118:PRO:HD3	4:B:226:PRO:HB3	1.91	0.52
1:C:82:ALA:HB1	1:C:113:PHE:HE2	1.74	0.52
2:D:106:ARG:HH12	2:D:107:THR:HG23	1.75	0.51
4:B:123:VAL:HG23	4:B:233:ALA:HB3	1.92	0.51
1:C:102:PRO:HA	1:C:154:ILE:HD13	1.92	0.51
2:D:112:HIS:O	2:D:166:PRO:HD2	2.11	0.50
1:C:11:SER:HG	1:C:22:TYR:HD2	1.60	0.50
3:A:154:TYR:CE1	4:B:175:GLU:HA	2.47	0.50
4:B:198:GLN:HA	4:B:238:ARG:O	2.12	0.49
4:B:169:ASP:HB2	4:B:186:LEU:CD1	2.43	0.49
3:A:31:TYR:HB3	3:A:93:SER:HB3	1.94	0.49
2:D:87:GLU:OE1	2:D:87:GLU:CA	2.61	0.49
2:D:143:VAL:HG22	2:D:162:LEU:HD13	1.95	0.49
4:B:175:GLU:O	4:B:176:GLN:HG3	2.12	0.49
1:C:14:GLN:OE1	1:C:115:PRO:HG2	2.12	0.48
2:D:25:ARG:HD2	2:D:43:ASP:OD1	2.12	0.48
3:A:168:PHE:CE2	4:B:136:LYS:HE2	2.47	0.48
4:B:207:GLN:HG3	4:B:230:ILE:HG23	1.96	0.47
3:A:85:SER:O	3:A:86:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:ILE:HG22	2:D:103:SER:N	2.30	0.47
4:B:24:THR:HG23	4:B:24:THR:O	2.13	0.47
4:B:68:SER:HB3	4:B:71:ASN:H	1.80	0.47
1:C:0:ILE:HG22	1:C:0:ILE:O	2.15	0.47
1:C:29:ASP:HB3	2:D:154:TRP:CE2	2.49	0.47
3:A:174:VAL:HG12	3:A:175:ALA:N	2.30	0.47
4:B:194:ALA:C	4:B:196:PHE:H	2.18	0.46
1:C:96:PRO:HG3	2:D:119:SER:CB	2.44	0.46
3:A:111:PRO:HG2	3:A:160:VAL:HG21	1.98	0.46
3:A:160:VAL:HG22	3:A:171:ASN:OD1	2.16	0.46
4:B:221:GLN:CD	4:B:222:ASP:H	2.19	0.46
1:C:66:VAL:HG22	2:D:9:TYR:CD2	2.51	0.46
2:D:134:ARG:NH1	2:D:139:GLU:OE2	2.49	0.46
3:A:151:SER:O	3:A:152:ASP:CB	2.60	0.45
4:B:33:TYR:CZ	4:B:43:LEU:HD13	2.51	0.45
1:C:123:ARG:HB2	1:C:161:TYR:CE1	2.50	0.45
3:A:161:LEU:C	3:A:161:LEU:HD12	2.37	0.45
4:B:225:LYS:HG2	4:B:227:VAL:HG13	1.97	0.45
2:D:66:GLU:O	2:D:70:ARG:HB2	2.17	0.45
4:B:23:GLN:OE1	4:B:27:HIS:HB2	2.17	0.45
3:A:159:CYS:CB	4:B:189:ARG:NH2	2.81	0.44
1:C:101:GLN:O	1:C:155:PRO:HD2	2.16	0.44
1:C:130:ASP:O	1:C:151:LEU:HD12	2.16	0.44
1:C:122:LEU:HD23	1:C:127:SER:HA	1.98	0.44
2:D:37:TYR:CE2	2:D:38:VAL:HG23	2.53	0.44
4:B:23:GLN:HG3	4:B:91:SER:HB3	1.98	0.44
1:C:135:THR:HG22	1:C:147:LYS:HG3	2.00	0.43
3:A:159:CYS:HB2	4:B:189:ARG:HH21	1.82	0.43
4:B:31:TYR:CD1	4:B:31:TYR:N	2.85	0.43
1:C:1:GLU:CD	1:C:1:GLU:N	2.66	0.43
4:B:219:TRP:CD1	4:B:225:LYS:HB2	2.53	0.43
1:C:26:PHE:CD1	2:D:87:GLU:OE2	2.71	0.43
1:C:138:PHE:HB2	1:C:146:HIS:CD2	2.54	0.43
4:B:203:HIS:HD2	4:B:234:GLU:OE2	2.01	0.43
2:D:114:ASN:C	2:D:164:MET:HE3	2.39	0.42
2:D:33:ASN:O	2:D:34:ARG:HB2	2.19	0.42
2:D:100:VAL:HG21	2:D:185:ILE:HG21	2.00	0.42
1:C:113:PHE:HA	1:C:114:PRO:C	2.39	0.42
1:C:135:THR:HG1	1:C:138:PHE:HE2	1.64	0.42
1:C:82:ALA:HB1	1:C:113:PHE:CE2	2.53	0.42
3:A:161:LEU:HD21	4:B:191:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:GLU:OE1	2:D:29:ARG:NH1	2.53	0.42
4:B:23:GLN:HE21	4:B:23:GLN:HB3	1.61	0.42
2:D:134:ARG:O	2:D:134:ARG:HG3	2.20	0.42
3:A:58:GLU:HG3	3:A:63:THR:CG2	2.49	0.41
4:B:200:PRO:HA	4:B:237:GLY:O	2.20	0.41
2:D:97:GLN:HA	2:D:98:PRO:HD3	1.90	0.41
2:D:181:LEU:HD23	2:D:181:LEU:HA	1.91	0.41
3:A:133:VAL:HG22	3:A:176:TRP:HB3	2.02	0.41
3:A:200:PRO:O	3:A:201:SER:CB	2.68	0.41
4:B:50:ALA:HA	4:B:66:ARG:HG3	2.02	0.41
3:A:56:LYS:HD2	3:A:65:PHE:CE1	2.56	0.41
2:D:109:ALA:O	2:D:112:HIS:HB2	2.20	0.41
1:C:50:GLN:NE2	1:C:50:GLN:HA	2.36	0.41
2:D:26:TYR:HB3	2:D:42:SER:HB3	2.02	0.41
2:D:115:THR:CB	2:D:163:GLU:OE1	2.60	0.41
3:A:20:LEU:HD23	3:A:88:TYR:HB2	2.02	0.41
1:C:135:THR:HG21	1:C:148:LEU:H	1.82	0.41
3:A:70:GLU:O	3:A:71:LYS:C	2.60	0.41
4:B:188:SER:C	4:B:189:ARG:HD3	2.40	0.41
3:A:156:THR:HG21	4:B:187:SER:OG	2.21	0.40
3:A:49:ILE:HD13	3:A:66:PHE:HB2	2.03	0.40
1:C:44:MET:HG2	2:D:154:TRP:CD1	2.56	0.40
1:C:110:ASP:OD1	1:C:146:HIS:HB3	2.22	0.40
2:D:82:ASN:O	2:D:87:GLU:HB2	2.22	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	C	177/182 (97%)	172 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	195/217 (90%)	189 (97%)	6 (3%)	0	100 100
3	A	197/205 (96%)	184 (93%)	11 (6%)	2 (1%)	15 37
4	B	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	34 60
All	All	805/845 (95%)	772 (96%)	30 (4%)	3 (0%)	34 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	129	SER
3	A	152	ASP
4	B	113	LEU

### 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	C	154/163 (94%)	144 (94%)	10 (6%)	17 38
2	D	175/189 (93%)	162 (93%)	13 (7%)	13 32
3	A	163/183 (89%)	156 (96%)	7 (4%)	29 57
4	B	196/206 (95%)	185 (94%)	11 (6%)	21 45
All	All	688/741 (93%)	647 (94%)	41 (6%)	19 42

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	GLU
1	C	15	SER
1	C	18	ASP
1	C	36	LEU
1	C	45	LEU
1	C	66	VAL
1	C	98	LEU
1	C	135	THR

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Mol	Chain	Res	Type
1	C	171	GLU
1	C	175	LEU
2	D	-21	LYS
2	D	-14	VAL
2	D	25	ARG
2	D	28	THR
2	D	53	LEU
2	D	87	GLU
2	D	92	LEU
2	D	95	LEU
2	D	107	THR
2	D	115	THR
2	D	164	MET
2	D	176	VAL
2	D	182	LYS
3	A	9	SER
3	A	11	THR
3	A	23	SER
3	A	63	THR
3	A	93	SER
3	A	189	ASN
3	A	192	ILE
4	B	18	THR
4	B	23	GLN
4	B	24	THR
4	B	26	ASN
4	B	37	THR
4	B	77	GLU
4	B	108	SER
4	B	167	CYS
4	B	180	ASN
4	B	189	ARG
4	B	195	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	50	GLN
2	D	6	HIS
2	D	89	HIS
2	D	137	GLN
3	A	189	ASN

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Mol	Chain	Res	Type
4	B	203	HIS

### 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 [\(i\)](#)

There are no ligands in this entry.

### 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 [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

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	C	179/182 (98%)	-0.09	1 (0%) 89 91	23, 43, 77, 107	0
2	D	199/217 (91%)	-0.05	4 (2%) 65 67	23, 45, 79, 103	0
3	A	199/205 (97%)	0.03	13 (6%) 18 17	25, 54, 106, 163	0
4	B	238/241 (98%)	-0.08	9 (3%) 40 39	25, 48, 88, 129	0
All	All	815/845 (96%)	-0.05	27 (3%) 46 46	23, 48, 91, 163	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	178	ALA	4.8
4	B	180	ASN	4.1
4	B	179	LEU	4.0
2	D	168	ARG	3.7
3	A	192	ILE	3.6
3	A	129	SER	3.6
3	A	191	SER	3.5
3	A	194	PRO	3.3
3	A	130	ASP	3.2
2	D	19	ASN	3.2
3	A	114	GLN	3.0
3	A	189	ASN	2.7
4	B	177	PRO	2.4
3	A	196	ASP	2.4
3	A	166	MET	2.4
4	B	181	ASP	2.3
2	D	169	GLY	2.3
3	A	199	PHE	2.3
4	B	218	GLU	2.2
4	B	216	ASN	2.2
2	D	171	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	193	ILE	2.2
3	A	195	GLU	2.1
3	A	190	ASN	2.1
4	B	214	SER	2.1
1	C	158	ASP	2.1
4	B	217	ASP	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 [\(i\)](#)

There are no ligands in this entry.

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.