



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:05 am BST

PDB ID : 6DFV
Title : Mouse diabetogenic TCR 8F10
Authors : Wang, Y.; Dai, S.
Deposited on : 2018-05-15
Resolution : 1.71 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 : 2.11
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) : 2.11

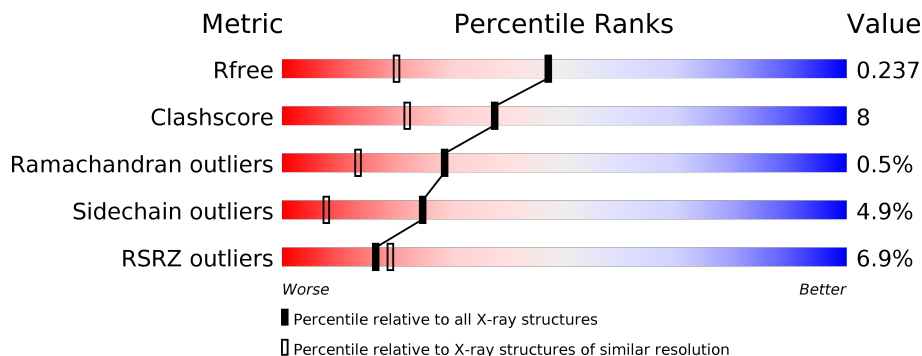
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	210	 13% 69% 14% 6% • 10%
1	C	210	 8% 79% 13% • 5%
2	B	241	 2% 88% 10% •
2	D	241	 4% 84% 14% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7147 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 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	190	1491	929	252	301	9	1	2	0
1	C	200	1569	984	264	312	9	1	4	0

- Molecule 2 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	240	1869	1177	329	357	6	2	1	0
2	D	240	1891	1187	334	364	6	1	1	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

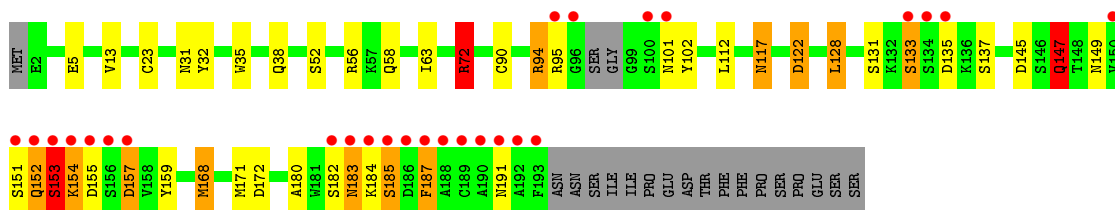
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	80	Total	O	0	0
			80	80		
4	C	89	Total	O	0	0
			89	89		
4	D	78	Total	O	0	0
			78	78		

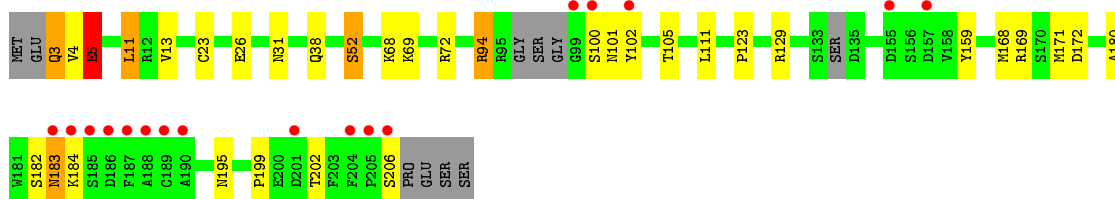
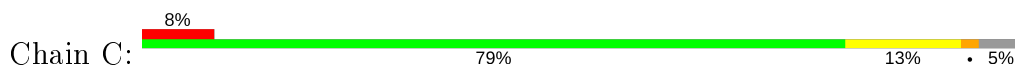
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

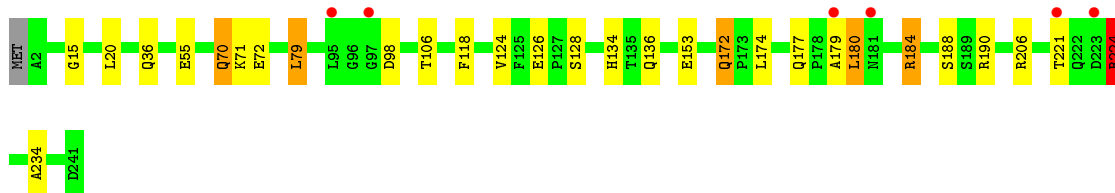
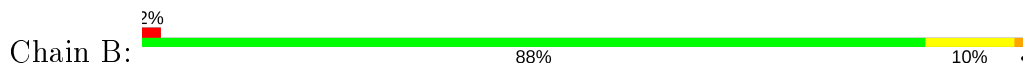
- Molecule 1: TCR alpha chain



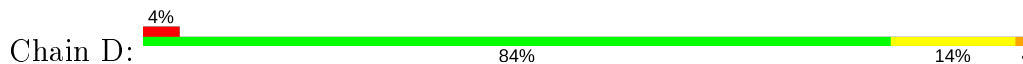
- Molecule 1: TCR alpha chain

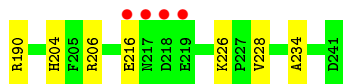


- Molecule 2: TCR beta chain



- Molecule 2: TCR beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.02Å 69.69Å 69.70Å 111.66° 111.03° 94.86°	Depositor
Resolution (Å)	48.21 – 1.71 48.21 – 1.71	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.21-1.71) 90.9 (48.21-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.71Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.171 , 0.231 0.181 , 0.237	Depositor DCC
R_{free} test set	4820 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	1.13	3/1524 (0.2%)	1.06	6/2058 (0.3%)
1	C	1.20	3/1611 (0.2%)	1.09	5/2179 (0.2%)
2	B	1.00	5/1920 (0.3%)	0.93	5/2617 (0.2%)
2	D	0.83	1/1942 (0.1%)	1.22	4/2644 (0.2%)
All	All	1.04	12/6997 (0.2%)	1.08	20/9498 (0.2%)

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	5
1	C	0	4
2	B	0	3
2	D	0	2
All	All	0	14

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	GLU	CD-OE1	25.37	1.53	1.25
1	A	147	GLN	CD-OE1	-25.16	0.68	1.24
1	C	5	GLU	CD-OE2	-23.38	0.99	1.25
2	B	153	GLU	CD-OE1	-22.26	1.01	1.25
1	A	147	GLN	CG-CD	16.45	1.88	1.51
1	A	147	GLN	CD-NE2	11.52	1.61	1.32
2	B	153	GLU	CD-OE2	10.91	1.37	1.25
2	B	172	GLN	CD-NE2	9.83	1.57	1.32
2	B	153	GLU	CG-CD	-9.78	1.37	1.51
2	D	58	ASP	CG-OD1	8.02	1.43	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	SER	CB-OG	-6.68	1.33	1.42
2	B	55	GLU	CD-OE2	6.30	1.32	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	58	ASP	OD1-CG-OD2	-40.88	45.63	123.30
1	C	5	GLU	OE1-CD-OE2	-26.43	91.59	123.30
2	B	172	GLN	OE1-CD-NE2	-14.39	88.80	121.90
1	A	147	GLN	CG-CD-OE1	-13.39	94.83	121.60
2	D	58	ASP	CB-CG-OD1	-13.12	106.49	118.30
1	A	147	GLN	CG-CD-NE2	11.01	143.12	116.70
1	A	168	MET	CG-SD-CE	-10.53	83.36	100.20
1	A	147	GLN	CB-CG-CD	-8.20	90.29	111.60
2	B	224	ARG	NE-CZ-NH2	7.84	124.22	120.30
2	D	206	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	C	5	GLU	CG-CD-OE1	6.42	131.13	118.30
2	B	206	ARG	NE-CZ-NH1	-6.12	117.24	120.30
2	B	153	GLU	OE1-CD-OE2	6.08	130.59	123.30
1	A	151	SER	N-CA-C	6.05	127.33	111.00
1	C	168	MET	CG-SD-CE	-5.94	90.69	100.20
1	C	169[A]	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	169[B]	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	D	183	SER	O-C-N	5.49	131.48	122.70
1	A	153	SER	N-CA-C	5.08	124.72	111.00
2	B	206	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	SER	Peptide
1	A	135	ASP	Peptide
1	A	191	ASN	Peptide
1	A	72	ARG	Sidechain
1	A	94	ARG	Sidechain
2	B	172	GLN	Sidechain
2	B	184	ARG	Sidechain
2	B	224	ARG	Sidechain
1	C	129	ARG	Sidechain
1	C	5	GLU	Sidechain
1	C	72	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	94	ARG	Sidechain
2	D	184[A]	ARG	Sidechain
2	D	58	ASP	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1491	0	1433	44	0
1	C	1569	0	1505	18	0
2	B	1869	0	1758	18	0
2	D	1891	0	1790	31	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
4	A	72	0	0	0	1
4	B	80	0	0	0	0
4	C	89	0	0	0	1
4	D	78	0	0	0	0
All	All	7147	0	6498	102	1

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 8.

All (102) 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:D:81:THR:O	2:D:110:VAL:HG21	1.51	1.09
1:A:147:GLN:OE1	1:A:147:GLN:CG	2.06	1.02
1:A:38:GLN:HE22	2:B:36:GLN:HE22	1.09	1.00
2:D:82:PRO:HA	2:D:110:VAL:HG23	1.42	0.98
1:C:3[A]:GLN:NE2	1:C:26:GLU:H	1.63	0.96
1:C:3[A]:GLN:HE22	1:C:26:GLU:H	1.06	0.93
1:C:38:GLN:HE22	2:D:36:GLN:HE22	1.16	0.90
1:A:147:GLN:OE1	1:A:147:GLN:NE2	2.05	0.88
2:D:82:PRO:HA	2:D:110:VAL:CG2	2.08	0.83
2:D:15:GLY:HA2	2:D:79:LEU:HD13	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:LEU:HB3	2:D:96:GLY:CA	2.16	0.76
2:D:95:LEU:HB3	2:D:96:GLY:HA3	1.69	0.75
1:C:38:GLN:HE22	2:D:36:GLN:NE2	1.85	0.74
1:A:145:ASP:CG	1:A:147:GLN:HE21	1.94	0.71
1:C:123:PRO:HB2	1:C:202:THR:HG22	1.72	0.71
2:D:2:ALA:HB1	2:D:26:ASN:OD1	1.91	0.70
1:C:199:PRO:O	1:C:202:THR:HG23	1.91	0.69
1:A:152:GLN:HG2	1:A:153:SER:N	2.07	0.69
1:A:95:ARG:NH1	1:A:101:ASN:HA	2.08	0.69
1:A:122:ASP:OD1	2:B:134:HIS:HE1	1.77	0.67
2:D:118:PHE:CE2	2:D:184[C]:ARG:NH1	2.62	0.67
2:D:81:THR:C	2:D:110:VAL:HG21	2.15	0.67
2:B:15:GLY:HA2	2:B:79:LEU:HD13	1.77	0.66
1:A:157:ASP:HB2	1:A:184:LYS:HD3	1.77	0.66
2:B:70:GLN:HA	2:B:70:GLN:HE21	1.60	0.66
2:D:15:GLY:HA2	2:D:79:LEU:CD1	2.26	0.65
2:D:95:LEU:CB	2:D:96:GLY:HA3	2.25	0.65
1:A:58:GLN:HG2	1:A:63:ILE:HG12	1.79	0.65
2:B:15:GLY:HA2	2:B:79:LEU:CD1	2.27	0.65
1:C:31:ASN:HD21	1:C:101:ASN:HD21	1.43	0.64
1:A:94:ARG:O	1:A:95:ARG:HG2	1.99	0.63
1:A:72:ARG:HH11	1:A:72:ARG:CG	2.11	0.63
1:A:153:SER:O	1:A:154:LYS:CB	2.47	0.63
1:C:182:SER:O	1:C:183:ASN:CB	2.47	0.62
2:D:70:GLN:HA	2:D:70:GLN:HE21	1.65	0.61
1:A:56:ARG:HE	1:A:58:GLN:HE21	1.49	0.60
2:D:188:SER:OG	2:D:190:ARG:NH2	2.33	0.59
1:A:182:SER:O	1:A:183:ASN:CB	2.49	0.59
2:D:159:ASN:HD21	2:D:204:HIS:H	1.51	0.59
1:C:11:LEU:HD22	1:C:13:VAL:CG2	2.33	0.59
1:A:185:SER:HA	1:A:187:PHE:N	2.18	0.58
1:A:157:ASP:HB2	1:A:184:LYS:CD	2.33	0.58
1:A:38:GLN:HE22	2:B:36:GLN:NE2	1.92	0.58
1:A:153:SER:O	1:A:154:LYS:HB3	2.04	0.58
1:C:3[A]:GLN:HE22	1:C:26:GLU:N	1.89	0.56
2:B:188:SER:OG	2:B:190:ARG:NH2	2.38	0.56
1:A:95:ARG:CZ	1:A:102:TYR:H	2.19	0.55
2:D:112:GLU:HA	2:D:112:GLU:OE1	2.08	0.54
1:C:11:LEU:HD22	1:C:13:VAL:HG23	1.90	0.54
2:D:159:ASN:ND2	2:D:204:HIS:H	2.05	0.54
1:A:56:ARG:HE	1:A:58:GLN:NE2	2.06	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:PRO:CA	2:D:110:VAL:HG23	2.29	0.53
2:D:77:LEU:N	2:D:77:LEU:HD12	2.24	0.53
1:A:152:GLN:HG2	1:A:153:SER:H	1.75	0.51
1:A:95:ARG:HH12	1:A:101:ASN:HA	1.75	0.51
2:B:179:ALA:C	2:B:180:LEU:HD23	2.31	0.51
1:A:155:ASP:HB2	1:A:157:ASP:OD1	2.11	0.50
1:A:72:ARG:HG2	1:A:72:ARG:HH11	1.77	0.49
2:D:95:LEU:CB	2:D:96:GLY:CA	2.88	0.49
1:A:182:SER:O	1:A:183:ASN:HB2	2.13	0.49
2:D:82:PRO:CA	2:D:110:VAL:CG2	2.85	0.49
1:A:31:ASN:HB2	1:A:52:SER:OG	2.13	0.49
1:A:185:SER:HA	1:A:187:PHE:HB3	1.93	0.48
1:A:122:ASP:OD1	2:B:134:HIS:CE1	2.63	0.48
2:D:176:GLU:HB2	2:D:184[A]:ARG:HB2	1.96	0.48
2:B:118:PHE:CD2	2:B:184:ARG:HD3	2.49	0.48
2:D:20:LEU:HD22	2:D:106:THR:HG21	1.96	0.47
2:B:20:LEU:HD22	2:B:106:THR:HG21	1.97	0.47
1:A:95:ARG:NH2	1:A:102:TYR:O	2.47	0.47
1:A:32:TYR:CE2	2:B:98:ASP:HB3	2.49	0.47
1:C:5:GLU:O	1:C:23:CYS:HA	2.14	0.47
1:A:153:SER:O	1:A:154:LYS:CG	2.63	0.47
2:D:110:VAL:HG23	2:D:110:VAL:O	2.15	0.47
1:A:94:ARG:O	1:A:95:ARG:CG	2.62	0.46
2:D:124:VAL:HG23	2:D:234:ALA:HB3	1.98	0.46
1:A:145:ASP:CG	1:A:147:GLN:NE2	2.67	0.46
1:C:171:MET:O	1:C:172:ASP:OD1	2.33	0.46
1:C:3[A]:GLN:HG3	1:C:4:VAL:HG23	1.97	0.45
1:A:72:ARG:CG	1:A:72:ARG:NH1	2.76	0.45
2:B:177:GLN:HE21	2:B:180:LEU:HD11	1.81	0.45
1:A:122:ASP:CG	1:A:122:ASP:O	2.54	0.45
1:A:5:GLU:O	1:A:23:CYS:HA	2.16	0.45
1:A:13:VAL:CG1	1:A:112:LEU:HD11	2.47	0.44
1:A:171:MET:O	1:A:172:ASP:OD1	2.35	0.44
1:A:117:ASN:HD22	1:A:117:ASN:C	2.19	0.44
2:B:174:LEU:C	2:B:174:LEU:HD12	2.38	0.44
1:A:35:TRP:CZ3	1:A:90:CYS:HB3	2.52	0.44
1:A:157:ASP:N	1:A:157:ASP:OD1	2.51	0.43
1:C:3[A]:GLN:CG	1:C:105:THR:HG21	2.49	0.43
1:C:159:TYR:O	1:C:180:ALA:HA	2.18	0.43
2:D:2:ALA:O	2:D:24:GLN:HA	2.19	0.42
1:C:31:ASN:HA	1:C:52:SER:OG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:O	1:A:180:ALA:HA	2.19	0.42
1:C:102:TYR:HE1	2:D:49:TYR:HH	1.64	0.42
2:B:124:VAL:HG23	2:B:234:ALA:HB3	2.02	0.41
2:B:79:LEU:C	2:B:79:LEU:HD12	2.41	0.41
2:D:32:TYR:O	2:D:90:CYS:HA	2.20	0.41
2:D:174:LEU:C	2:D:174:LEU:HD12	2.41	0.41
1:A:128:LEU:HB3	2:B:126:GLU:O	2.21	0.40
1:A:72:ARG:HG2	1:A:72:ARG:NH1	2.36	0.40
2:B:71:LYS:HG3	2:B:72:GLU:HG3	2.04	0.40
2:D:226:LYS:HD3	2:D:228:VAL:CG1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:343:HOH:O	4:C:412:HOH:O[1_554]	2.19	0.01

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	188/210 (90%)	173 (92%)	12 (6%)	3 (2%)	9	1
1	C	197/210 (94%)	189 (96%)	7 (4%)	1 (0%)	29	13
2	B	239/241 (99%)	233 (98%)	6 (2%)	0	100	100
2	D	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
All	All	863/902 (96%)	826 (96%)	33 (4%)	4 (0%)	29	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	SER
1	A	154	LYS
1	A	152	GLN
1	C	183	ASN

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	169/189 (89%)	155 (92%)	14 (8%)	11 2
1	C	178/189 (94%)	167 (94%)	11 (6%)	18 5
2	B	197/205 (96%)	190 (96%)	7 (4%)	35 15
2	D	203/205 (99%)	198 (98%)	5 (2%)	47 27
All	All	747/788 (95%)	710 (95%)	37 (5%)	25 7

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	117	ASN
1	A	122	ASP
1	A	128	LEU
1	A	131	SER
1	A	133	SER
1	A	137	SER
1	A	147	GLN
1	A	149	ASN
1	A	157	ASP
1	A	168	MET
1	A	183	ASN
1	A	185	SER
1	A	187	PHE
2	B	70	GLN
2	B	79	LEU
2	B	128	SER
2	B	136	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	180	LEU
2	B	221	THR
2	B	224	ARG
1	C	3[A]	GLN
1	C	3[B]	GLN
1	C	11	LEU
1	C	68	LYS
1	C	69	LYS
1	C	94	ARG
1	C	100	SER
1	C	111	LEU
1	C	184	LYS
1	C	195	ASN
1	C	206	SER
2	D	38	THR
2	D	70	GLN
2	D	79	LEU
2	D	182	ASP
2	D	216	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	58	GLN
1	A	117	ASN
1	A	147	GLN
1	A	152	GLN
1	A	183	ASN
2	B	27	ASN
2	B	46	HIS
2	B	70	GLN
2	B	134	HIS
2	B	177	GLN
2	B	204	HIS
1	C	14	GLN
1	C	101	ASN
2	D	27	ASN
2	D	36	GLN
2	D	70	GLN
2	D	100	GLN
2	D	116	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	159	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
3	EDO	B	301	-	3,3,3	0.49	0	2,2,2	0.38	0
3	EDO	C	301	-	3,3,3	0.47	0	2,2,2	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	301	-	-	0/1/1/1	-
3	EDO	C	301	-	-	0/1/1/1	-

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	190/210 (90%)	0.60	27 (14%) 2 2	25, 40, 86, 108	1 (0%)
1	C	200/210 (95%)	0.51	17 (8%) 10 12	24, 38, 75, 94	1 (0%)
2	B	240/241 (99%)	0.06	6 (2%) 57 61	24, 38, 69, 91	2 (0%)
2	D	240/241 (99%)	0.15	10 (4%) 36 40	23, 37, 58, 81	1 (0%)
All	All	870/902 (96%)	0.31	60 (6%) 16 19	23, 38, 72, 108	5 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	PHE	6.7
1	A	186	ASP	6.4
1	A	183	ASN	5.8
2	D	96	GLY	5.8
2	D	217	ASN	5.6
1	A	185	SER	5.3
1	A	191	ASN	5.1
1	C	187	PHE	4.5
1	C	99	GLY	4.4
1	A	190	ALA	4.4
1	A	189	CYS	4.3
1	C	185	SER	4.3
1	C	186	ASP	4.3
2	D	216	GLU	4.2
1	A	155	ASP	4.0
1	A	152	GLN	3.9
2	B	95	LEU	3.6
1	C	205	PRO	3.5
1	A	154	LYS	3.5
1	C	204	PHE	3.5
1	A	157	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	206	SER	3.4
1	C	102	TYR	3.3
1	A	182	SER	3.3
2	B	223	ASP	3.2
1	A	96	GLY	3.2
1	A	135	ASP	3.1
1	C	157	ASP	3.1
1	A	188	ALA	3.0
1	C	188	ALA	3.0
1	A	100	SER	3.0
1	A	184	LYS	3.0
1	A	134	SER	2.9
1	A	153	SER	2.9
1	C	189	CYS	2.8
1	C	155	ASP	2.8
2	D	219	GLU	2.8
1	C	183	ASN	2.8
1	C	184	LYS	2.8
2	D	176	GLU	2.8
2	D	95	LEU	2.8
2	D	181	ASN	2.7
1	C	201	ASP	2.7
1	C	100	SER	2.7
1	A	95	ARG	2.7
2	D	218	ASP	2.7
2	B	179	ALA	2.6
1	A	101	ASN	2.3
2	B	97	GLY	2.3
1	A	133	SER	2.3
2	B	181	ASN	2.3
2	B	221	THR	2.3
1	A	151	SER	2.2
1	A	192	ALA	2.2
1	A	193	PHE	2.2
1	A	150	VAL	2.1
1	A	156	SER	2.1
2	D	112	GLU	2.1
1	C	190	ALA	2.1
2	D	163	VAL	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 carbohydrates 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	C	301	4/4	0.83	0.19	45,46,46,54	0
3	EDO	B	301	4/4	0.93	0.19	42,42,43,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.