Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:30 PM BST

PDB ID	:	6DFS
Title	:	mouse TCR I.29 in complex with IAg7-p8E9E6ss
Authors	:	Wang, Y.; Dai, S.
Deposited on	:	2018-05-15
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

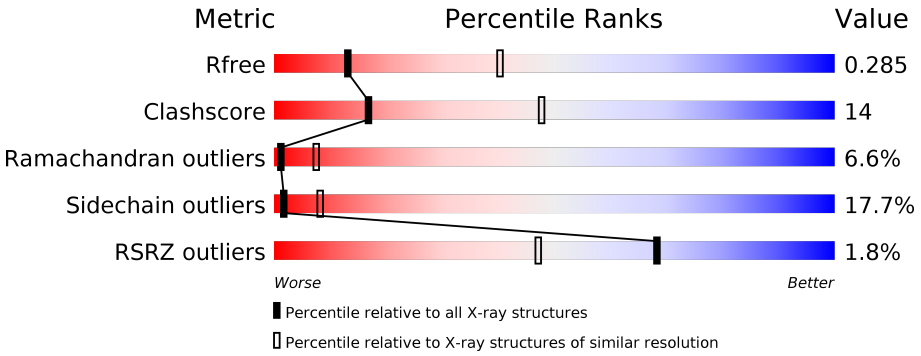
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 >=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	210	56% 33% 9% •
2	B	242	% 56% 32% 10% •
3	C	183	% 58% 32% 8% ••
4	D	215	5% 34% 31% 5% 30%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6260 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 mouse TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1606	1004	269	325	8			

- Molecule 2 is a protein called mouse TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1922	1217	335	361	9			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	181	Total	C	N	O	S	0	0	0
			1449	939	234	273	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	64	CYS	ASN	conflict	UNP P04228

- Molecule 4 is a protein called H2-Ab1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	150	Total	C	N	O	S	0	1	0
			1250	787	222	234	7			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-28	HIS	-	expression tag	UNP Q31135
D	-27	LEU	-	expression tag	UNP Q31135
D	-26	VAL	-	expression tag	UNP Q31135

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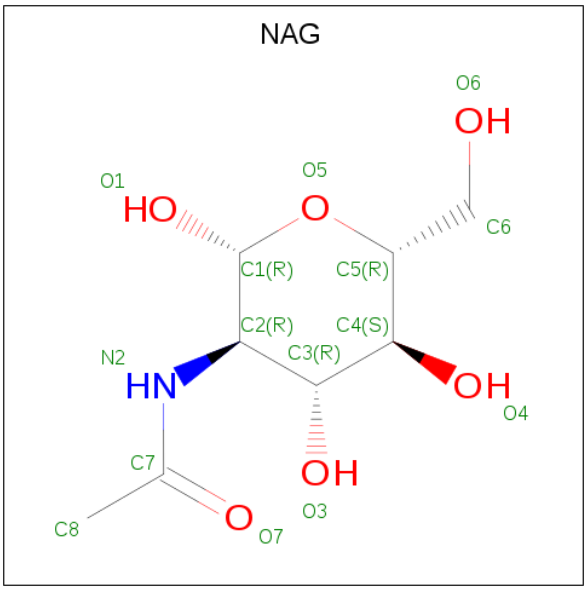
Chain	Residue	Modelled	Actual	Comment	Reference
D	-25	GLU	-	expression tag	UNP Q31135
D	-24	ARG	-	expression tag	UNP Q31135
D	-23	LEU	-	expression tag	UNP Q31135
D	-22	TYR	-	expression tag	UNP Q31135
D	-21	LEU	-	expression tag	UNP Q31135
D	-20	VAL	-	expression tag	UNP Q31135
D	-19	CYS	-	expression tag	UNP Q31135
D	-18	GLY	-	expression tag	UNP Q31135
D	-17	GLU	-	expression tag	UNP Q31135
D	-16	GLU	-	expression tag	UNP Q31135
D	-15	GLY	-	expression tag	UNP Q31135
D	-14	ALA	-	expression tag	UNP Q31135
D	-8	GLY	-	expression tag	UNP Q31135
D	-7	GLY	-	expression tag	UNP Q31135
D	-6	GLY	-	expression tag	UNP Q31135
D	-5	SER	-	expression tag	UNP Q31135
D	-4	LEU	-	expression tag	UNP Q31135
D	-3	VAL	-	expression tag	UNP Q31135
D	-2	GLY	-	expression tag	UNP Q31135
D	-1	GLY	-	expression tag	UNP Q31135
D	0	SER	-	expression tag	UNP Q31135
D	1	GLY	-	expression tag	UNP Q31135
D	2	GLY	-	expression tag	UNP Q31135
D	3	GLY	-	expression tag	UNP Q31135

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

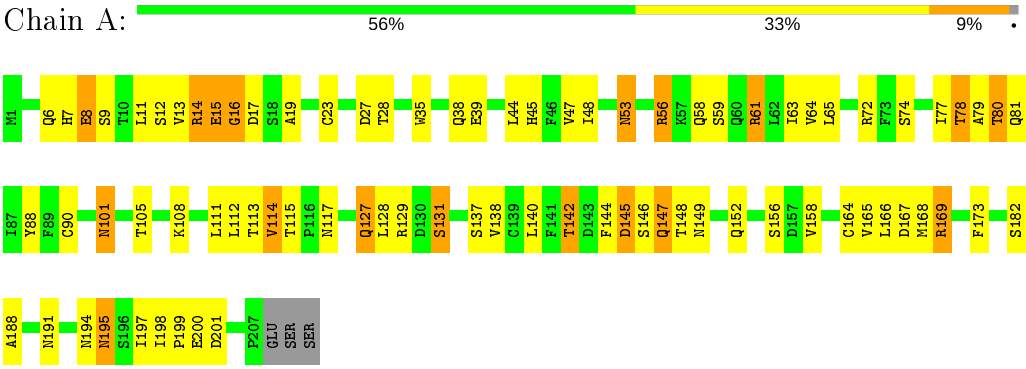
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	4	Total	O	0	0
			4	4		
6	C	6	Total	O	0	0
			6	6		
6	D	3	Total	O	0	0
			3	3		

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.

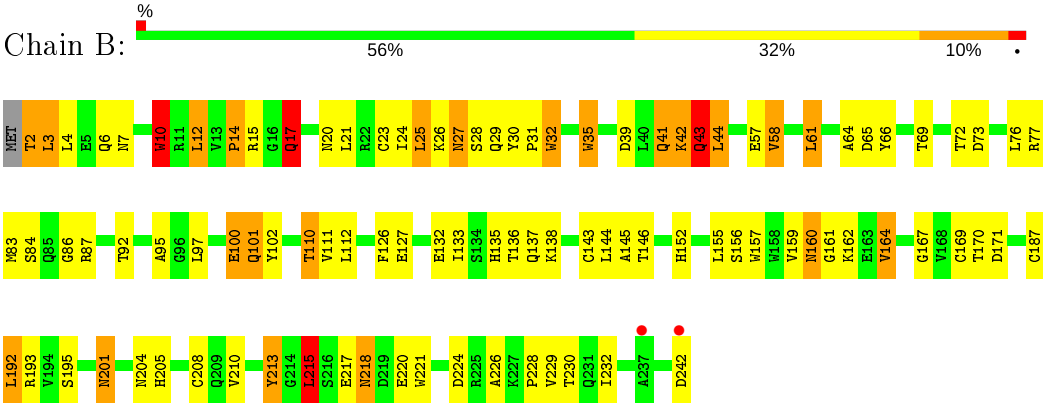
- Molecule 1: mouse TCR alpha chain

Chain A:



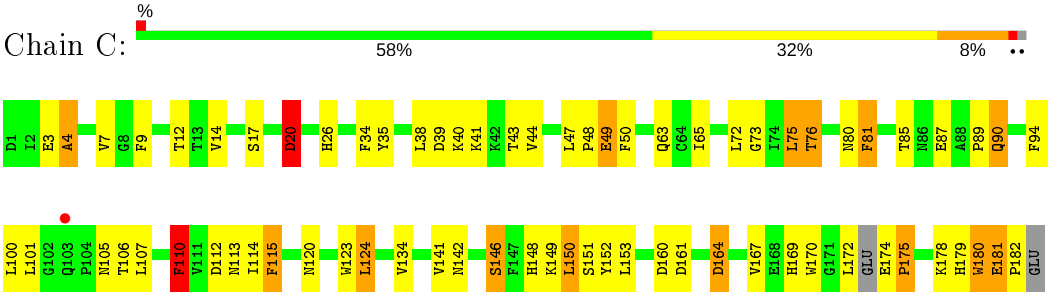
- Molecule 2: mouse TCR beta chain

Chain B:



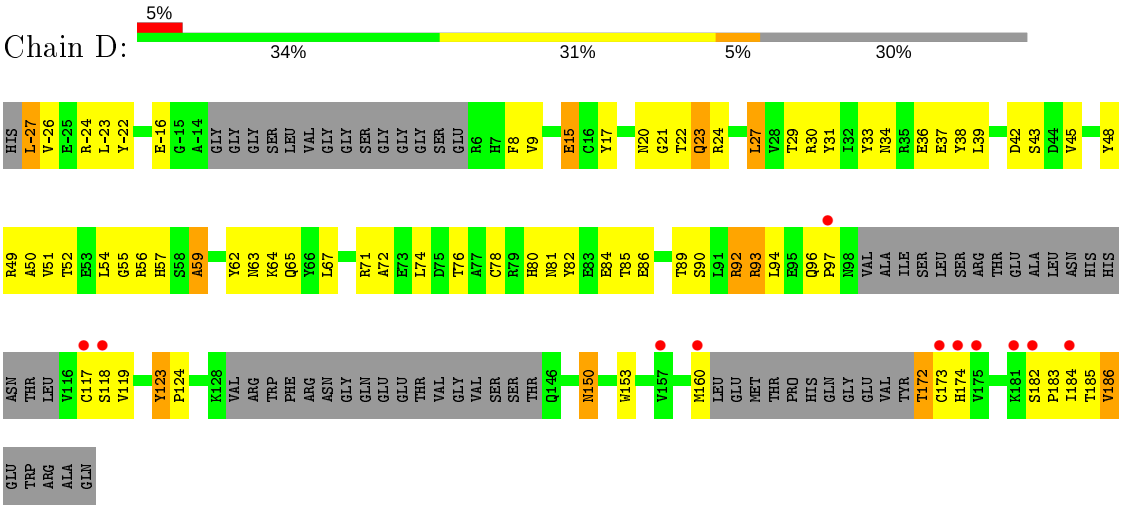
- Molecule 3: H-2 class II histocompatibility antigen, A-D alpha chain

Chain C:



- Molecule 4: H2-Ab1 protein

Chain D:


5%
34%
31%
5%
30%
HIS L-27 V-26 E-25 R-24 L-23 Y-22 E-16 G-15 A-14 GLY GLY GLY SER LEU VAL GLY GLY SER GLY GLY GLY SER GLU R6 H7 F8 V9 E15 C16 Y17 N20 G21 T22 Q23 R24 L27 V28 T29 R30 Y31 I32 Y33 N34 R35 E36 E37 Y38 L39 D42 S43 D44 V45 Y48
R49 A50 V51 T52 E53 L54 G55 R56 H57 S58 A59 Y62 N63 K64 Q65 Y66 L67 R71 A72 E73 L74 D75 T76 A77 C78 R79 H80 N81 Y82 E83 E84 T85 E86 T89 S90 L91 R92 R93 L94 E95 Q96 P97 N98 VAL ALA ILE SER LEU SER ARG THR GLU ALA LEU ASN HIS HIS
ASN THR LEU V116 C117 S118 V119 Y123 P124 K128 VAL ARG TRP PHE ARG ASN GLY GLN GLU GLU THR VAL GLY VAL SER SER THR Q146 N150 W153 V157 M160 LEU GLU MET THR PRO HIS GLN GLY GLU VAL TYR T172 C173 H174 V175 K181 S182 P183 I184 T185 V186
GLU TRP ARG ALA GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	269.52Å 269.52Å 45.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 3.10 46.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.01-3.10) 96.2 (46.68-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.240 , 0.285 0.244 , 0.285	Depositor DCC
R_{free} test set	1713 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6260	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: NAG

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	0.95	0/1640	1.11	3/2225 (0.1%)
2	B	0.82	2/1975 (0.1%)	1.02	2/2698 (0.1%)
3	C	0.81	0/1494	0.96	2/2042 (0.1%)
4	D	0.88	0/1275	1.00	2/1722 (0.1%)
All	All	0.86	2/6384 (0.0%)	1.03	9/8687 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
3	C	0	2
4	D	0	3
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	10	TRP	CB-CG	6.51	1.61	1.50
2	B	32	TRP	CB-CG	-5.84	1.39	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	-27	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	61	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	101	ASN	CB-CA-C	-5.58	99.24	110.40
2	B	215	LEU	CA-CB-CG	5.57	128.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	20	ASP	CB-CA-C	5.40	121.20	110.40
2	B	77	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	72	ARG	NE-CZ-NH2	5.32	122.96	120.30
4	D	123	TYR	C-N-CD	-5.09	109.41	120.60
3	C	110	PHE	CB-CG-CD1	5.05	124.34	120.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ALA	Peptide
1	A	39	GLU	Peptide
1	A	65	LEU	Peptide
3	C	178	LYS	Peptide
3	C	20	ASP	Peptide
4	D	21	GLY	Peptide
4	D	49	ARG	Peptide
4	D	92	ARG	Peptide

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	1606	0	1527	44	0
2	B	1922	0	1823	64	0
3	C	1449	0	1372	40	0
4	D	1250	0	1188	38	0
5	C	14	0	13	0	0
6	A	6	0	0	1	0
6	B	4	0	0	0	0
6	C	6	0	0	0	0
6	D	3	0	0	0	0
All	All	6260	0	5923	172	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 14.

All (172) 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)
1:A:6:GLN:HG2	1:A:23:CYS:SG	2.19	0.82
3:C:87:GLU:HB3	3:C:113:ASN:HD21	1.47	0.78
1:A:56:ARG:NH1	1:A:58:GLN:OE1	2.18	0.77
4:D:30:ARG:NH1	4:D:37:GLU:OE1	2.17	0.75
4:D:50:ALA:HB2	4:D:55:GLY:O	1.88	0.74
4:D:123:TYR:CD1	4:D:124:PRO:HA	2.26	0.70
4:D:64:LYS:O	4:D:65:GLN:HG2	1.92	0.68
1:A:14:ARG:O	1:A:15:GLU:O	2.12	0.66
3:C:149:LYS:O	3:C:150:LEU:HD12	1.95	0.66
4:D:81:ASN:O	4:D:85:THR:OG1	2.14	0.65
4:D:-24:ARG:NH1	4:D:86:GLU:OE2	2.30	0.65
1:A:77:ILE:HD11	1:A:88:TYR:CE2	2.31	0.64
2:B:218:ASN:HD22	2:B:218:ASN:C	2.01	0.63
1:A:140:LEU:HD22	1:A:142:THR:OG1	1.99	0.62
2:B:3:LEU:HD11	2:B:30:TYR:CD2	2.34	0.62
1:A:7:HIS:O	1:A:8:GLU:HG2	1.99	0.62
1:A:61:ARG:O	1:A:78:THR:HB	2.00	0.62
3:C:38:LEU:HD13	3:C:65:ILE:HG13	1.83	0.61
4:D:174:HIS:HA	4:D:185:THR:HG22	1.83	0.60
2:B:215:LEU:HD12	2:B:229:VAL:HA	1.81	0.60
4:D:43:SER:HB2	4:D:74:LEU:HD12	1.83	0.59
4:D:64:LYS:O	4:D:65:GLN:CG	2.50	0.59
1:A:173:PHE:CE2	2:B:138:LYS:HE3	2.38	0.59
3:C:20:ASP:O	3:C:20:ASP:OD1	2.19	0.59
2:B:110:THR:OG1	2:B:152:HIS:NE2	2.37	0.58
2:B:14:PRO:O	2:B:17:GLN:HB2	2.03	0.57
1:A:53:ASN:OD1	1:A:53:ASN:N	2.37	0.57
1:A:13:VAL:O	1:A:114:VAL:HA	2.04	0.57
2:B:27:ASN:OD1	2:B:27:ASN:C	2.43	0.57
2:B:213:TYR:HA	2:B:230:THR:HG23	1.85	0.56
2:B:35:TRP:CE2	2:B:78:LEU:HB2	2.41	0.56
2:B:155:LEU:HD12	2:B:210:VAL:HG22	1.86	0.56
3:C:112:ASP:OD1	3:C:113:ASN:N	2.37	0.55
3:C:181:GLU:CB	3:C:182:PRO:CD	2.85	0.55
4:D:94:LEU:HD22	4:D:124:PRO:HD2	1.89	0.55
3:C:169:HIS:CG	3:C:170:TRP:H	2.25	0.55
2:B:157:TRP:CE3	2:B:192:LEU:HD23	2.42	0.54
2:B:35:TRP:CE2	2:B:76:LEU:HD23	2.43	0.54
1:A:198:ILE:HB	1:A:199:PRO:HD2	1.89	0.54
3:C:174:GLU:N	3:C:175:PRO:HD2	2.23	0.54
1:A:138:VAL:HG13	2:B:126:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:ASN:HB2	3:C:146:SER:OG	2.08	0.53
2:B:4:LEU:HD22	2:B:23:CYS:SG	2.49	0.53
1:A:45:HIS:HB2	6:A:306:HOH:O	2.08	0.53
1:A:7:HIS:O	1:A:8:GLU:CG	2.56	0.53
3:C:7:VAL:HG22	4:D:17:TYR:HD1	1.74	0.53
4:D:36:GLU:HG2	4:D:52:THR:HG21	1.91	0.53
2:B:41:GLN:C	2:B:42:LYS:O	2.47	0.53
3:C:87:GLU:CB	3:C:113:ASN:HD21	2.20	0.52
3:C:35:TYR:CE2	3:C:44:VAL:HG11	2.45	0.52
3:C:38:LEU:CD1	3:C:65:ILE:HG13	2.40	0.52
4:D:27:LEU:HD12	4:D:78:CYS:SG	2.49	0.52
3:C:80:ASN:O	3:C:81:PHE:HB2	2.09	0.52
1:A:80:THR:HB	1:A:114:VAL:HG21	1.91	0.52
1:A:173:PHE:CE2	2:B:138:LYS:CE	2.93	0.52
2:B:65:ASP:OD2	2:B:82:ASN:ND2	2.42	0.52
3:C:134:VAL:HA	3:C:152:TYR:O	2.09	0.52
2:B:61:LEU:O	2:B:64:ALA:O	2.28	0.51
4:D:50:ALA:CB	4:D:55:GLY:O	2.58	0.51
4:D:42:ASP:HB3	4:D:45:VAL:HG23	1.93	0.51
3:C:114:ILE:O	3:C:115:PHE:HB2	2.11	0.51
2:B:42:LYS:O	2:B:43:GLN:CB	2.58	0.50
3:C:142:ASN:OD1	3:C:148:HIS:ND1	2.38	0.50
1:A:165:VAL:O	2:B:169:CYS:SG	2.70	0.50
2:B:2:THR:O	2:B:4:LEU:N	2.44	0.50
2:B:42:LYS:O	2:B:43:GLN:HB3	2.12	0.50
1:A:61:ARG:NH2	1:A:84:ASP:OD2	2.44	0.50
3:C:63:GLN:OE1	4:D:-22:TYR:OH	2.19	0.49
3:C:47:LEU:HD11	4:D:153:TRP:CD1	2.47	0.49
4:D:48:TYR:CD2	4:D:62:TYR:HB3	2.47	0.49
1:A:6:GLN:CG	1:A:23:CYS:SG	2.95	0.49
2:B:10:TRP:CZ3	2:B:213:TYR:CE1	3.00	0.49
2:B:41:GLN:O	2:B:42:LYS:O	2.30	0.49
1:A:35:TRP:CZ3	1:A:90:CYS:HB3	2.47	0.49
2:B:32:TRP:CH2	2:B:97:LEU:HD21	2.48	0.49
4:D:150:ASN:OD1	4:D:150:ASN:N	2.44	0.49
2:B:12:LEU:HD22	2:B:112:LEU:HD22	1.95	0.48
1:A:195:ASN:N	1:A:195:ASN:OD1	2.46	0.48
1:A:16:GLY:HA2	1:A:79:ALA:HA	1.96	0.48
2:B:201:ASN:HD21	2:B:204:ASN:ND2	2.12	0.48
2:B:159:VAL:HG23	2:B:164:VAL:HG11	1.96	0.48
1:A:168:MET:HA	1:A:169:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:TYR:HB2	4:D:39:LEU:HB3	1.95	0.47
3:C:76:THR:HA	4:D:33:TYR:OH	2.14	0.47
4:D:59:ALA:O	4:D:63:ASN:ND2	2.47	0.47
2:B:192:LEU:C	2:B:192:LEU:HD12	2.35	0.47
1:A:168:MET:CE	2:B:193:ARG:O	2.63	0.47
2:B:39:ASP:C	2:B:39:ASP:OD1	2.52	0.47
3:C:167:VAL:O	3:C:167:VAL:HG12	2.15	0.47
2:B:20:ASN:HB3	2:B:79:GLN:HA	1.96	0.47
3:C:180:TRP:CD1	3:C:181:GLU:N	2.82	0.47
3:C:34:PHE:CD2	3:C:43:THR:HG23	2.49	0.47
4:D:172:THR:HG22	4:D:186:VAL:C	2.35	0.47
1:A:168:MET:HA	1:A:169:ARG:CB	2.45	0.46
1:A:127:GLN:C	1:A:128:LEU:HD12	2.35	0.46
4:D:63:ASN:HA	4:D:67:LEU:HB2	1.96	0.46
1:A:158:VAL:HG22	1:A:182:SER:HB2	1.96	0.46
3:C:123:TRP:CG	3:C:153:LEU:HD22	2.51	0.46
1:A:80:THR:CG2	1:A:114:VAL:HG21	2.45	0.46
2:B:100:GLU:HG3	2:B:102:TYR:CE1	2.51	0.45
4:D:82:TYR:C	4:D:82:TYR:CD1	2.89	0.45
2:B:26:LYS:O	2:B:27:ASN:HB2	2.16	0.45
3:C:114:ILE:HG22	3:C:115:PHE:N	2.31	0.45
4:D:97:PRO:HB3	4:D:119:VAL:HG22	1.98	0.45
2:B:10:TRP:CE3	2:B:213:TYR:CE1	3.04	0.45
2:B:221:TRP:CZ2	2:B:228:PRO:HD3	2.52	0.45
4:D:67:LEU:O	4:D:71:ARG:HG3	2.17	0.45
1:A:82:PRO:HA	1:A:114:VAL:HG12	1.99	0.45
2:B:100:GLU:HG3	2:B:102:TYR:CZ	2.52	0.44
2:B:92:THR:OG1	2:B:101:GLN:HG3	2.16	0.44
3:C:110:PHE:C	3:C:110:PHE:CD1	2.91	0.44
3:C:169:HIS:CG	3:C:170:TRP:N	2.86	0.44
4:D:72:ALA:O	4:D:76:THR:HG23	2.17	0.44
2:B:35:TRP:CE2	2:B:76:LEU:CD2	3.00	0.44
1:A:47:VAL:HG12	1:A:48:ILE:HG22	2.00	0.44
2:B:171:ASP:HB2	2:B:188:LEU:CD1	2.47	0.44
1:A:44:LEU:HD21	2:B:44:LEU:HD21	2.00	0.44
2:B:26:LYS:O	2:B:27:ASN:CB	2.63	0.44
2:B:27:ASN:OD1	2:B:28:SER:N	2.51	0.44
4:D:67:LEU:CD1	4:D:71:ARG:HD2	2.47	0.44
1:A:147:GLN:OE1	1:A:147:GLN:HA	2.17	0.44
3:C:172:LEU:O	3:C:172:LEU:HD12	2.17	0.44
2:B:145:ALA:HB3	2:B:188:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:HIS:HB2	3:C:34:PHE:CE1	2.52	0.43
4:D:89:THR:OG1	4:D:90:SER:N	2.52	0.43
2:B:110:THR:HG1	2:B:152:HIS:HE2	1.59	0.43
2:B:170:THR:HG22	2:B:171:ASP:N	2.34	0.43
3:C:181:GLU:CB	3:C:182:PRO:HD2	2.48	0.43
2:B:160:ASN:O	2:B:162:LYS:N	2.51	0.43
2:B:35:TRP:NE1	2:B:78:LEU:HB2	2.32	0.43
2:B:58:VAL:HA	2:B:66:TYR:O	2.19	0.43
4:D:-26:VAL:HG11	4:D:84:GLU:O	2.19	0.43
2:B:12:LEU:HD22	2:B:112:LEU:HB2	2.01	0.42
2:B:171:ASP:HB2	2:B:188:LEU:HD12	2.00	0.42
3:C:9:PHE:CE1	4:D:15:GLU:HG3	2.54	0.42
1:A:131:SER:HB2	2:B:127:GLU:OE2	2.19	0.42
4:D:-23:LEU:HD12	4:D:80:HIS:CD2	2.54	0.42
2:B:25:LEU:HD21	2:B:30:TYR:O	2.19	0.42
3:C:124:LEU:HB2	3:C:164:ASP:HB3	2.00	0.42
2:B:189:SER:OG	2:B:191:ARG:NH2	2.47	0.42
1:A:80:THR:CB	1:A:114:VAL:HG21	2.50	0.42
2:B:143:CYS:SG	2:B:208:CYS:SG	3.17	0.42
3:C:174:GLU:N	3:C:175:PRO:CD	2.83	0.42
2:B:132:GLU:O	2:B:136:THR:OG1	2.31	0.41
2:B:31:PRO:HD2	2:B:95:ALA:HA	2.02	0.41
2:B:84:SER:O	2:B:111:VAL:HG21	2.20	0.41
1:A:44:LEU:N	1:A:44:LEU:HD12	2.35	0.41
3:C:142:ASN:ND2	3:C:146:SER:OG	2.38	0.41
2:B:145:ALA:O	2:B:187:CYS:HA	2.21	0.41
4:D:93:ARG:NH1	4:D:153:TRP:HB3	2.36	0.41
1:A:167:ASP:O	2:B:167:GLY:N	2.53	0.41
1:A:38:GLN:O	1:A:86:ALA:HB1	2.20	0.41
4:D:-22:TYR:CG	4:D:-22:TYR:O	2.73	0.41
1:A:111:LEU:HD23	1:A:112:LEU:N	2.36	0.41
3:C:47:LEU:O	3:C:49:GLU:N	2.53	0.41
2:B:27:ASN:OD1	2:B:29:GLN:N	2.47	0.41
2:B:218:ASN:ND2	2:B:218:ASN:C	2.72	0.41
3:C:105:ASN:OD1	3:C:106:THR:N	2.52	0.41
2:B:2:THR:HG23	2:B:3:LEU:HD23	2.02	0.41
4:D:20:ASN:HB3	4:D:23:GLN:HG3	2.03	0.41
1:A:191:ASN:O	1:A:194:ASN:HB2	2.21	0.40
1:A:19:ALA:CB	1:A:112:LEU:HD11	2.51	0.40
1:A:81:GLN:O	1:A:83:GLU:N	2.54	0.40
3:C:72:LEU:O	3:C:75:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:GLU:O	3:C:4:ALA:CB	2.69	0.40
1:A:15:GLU:O	1:A:17:ASP:N	2.55	0.40
3:C:150:LEU:HB3	3:C:152:TYR:HE1	1.86	0.40
3:C:75:LEU:HD11	4:D:38:TYR:CE1	2.57	0.40
1:A:145:ASP:OD1	1:A:145:ASP:C	2.59	0.40
1:A:144:PHE:CD2	1:A:148:THR:HG22	2.56	0.40
2:B:215:LEU:O	2:B:229:VAL:HG23	2.22	0.40
4:D:37:GLU:OE2	4:D:51:VAL:HG21	2.21	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	205/210 (98%)	170 (83%)	24 (12%)	11 (5%)	2 12
2	B	239/242 (99%)	200 (84%)	25 (10%)	14 (6%)	1 10
3	C	177/183 (97%)	135 (76%)	23 (13%)	19 (11%)	0 2
4	D	141/215 (66%)	110 (78%)	25 (18%)	6 (4%)	2 16
All	All	762/850 (90%)	615 (81%)	97 (13%)	50 (7%)	1 7

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	101	ASN
1	A	169	ARG
1	A	187	PHE
1	A	200	GLU
2	B	3	LEU
2	B	43	GLN

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Mol	Chain	Res	Type
2	B	161	GLY
2	B	226	ALA
3	C	4	ALA
3	C	48	PRO
3	C	81	PHE
3	C	89	PRO
3	C	175	PRO
3	C	180	TRP
3	C	181	GLU
4	D	22	THR
4	D	24	ARG
4	D	183	PRO
1	A	16	GLY
1	A	152	GLN
2	B	27	ASN
2	B	42	LYS
2	B	73	ASP
2	B	86	GLY
2	B	137	GLN
3	C	95	PRO
3	C	101	LEU
3	C	146	SER
1	A	8	GLU
2	B	100	GLU
2	B	160	ASN
3	C	90	GLN
4	D	184	ILE
1	A	131	SER
1	A	184	LYS
2	B	17	GLN
3	C	20	ASP
3	C	41	LYS
3	C	115	PHE
4	D	59	ALA
3	C	12	THR
3	C	73	GLY
3	C	85	THR
3	C	96	LYS
3	C	179	HIS
4	D	34	ASN
1	A	82	PRO
2	B	14	PRO

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Mol	Chain	Res	Type
2	B	133	ILE

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	182/189 (96%)	147 (81%)	35 (19%)	1 6
2	B	205/213 (96%)	164 (80%)	41 (20%)	1 5
3	C	160/165 (97%)	137 (86%)	23 (14%)	3 14
4	D	136/188 (72%)	114 (84%)	22 (16%)	2 10
All	All	683/755 (90%)	562 (82%)	121 (18%)	2 8

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	11	LEU
1	A	12	SER
1	A	14	ARG
1	A	27	ASP
1	A	28	THR
1	A	53	ASN
1	A	56	ARG
1	A	59	SER
1	A	63	ILE
1	A	64	VAL
1	A	74	SER
1	A	78	THR
1	A	80	THR
1	A	105	THR
1	A	108	LYS
1	A	113	THR
1	A	114	VAL
1	A	115	THR
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	127	GLN
1	A	129	ARG
1	A	137	SER
1	A	142	THR
1	A	145	ASP
1	A	146	SER
1	A	147	GLN
1	A	149	ASN
1	A	156	SER
1	A	164	CYS
1	A	166	LEU
1	A	185	SER
1	A	195	ASN
1	A	197	ILE
1	A	201	ASP
2	B	2	THR
2	B	6	GLN
2	B	7	ASN
2	B	10	TRP
2	B	12	LEU
2	B	15	ARG
2	B	17	GLN
2	B	21	LEU
2	B	24	ILE
2	B	25	LEU
2	B	35	TRP
2	B	41	GLN
2	B	43	GLN
2	B	44	LEU
2	B	57	GLU
2	B	58	VAL
2	B	61	LEU
2	B	69	THR
2	B	72	THR
2	B	83	MET
2	B	87	ARG
2	B	101	GLN
2	B	110	THR
2	B	135	HIS
2	B	144	LEU
2	B	146	THR
2	B	156	SER

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Mol	Chain	Res	Type
2	B	164	VAL
2	B	191	ARG
2	B	192	LEU
2	B	195	SER
2	B	201	ASN
2	B	205	HIS
2	B	213	TYR
2	B	215	LEU
2	B	217	GLU
2	B	218	ASN
2	B	220	GLU
2	B	224	ASP
2	B	232	ILE
2	B	242	ASP
3	C	14	VAL
3	C	17	SER
3	C	20	ASP
3	C	39	ASP
3	C	40	LYS
3	C	49	GLU
3	C	50	PHE
3	C	75	LEU
3	C	76	THR
3	C	90	GLN
3	C	94	PHE
3	C	97	SER
3	C	100	LEU
3	C	107	LEU
3	C	110	PHE
3	C	120	ASN
3	C	124	LEU
3	C	141	VAL
3	C	150	LEU
3	C	151	SER
3	C	160	ASP
3	C	161	ASP
3	C	164	ASP
4	D	-27	LEU
4	D	-16	GLU
4	D	8	PHE
4	D	9	VAL
4	D	15	GLU

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Mol	Chain	Res	Type
4	D	23	GLN
4	D	27	LEU
4	D	29	THR
4	D	54	LEU
4	D	56	ARG
4	D	57	HIS
4	D	92	ARG
4	D	93	ARG
4	D	96	GLN
4	D	117	CYS
4	D	118	SER
4	D	150	ASN
4	D	160	MET
4	D	172	THR
4	D	173	CYS
4	D	182	SER
4	D	186	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	194	ASN
2	B	41	GLN
2	B	43	GLN
2	B	204	ASN
2	B	218	ASN
3	C	16	GLN
3	C	90	GLN
3	C	113	ASN
3	C	179	HIS
4	D	65	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
5	NAG	C	201	3	14,14,15	1.15	1 (7%)	17,19,21	1.69	3 (17%)

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
5	NAG	C	201	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	NAG	C1-C2	2.99	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	201	NAG	O5-C5-C6	4.03	113.52	107.20
5	C	201	NAG	C2-N2-C7	3.45	127.81	122.90
5	C	201	NAG	O7-C7-N2	2.10	125.81	121.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	201	NAG	O5-C5-C6-O6
5	C	201	NAG	C4-C5-C6-O6

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	207/210 (98%)	-0.48	0 100 100	17, 46, 99, 128	0
2	B	241/242 (99%)	-0.30	2 (0%) 86 72	20, 66, 119, 131	0
3	C	181/183 (98%)	-0.29	1 (0%) 89 78	24, 72, 125, 145	0
4	D	150/215 (69%)	0.20	11 (7%) 15 6	25, 80, 141, 151	0
All	All	779/850 (91%)	-0.25	14 (1%) 68 47	17, 66, 127, 151	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	157	VAL	3.9
4	D	175	VAL	3.4
4	D	118	SER	3.3
4	D	117	CYS	2.7
4	D	181	LYS	2.6
2	B	242	ASP	2.6
4	D	184	ILE	2.6
4	D	182	SER	2.4
4	D	174	HIS	2.3
4	D	173	CYS	2.3
4	D	97	PRO	2.2
4	D	160	MET	2.2
2	B	237	ALA	2.1
3	C	103	GLN	2.1

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 (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
5	NAG	C	201	14/15	0.89	0.15	67,77,81,86	0

6.5 Other polymers (i)

There are no such residues in this entry.