



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:38 AM UTC

PDB ID : 6DFV / pdb\_00006dfv  
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](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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

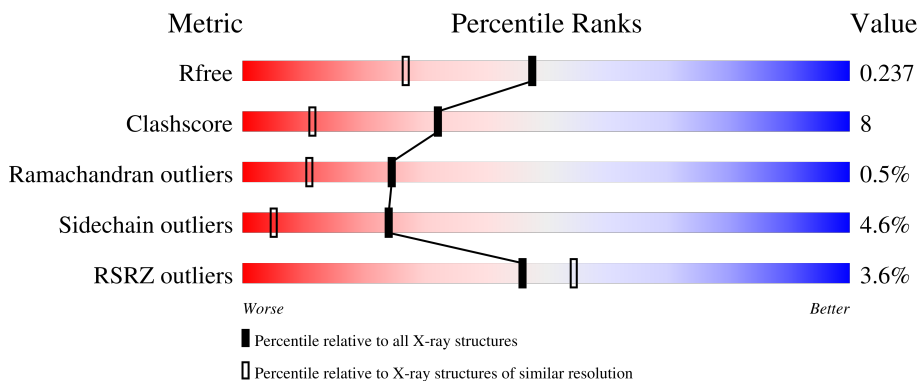
# 1 Overall quality at a glance

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))
$R_{free}$	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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  $\geq 3$ , 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	
1	C	210	
2	B	241	
2	D	241	

## 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.

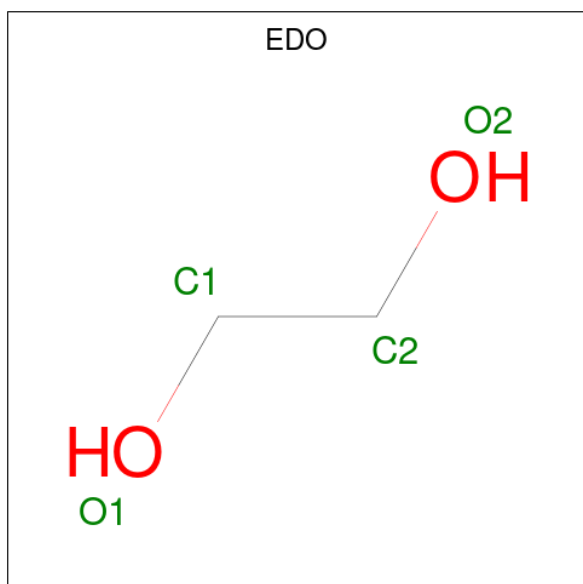
- Molecule 1 is a protein called TCR alpha chain.

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 (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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		

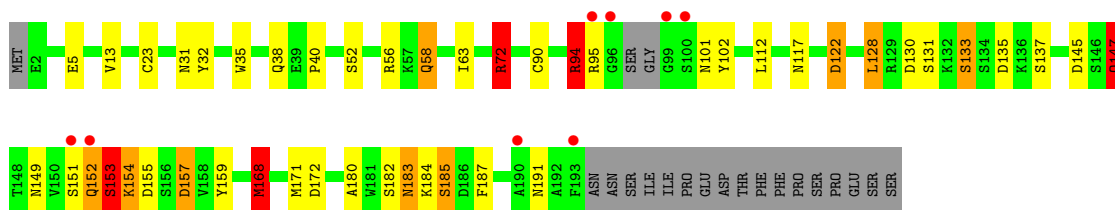
- Molecule 4 is water.

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		

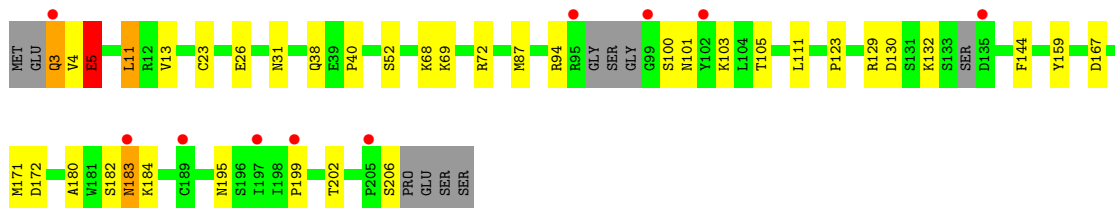
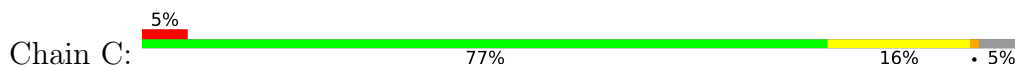
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

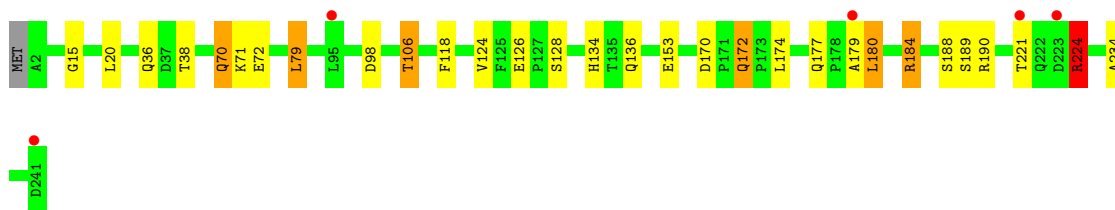
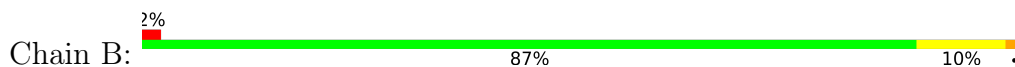
- Molecule 1: TCR alpha chain



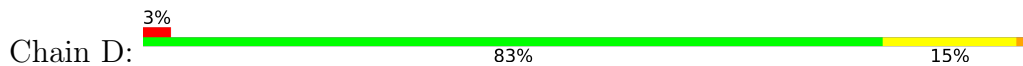
- Molecule 1: TCR alpha chain

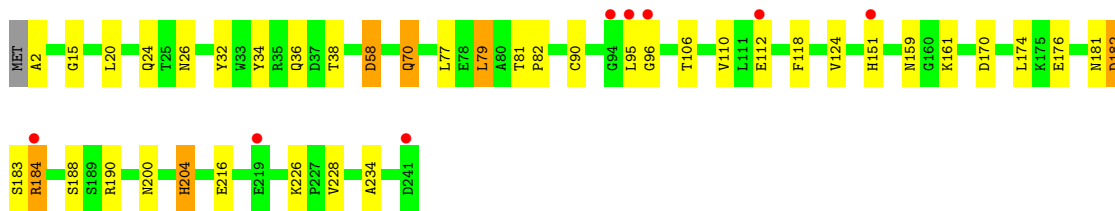


- Molecule 2: TCR beta chain



- Molecule 2: TCR beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (4.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<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](#)

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	1.43	5/1524 (0.3%)	1.31	8/2058 (0.4%)
1	C	1.24	5/1611 (0.3%)	1.18	5/2179 (0.2%)
2	B	1.16	6/1920 (0.3%)	1.30	8/2617 (0.3%)
2	D	1.14	6/1942 (0.3%)	1.27	7/2644 (0.3%)
All	All	1.24	22/6997 (0.3%)	1.27	28/9498 (0.3%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLN	CD-OE1	-28.93	0.68	1.23
1	C	5	GLU	CD-OE1	14.85	1.53	1.25
1	A	147	GLN	CG-CD	14.74	1.88	1.52
1	A	147	GLN	CD-NE2	13.53	1.61	1.33
1	C	5	GLU	CD-OE2	-13.38	0.99	1.25
2	B	153	GLU	CD-OE1	-12.73	1.01	1.25
2	B	172	GLN	CD-NE2	11.51	1.57	1.33
2	D	58	ASP	CG-OD1	9.71	1.43	1.25
2	B	153	GLU	CD-OE2	6.47	1.37	1.25
1	A	147	GLN	C-O	-6.32	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	204	HIS	CE1-NE2	6.14	1.38	1.32
2	B	106	THR	C-O	-6.03	1.17	1.24
2	B	153	GLU	CG-CD	-5.91	1.37	1.52
1	C	144	PHE	N-CA	5.74	1.52	1.45
2	D	151	HIS	CE1-NE2	5.49	1.38	1.32
1	C	103	LYS	N-CA	5.47	1.52	1.46
1	A	58	GLN	C-O	5.18	1.30	1.23
2	D	200	ASN	C-N	5.15	1.38	1.33
2	B	172	GLN	C-O	-5.07	1.18	1.24
1	C	40	PRO	N-CA	-5.04	1.41	1.47
2	D	34	TYR	N-CA	-5.02	1.39	1.45
2	D	161	LYS	N-CA	5.01	1.52	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	GLN	OE1-CD-NE2	-33.80	88.80	122.60
2	D	58	ASP	OD1-CG-OD2	-32.20	45.63	122.90
1	A	147	GLN	CG-CD-NE2	17.81	143.12	116.40
1	A	147	GLN	CB-CG-CD	-13.12	90.29	112.60
1	C	5	GLU	OE1-CD-OE2	-13.05	91.59	122.90
1	A	147	GLN	CG-CD-OE1	-12.99	94.83	120.80
1	C	5	GLU	CB-CG-CD	8.79	127.54	112.60
1	A	168	MET	CG-SD-CE	-7.97	83.36	100.90
1	A	151	SER	N-CA-C	7.76	127.33	110.80
1	A	130	ASP	CA-CB-CG	6.78	119.38	112.60
2	B	153	GLU	CB-CG-CD	6.73	124.03	112.60
1	A	153	SER	N-CA-C	6.54	124.72	110.80
2	D	183	SER	O-C-N	-6.44	115.33	123.06
1	C	167	ASP	CA-CB-CG	6.28	118.88	112.60
2	B	170	ASP	CA-C-N	5.81	125.50	119.05
2	B	170	ASP	C-N-CA	5.81	125.50	119.05
2	B	38	THR	CA-CB-OG1	-5.81	100.89	109.60
2	B	224	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	C	5	GLU	CG-CD-OE1	5.54	131.13	118.40
1	C	130	ASP	CA-CB-CG	5.50	118.10	112.60
2	B	170	ASP	CA-CB-CG	5.22	117.82	112.60
2	D	58	ASP	CB-CG-OD1	-5.18	106.49	118.40
1	A	94	ARG	CA-C-O	-5.17	115.71	121.81
2	D	170	ASP	CA-CB-CG	5.09	117.69	112.60
2	B	172	GLN	CG-CD-NE2	-5.05	108.82	116.40
2	D	182	ASP	CA-CB-CG	5.01	117.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	181	ASN	CA-C-N	5.00	131.44	122.38
2	D	181	ASN	C-N-CA	5.00	131.44	122.38

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
1	C	94	ARG	Sidechain
2	D	184[A]	ARG	Sidechain
2	D	58	ASP	Sidechain

## 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	1491	0	1433	46	0
1	C	1569	0	1505	18	0
2	B	1869	0	1758	19	0
2	D	1891	0	1790	32	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	107	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 (107) 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
2:D:95:LEU:HB3	2:D:96:GLY:CA	2.16	0.76
1:A:145:ASP:CG	1:A:147:GLN:HE21	1.94	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
2:D:81:THR:C	2:D:110:VAL:HG21	2.15	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:95:ARG:NH1	1:A:101:ASN:HA	2.08	0.69
1:A:152:GLN:HG2	1:A:153:SER:N	2.07	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: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:HE21	2:B:70:GLN:HA	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:CG	1:A:72:ARG:HH11	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:HE21	2:D:70:GLN:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:179:ALA:C	2:B:180:LEU:HD23	2.31	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
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:95:ARG:HH12	1:A:101:ASN:HA	1.75	0.51
1:A:152:GLN:HG2	1:A:153:SER:H	1.75	0.51
1:A:155:ASP:HB2	1:A:157:ASP:OD1	2.11	0.50
1:A:145:ASP:CG	1:A:147:GLN:NE2	2.67	0.50
1:A:72:ARG:HH11	1:A:72:ARG:HG2	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
1:A:122:ASP:CG	1:A:122:ASP:O	2.54	0.49
2:D:82:PRO:CA	2:D:110:VAL:CG2	2.85	0.49
1:A:117:ASN:HD22	1:A:117:ASN:C	2.19	0.49
2:B:174:LEU:C	2:B:174:LEU:HD12	2.38	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:32:TYR:CE2	2:B:98:ASP:HB3	2.49	0.47
1:A:95:ARG:NH2	1:A:102:TYR:O	2.47	0.47
1:A:153:SER:O	1:A:154:LYS:CG	2.63	0.47
1:C:5:GLU:O	1:C:23:CYS:HA	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:LEU:C	2:B:79:LEU:HD12	2.41	0.46
2:D:174:LEU:C	2:D:174:LEU:HD12	2.41	0.46
2:D:124:VAL:HG23	2:D:234:ALA:HB3	1.98	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: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:C:87:MET:HE2	1:C:87:MET:HB2	1.89	0.44
1:A:35:TRP:CZ3	1:A:90:CYS:HB3	2.52	0.44
1:A:157:ASP:OD1	1:A:157:ASP:N	2.51	0.43
2:D:79:LEU:C	2:D:79:LEU:HD12	2.44	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:A:117:ASN:C	1:A:117:ASN:ND2	2.78	0.42
1:C:31:ASN:HA	1:C:52:SER:OG	2.20	0.42
1:A:159:TYR:O	1:A:180:ALA:HA	2.19	0.42
2:B:124:VAL:HG23	2:B:234:ALA:HB3	2.02	0.41
2:D:32:TYR:O	2:D:90:CYS:HA	2.20	0.41
2:D:188:SER:HG	2:D:190:ARG:HH22	1.63	0.41
1:A:40:PRO:HD2	1:A:168:MET:HE2	2.03	0.41
2:B:189:SER:C	2:B:190:ARG:HD3	2.46	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%)	7	1
1	C	197/210 (94%)	189 (96%)	7 (4%)	1 (0%)	24	11
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%)	24	11

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%)	157 (93%)	12 (7%)	13	2
1	C	178/189 (94%)	167 (94%)	11 (6%)	16	2
2	B	197/205 (96%)	190 (96%)	7 (4%)	31	8
2	D	203/205 (99%)	198 (98%)	5 (2%)	42	18
All	All	747/788 (95%)	712 (95%)	35 (5%)	24	4

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
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
2	B	70	GLN
2	B	79	LEU
2	B	128	SER
2	B	136	GLN
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	100	SER
1	C	111	LEU
1	C	132	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	58	GLN

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Mol	Chain	Res	Type
1	A	60	GLN
1	A	117	ASN
1	A	120	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	199	GLN
2	B	204	HIS
1	C	60	GLN
1	C	101	ASN
1	C	147	GLN
2	D	9	ASN
2	D	27	ASN
2	D	36	GLN
2	D	70	GLN
2	D	116	ASN
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 oligosaccharides 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	0.47	0	2,2,2	0.30	0
3	EDO	C	301	-	3,3,3	0.46	0	2,2,2	0.49	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 [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	A	190/210 (90%)	0.21	8 (4%) 40 48	15, 40, 86, 108	3 (1%)
1	C	200/210 (95%)	0.29	10 (5%) 34 40	15, 38, 75, 94	5 (2%)
2	B	240/241 (99%)	0.09	5 (2%) 63 72	18, 38, 69, 91	3 (1%)
2	D	240/241 (99%)	0.16	8 (3%) 49 58	22, 37, 58, 81	2 (0%)
All	All	870/902 (96%)	0.18	31 (3%) 46 54	15, 38, 72, 108	13 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	219	GLU	4.5
2	D	184[A]	ARG	4.3
1	A	152	GLN	3.9
2	D	112	GLU	3.8
2	B	95	LEU	3.7
2	D	95	LEU	3.7
2	D	96	GLY	3.6
1	C	102	TYR	3.6
2	D	94	GLY	3.5
1	C	99	GLY	3.1
2	B	223	ASP	3.0
2	B	179	ALA	2.9
1	A	96	GLY	2.9
1	C	135	ASP	2.8
1	C	189	CYS	2.8
1	C	3[A]	GLN	2.7
1	C	197	ILE	2.6
2	B	221	THR	2.5
2	B	241	ASP	2.5
1	A	99	GLY	2.5
1	C	95	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	205	PRO	2.5
1	A	100	SER	2.4
1	A	190	ALA	2.4
1	A	193	PHE	2.2
2	D	241	ASP	2.1
1	C	183	ASN	2.1
1	C	199	PRO	2.1
2	D	151	HIS	2.1
1	A	95	ARG	2.0
1	A	151	SER	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 oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	C	301	4/4	0.84	0.15	45,46,46,54	0
3	EDO	B	301	4/4	0.94	0.09	42,42,43,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.