Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 03:12 PM EDT

PDB ID	:	6DFQ
Title	:	mouse diabetogenic TCR I.29
Authors	:	Wang, Y.; Dai, S.
Deposited on	:	2018-05-15
Resolution	:	2.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

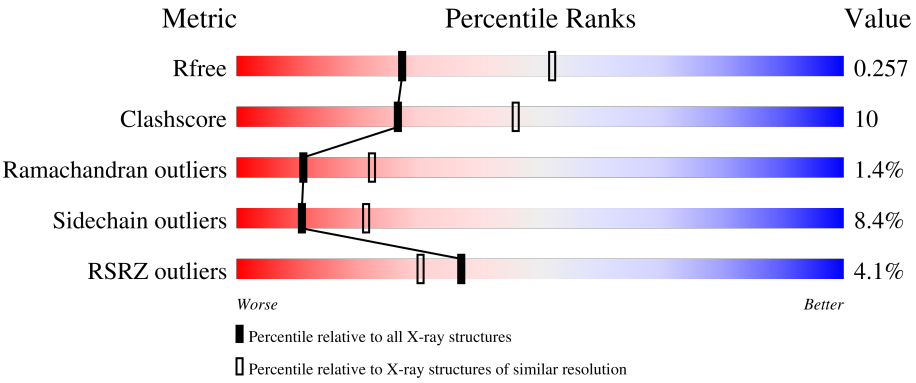
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	210	% 70% 18% 5% 7%
1	C	210	2% 70% 20% • • 5%
1	E	210	3% 71% 19% 5% 5%
1	G	210	9% 55% 20% 5% 20%
2	B	242	6% 78% 18% • •

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Mol	Chain	Length	Quality of chain
2	D	242	2% 70% 26%
2	F	242	2% 76% 19%
2	H	242	6% 69% 23%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13683 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
1	E	199	Total	C	N	O	S	0	0	0
			1544	971	258	309	6			
1	A	195	Total	C	N	O	S	0	0	0
			1515	956	248	304	7			
1	C	200	Total	C	N	O	S	0	0	0
			1552	978	258	308	8			
1	G	167	Total	C	N	O	S	0	1	0
			1304	822	219	258	5			

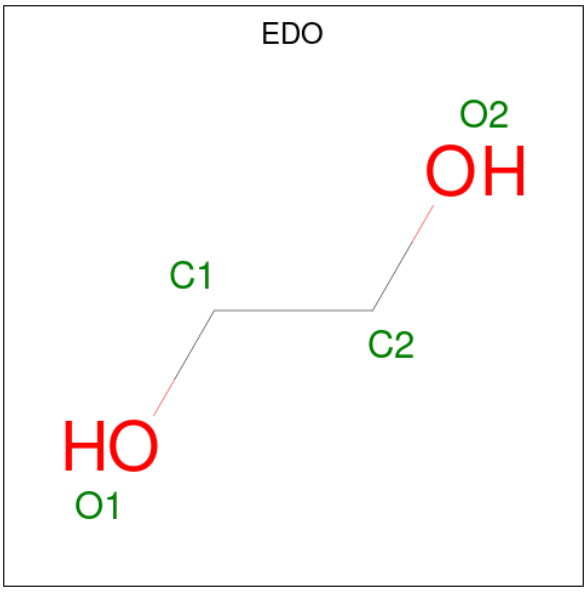
- Molecule 2 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	238	Total	C	N	O	S	0	0	0
			1919	1217	339	354	9			
2	B	239	Total	C	N	O	S	0	2	0
			1921	1222	331	358	10			
2	D	237	Total	C	N	O	S	0	2	0
			1915	1219	335	351	10			
2	H	234	Total	C	N	O	S	0	0	0
			1836	1173	319	335	9			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

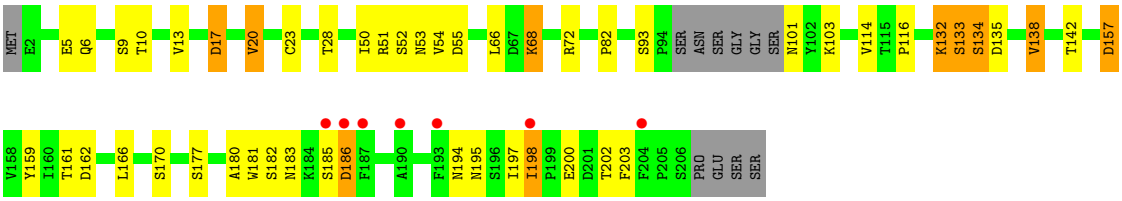
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	27	Total O 27 27	0	0
5	F	41	Total O 41 41	0	0
5	A	22	Total O 22 22	0	0
5	B	14	Total O 14 14	0	0
5	C	21	Total O 21 21	0	0
5	D	11	Total O 11 11	0	0
5	G	23	Total O 23 23	0	0
5	H	9	Total O 9 9	0	0

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.

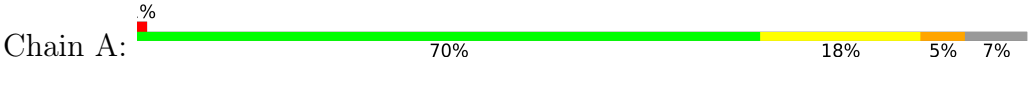
• Molecule 1: TCR alpha chain

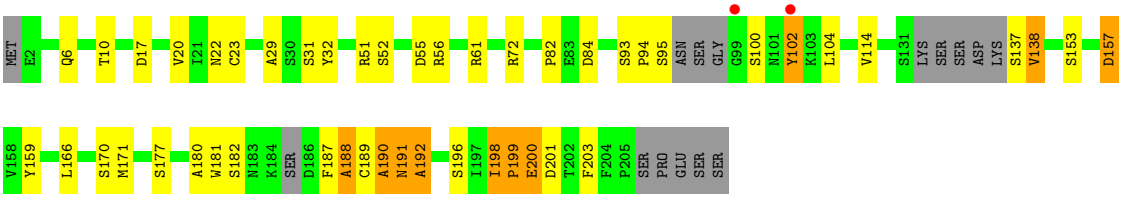
Chain E:



• Molecule 1: TCR alpha chain

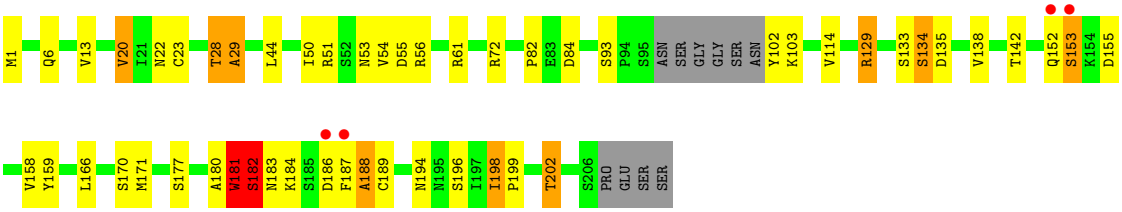
Chain A:





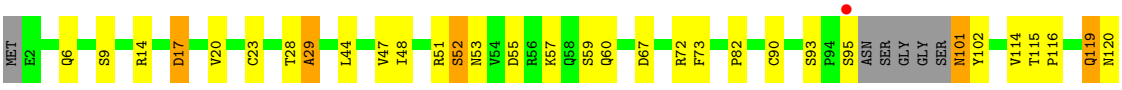
• Molecule 1: TCR alpha chain

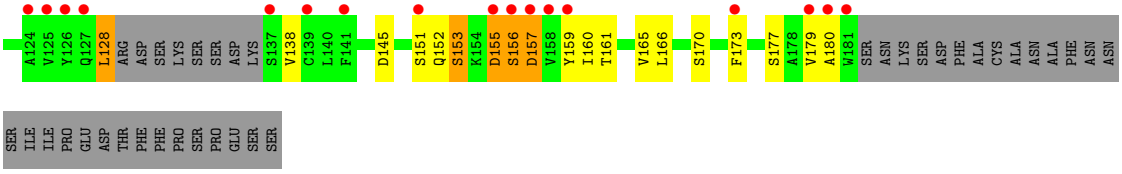
Chain C:



• Molecule 1: TCR alpha chain

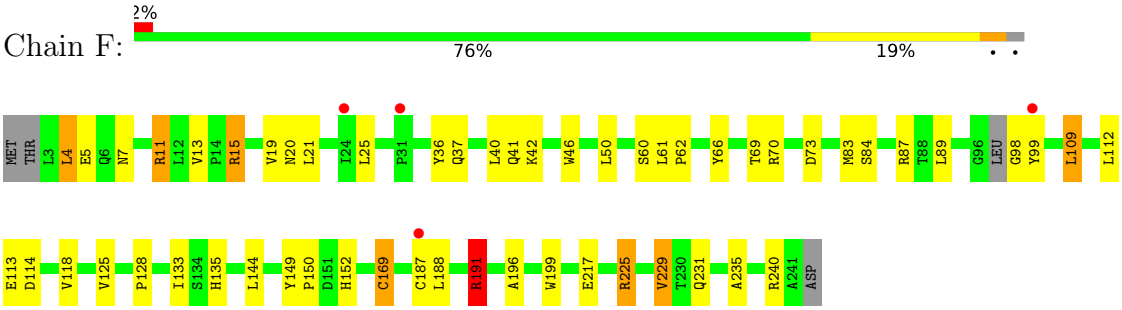
Chain G:





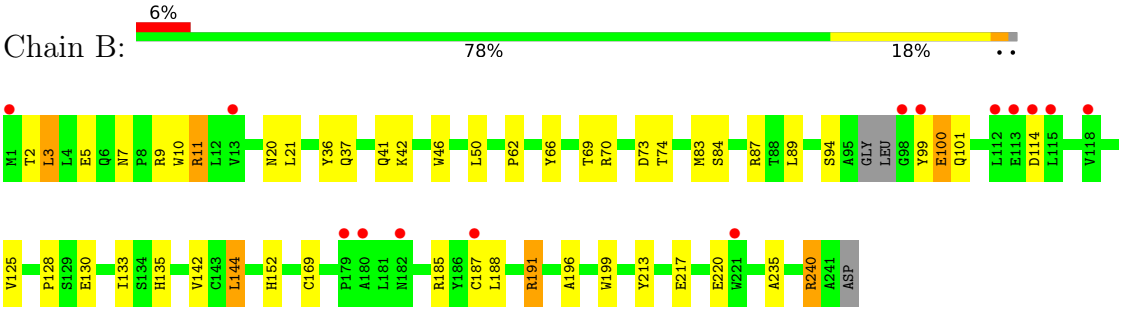
• Molecule 2: TCR beta chain

Chain F:



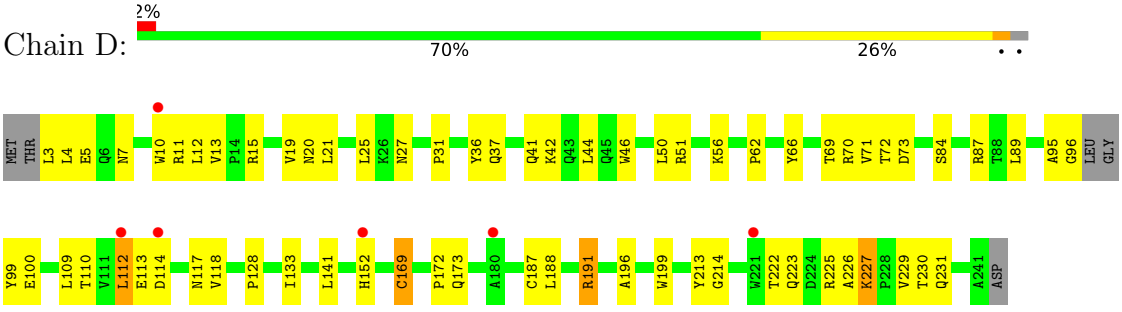
• Molecule 2: TCR beta chain

Chain B:



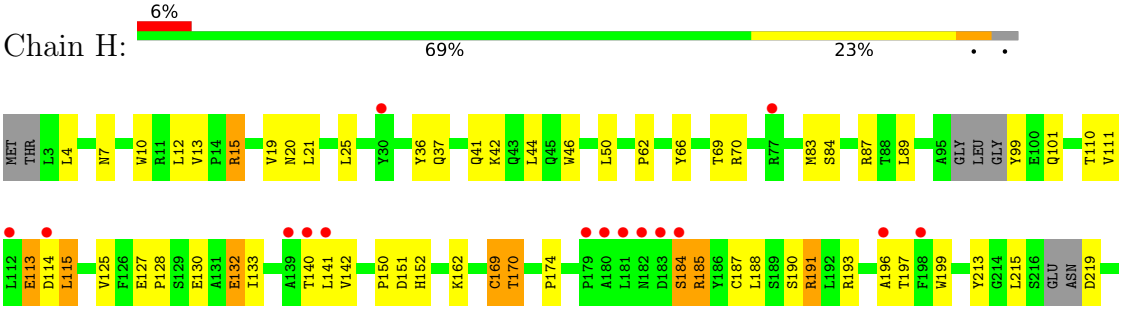
• Molecule 2: TCR beta chain

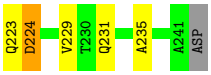
Chain D:



• Molecule 2: TCR beta chain

Chain H:




Q223
D224
V229
T230
Q231
A235
A241
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.11Å 117.63Å 234.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.60 47.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.60-2.60) 98.2 (47.55-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.220 , 0.253 0.229 , 0.257	Depositor DCC
R_{free} test set	4079 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13683	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: EDO, CA

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	0.53	0/1545	0.83	3/2095 (0.1%)
1	C	0.56	0/1584	0.80	1/2147 (0.0%)
1	E	0.57	0/1576	0.82	1/2139 (0.0%)
1	G	0.53	0/1332	0.81	1/1808 (0.1%)
2	B	0.47	0/1979	0.69	0/2699
2	D	0.48	0/1969	0.72	0/2686
2	F	0.51	0/1971	0.71	0/2685
2	H	0.45	0/1886	0.71	0/2576
All	All	0.51	0/13842	0.76	6/18835 (0.0%)

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
1	C	0	8
1	E	0	4
1	G	0	6
2	B	0	6
2	D	0	3
2	F	0	4
2	H	0	3
All	All	0	37

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	170	SER	CA-C-N	9.07	137.16	117.20
1	A	170	SER	C-N-CA	7.24	139.80	121.70
1	E	17	ASP	CB-CA-C	6.98	124.36	110.40
1	G	17	ASP	CB-CA-C	6.69	123.78	110.40
1	A	170	SER	O-C-N	-6.09	112.95	122.70
1	C	181	TRP	C-N-CA	5.19	134.68	121.70

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ALA	Peptide
1	A	51	ARG	Sidechain
1	A	56	ARG	Sidechain
2	B	11	ARG	Sidechain
2	B	185	ARG	Sidechain
2	B	191	ARG	Sidechain
2	B	240	ARG	Sidechain
2	B	62	PRO	Peptide
2	B	9	ARG	Sidechain
1	C	1	MET	Peptide
1	C	129	ARG	Sidechain
1	C	170	SER	Peptide
1	C	181	TRP	Peptide
1	C	182	SER	Peptide
1	C	29	ALA	Peptide
1	C	51	ARG	Sidechain
1	C	56	ARG	Sidechain
2	D	15	ARG	Sidechain
2	D	191	ARG	Sidechain
2	D	62	PRO	Peptide
1	E	133	SER	Peptide
1	E	135	ASP	Peptide
1	E	170	SER	Peptide
1	E	51	ARG	Sidechain
2	F	11	ARG	Sidechain
2	F	15	ARG	Sidechain
2	F	191	ARG	Sidechain
2	F	62	PRO	Peptide
1	G	14[A]	ARG	Sidechain
1	G	14[B]	ARG	Sidechain
1	G	170	SER	Peptide
1	G	29	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	G	51	ARG	Sidechain
1	G	72	ARG	Sidechain
2	H	15	ARG	Sidechain
2	H	191	ARG	Sidechain
2	H	62	PRO	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	1515	0	1419	34	0
1	C	1552	0	1485	40	0
1	E	1544	0	1461	30	0
1	G	1304	0	1246	39	0
2	B	1921	0	1833	36	0
2	D	1915	0	1826	47	0
2	F	1919	0	1847	38	0
2	H	1836	0	1742	39	0
3	C	1	0	0	0	0
4	G	8	0	12	0	0
5	A	22	0	0	3	0
5	B	14	0	0	0	0
5	C	21	0	0	2	0
5	D	11	0	0	1	0
5	E	27	0	0	2	0
5	F	41	0	0	4	0
5	G	23	0	0	1	0
5	H	9	0	0	0	0
All	All	13683	0	12871	271	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 10.

All (271) 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:187:PHE:HA	1:A:188:ALA:HB2	1.36	1.07
2:B:99:TYR:HB3	2:B:100:GLU:HA	1.33	1.07
1:C:187:PHE:HA	1:C:188:ALA:HB2	1.34	1.05
1:A:32:TYR:CD2	2:B:99:TYR:HD2	1.77	1.02
2:H:151:ASP:OD1	2:H:174:PRO:HG2	1.62	0.97
2:F:15:ARG:HH11	2:F:15:ARG:HB3	1.33	0.94
2:D:12:LEU:HD22	2:D:112:LEU:HD22	1.52	0.90
1:A:32:TYR:CE2	2:B:99:TYR:HD2	1.91	0.88
1:E:161:THR:HG21	2:F:191:ARG:HH12	1.38	0.88
1:C:133:SER:CB	1:C:134:SER:HA	2.08	0.84
1:G:152:GLN:O	1:G:153:SER:O	1.96	0.83
1:G:128:LEU:HD13	1:G:138:VAL:HG23	1.58	0.83
1:A:32:TYR:CD2	2:B:99:TYR:CD2	2.66	0.83
1:C:134:SER:H	1:C:135:ASP:HA	1.44	0.82
1:C:133:SER:HB2	1:C:134:SER:HA	1.61	0.80
1:G:47:VAL:HG23	1:G:48:ILE:HG22	1.63	0.80
2:B:99:TYR:HB3	2:B:100:GLU:CA	2.12	0.80
1:C:199:PRO:O	1:C:202:THR:HG23	1.83	0.79
1:G:160:ILE:HD12	1:G:180:ALA:HB2	1.66	0.78
2:F:118:VAL:O	2:F:225:ARG:NH2	2.18	0.77
1:C:187:PHE:HA	1:C:188:ALA:CB	2.14	0.77
1:A:32:TYR:CE2	2:B:99:TYR:CD2	2.74	0.76
2:H:115:LEU:HD22	2:H:215:LEU:HD11	1.67	0.75
1:G:128:LEU:HD12	1:G:128:LEU:N	2.02	0.74
1:C:134:SER:N	1:C:135:ASP:HA	2.04	0.73
2:D:118:VAL:O	2:D:225:ARG:NH2	2.21	0.72
1:A:6:GLN:HG3	1:A:23:CYS:SG	2.29	0.71
1:E:6:GLN:HG3	1:E:23:CYS:SG	2.30	0.71
1:C:6:GLN:HG3	1:C:23:CYS:SG	2.30	0.70
1:G:67:ASP:OD1	5:G:401:HOH:O	2.10	0.70
1:A:187:PHE:HA	1:A:188:ALA:CB	2.18	0.69
1:E:197:ILE:O	1:E:198:ILE:HG22	1.93	0.69
1:G:6:GLN:HG3	1:G:90:CYS:SG	2.33	0.68
1:G:6:GLN:HG2	1:G:23:CYS:SG	2.33	0.68
1:C:44:LEU:HD21	2:D:44:LEU:HD11	1.75	0.68
2:H:170:THR:HG22	2:H:190:SER:HB2	1.75	0.68
1:E:161:THR:HG22	1:E:162:ASP:O	1.92	0.68
1:E:157:ASP:O	1:E:182:SER:OG	2.12	0.68
1:G:59:SER:O	1:G:60:GLN:HG3	1.93	0.67
2:D:128:PRO:HD3	2:D:141:LEU:HD22	1.77	0.66
2:F:89:LEU:HD23	2:F:109:LEU:HD22	1.78	0.66
1:C:61:ARG:NH2	1:C:84:ASP:OD2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:ASP:OD1	2:H:174:PRO:CG	2.41	0.66
1:A:17:ASP:OD2	5:A:301:HOH:O	2.13	0.65
2:D:13:VAL:HG22	2:D:19:VAL:HG21	1.78	0.65
1:A:61:ARG:NH2	1:A:84:ASP:OD2	2.29	0.65
1:A:104:LEU:HD21	2:B:99:TYR:CE2	2.31	0.65
1:C:53:ASN:HB2	1:C:54:VAL:HG13	1.78	0.65
1:E:161:THR:HG21	2:F:191:ARG:NH1	2.10	0.64
1:G:160:ILE:O	1:G:161:THR:OG1	2.15	0.63
2:H:13:VAL:HG11	2:H:19:VAL:CG2	2.30	0.62
1:G:128:LEU:HB3	2:H:127:GLU:O	2.00	0.62
1:E:194:ASN:O	1:E:195:ASN:HB3	2.00	0.61
1:A:190:ALA:HB3	1:A:191:ASN:HB3	1.82	0.61
1:A:157:ASP:O	1:A:182:SER:OG	2.15	0.61
2:D:172:PRO:HG2	2:D:173:GLN:OE1	2.00	0.61
1:C:54:VAL:HG11	1:G:57:LYS:HD3	1.82	0.61
2:H:133:ILE:HG23	2:H:196:ALA:HB1	1.84	0.60
2:D:223:GLN:HB3	5:D:309:HOH:O	2.01	0.60
2:D:133:ILE:HG23	2:D:196:ALA:HB1	1.83	0.60
1:E:198:ILE:HD11	1:E:202:THR:HG21	1.83	0.59
1:G:128:LEU:HD12	1:G:138:VAL:O	2.02	0.59
1:G:128:LEU:HD12	1:G:128:LEU:H	1.67	0.59
2:F:150:PRO:HG2	2:F:152:HIS:CD2	2.38	0.58
1:A:137:SER:N	5:A:303:HOH:O	2.35	0.58
1:C:184:LYS:HB3	1:C:186:ASP:OD1	2.03	0.58
2:F:13:VAL:HG22	2:F:19:VAL:HG21	1.85	0.58
2:B:133:ILE:HG23	2:B:196:ALA:HB1	1.86	0.58
1:E:185:SER:O	1:E:186:ASP:CB	2.52	0.58
2:D:110:THR:HG1	2:D:152:HIS:HE2	1.50	0.58
2:F:133:ILE:HG23	2:F:196:ALA:HB1	1.86	0.58
1:G:155:ASP:C	1:G:157:ASP:H	2.07	0.57
1:E:183:ASN:HB2	5:E:302:HOH:O	2.04	0.57
1:A:166:LEU:HB3	2:B:169:CYS:HB2	1.87	0.57
1:C:155:ASP:O	1:C:158:VAL:HG12	2.05	0.57
1:G:119:GLN:HG2	1:G:120:ASN:H	1.70	0.57
2:H:128:PRO:HD3	2:H:141:LEU:HD23	1.86	0.56
1:A:187:PHE:CA	1:A:188:ALA:HB2	2.24	0.56
1:A:190:ALA:HB3	1:A:191:ASN:CB	2.36	0.56
2:D:10[B]:TRP:HZ2	2:D:214:GLY:O	1.89	0.56
2:B:3:LEU:HD12	2:B:3:LEU:O	2.06	0.56
2:H:66:TYR:OH	2:H:87:ARG:HD3	2.07	0.55
1:A:22:ASN:CG	1:G:17:ASP:HB2	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:PRO:HD3	2:D:141:LEU:CD2	2.36	0.55
1:E:194:ASN:O	1:E:195:ASN:CB	2.53	0.55
1:C:72:ARG:NH1	5:C:404:HOH:O	2.40	0.54
2:F:11:ARG:NH2	5:F:302:HOH:O	2.37	0.54
2:H:184:SER:O	2:H:185:ARG:CB	2.57	0.53
2:B:99:TYR:HA	2:B:100:GLU:C	2.29	0.53
2:D:95:ALA:O	2:D:96:GLY:C	2.46	0.53
1:G:6:GLN:CG	1:G:23:CYS:SG	2.96	0.53
1:G:115:THR:HB	1:G:116:PRO:HD2	1.91	0.53
2:H:223:GLN:O	2:H:224:ASP:CB	2.57	0.52
2:H:15:ARG:HH11	2:H:113:GLU:CD	2.13	0.52
1:C:199:PRO:HB2	1:C:202:THR:HG22	1.92	0.52
2:H:132:GLU:OE2	2:H:140:THR:N	2.41	0.52
2:B:99:TYR:CB	2:B:100:GLU:HA	2.20	0.52
1:C:134:SER:H	1:C:135:ASP:CA	2.20	0.52
1:G:44:LEU:HD21	2:H:44:LEU:HD11	1.92	0.52
1:G:166:LEU:HB3	2:H:169:CYS:HB3	1.92	0.52
1:C:187:PHE:CA	1:C:188:ALA:HB2	2.25	0.51
2:F:66:TYR:OH	2:F:87:ARG:HD3	2.11	0.51
1:A:31:SER:OG	1:A:95:SER:C	2.48	0.51
2:D:187:CYS:SG	2:D:188:LEU:N	2.84	0.51
1:A:181:TRP:CZ2	2:B:187:CYS:SG	3.03	0.51
1:C:198:ILE:HG12	1:C:202:THR:HG21	1.93	0.51
1:E:133:SER:HA	1:E:134:SER:OG	2.10	0.51
1:E:203:PHE:HD2	2:F:135:HIS:CD2	2.28	0.51
2:F:41:GLN:O	2:F:42:LYS:HB2	2.11	0.51
2:D:25:LEU:HD23	2:D:25:LEU:C	2.31	0.51
2:D:66:TYR:OH	2:D:87:ARG:HD3	2.11	0.51
1:A:191:ASN:O	1:A:192:ALA:HB2	2.11	0.51
2:B:5[A]:GLU:OE2	2:B:5[A]:GLU:HA	2.11	0.51
2:F:187:CYS:SG	2:F:188:LEU:N	2.84	0.51
2:B:99:TYR:HA	2:B:100:GLU:O	2.10	0.51
1:C:181:TRP:CZ2	2:D:187:CYS:SG	3.05	0.50
1:G:52:SER:O	1:G:53:ASN:HB2	2.11	0.50
2:B:66:TYR:OH	2:B:87:ARG:HD3	2.11	0.50
1:C:50:ILE:HD11	1:C:54:VAL:HG23	1.92	0.50
2:H:41:GLN:O	2:H:42:LYS:HB2	2.10	0.50
2:F:13:VAL:CG2	2:F:19:VAL:HG21	2.42	0.50
2:F:98:GLY:HA2	5:F:309:HOH:O	2.12	0.50
2:H:187:CYS:SG	2:H:188:LEU:N	2.84	0.50
2:B:187:CYS:SG	2:B:188:LEU:N	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:LEU:HD21	2:D:27:ASN:C	2.33	0.49
2:D:31:PRO:HB2	2:D:51:ARG:CZ	2.42	0.49
2:H:13:VAL:HG23	2:H:111:VAL:HG22	1.94	0.49
2:D:229:VAL:HG12	2:D:230:THR:O	2.12	0.49
2:B:41:GLN:O	2:B:42:LYS:HB2	2.11	0.49
2:H:128:PRO:HD3	2:H:141:LEU:CD2	2.43	0.49
2:F:15:ARG:HH11	2:F:15:ARG:CB	2.15	0.49
1:A:22:ASN:OD1	1:G:17:ASP:HB2	2.13	0.49
2:D:71:VAL:HG23	2:D:72:THR:HG23	1.94	0.48
2:F:133:ILE:HG23	2:F:196:ALA:CB	2.43	0.48
2:H:133:ILE:HG23	2:H:196:ALA:CB	2.44	0.48
1:E:20:VAL:HG22	1:C:20:VAL:HG22	1.96	0.48
1:E:82:PRO:HA	1:E:114:VAL:HB	1.95	0.48
1:C:196:SER:O	1:C:198:ILE:HG22	2.14	0.48
2:D:37:GLN:OE1	2:D:87:ARG:NH1	2.46	0.48
2:D:25:LEU:HD21	2:D:27:ASN:O	2.13	0.48
1:E:17:ASP:HB2	1:C:22:ASN:CG	2.34	0.48
1:A:198:ILE:O	1:A:200:GLU:N	2.46	0.48
1:E:197:ILE:CD1	1:E:197:ILE:N	2.77	0.48
2:F:37:GLN:OE1	2:F:87:ARG:NH1	2.47	0.47
1:G:173:PHE:HE2	2:H:193:ARG:HH21	1.59	0.47
1:E:159:TYR:O	1:E:180:ALA:HA	2.14	0.47
1:C:72:ARG:NH2	5:C:401:HOH:O	2.22	0.47
2:D:13:VAL:CG2	2:D:19:VAL:HG21	2.42	0.47
2:F:128:PRO:HD2	2:F:199:TRP:CZ2	2.50	0.47
2:D:41:GLN:O	2:D:42:LYS:HB2	2.12	0.47
2:D:133:ILE:HG23	2:D:196:ALA:CB	2.44	0.47
1:G:101:ASN:O	1:G:102:TYR:HB2	2.14	0.47
1:A:188:ALA:HB1	1:A:191:ASN:ND2	2.29	0.47
2:H:128:PRO:HD2	2:H:199:TRP:CZ2	2.49	0.47
2:B:37:GLN:OE1	2:B:87:ARG:NH1	2.47	0.47
1:A:104:LEU:CD2	2:B:99:TYR:CE2	2.98	0.47
1:A:203:PHE:HD2	2:B:135:HIS:CD2	2.33	0.47
2:H:170:THR:HG22	2:H:190:SER:CB	2.45	0.47
1:A:191:ASN:C	1:A:191:ASN:HD22	2.17	0.47
1:E:166:LEU:HB3	2:F:169:CYS:HB3	1.96	0.46
2:D:89:LEU:HD12	2:D:109:LEU:HD22	1.97	0.46
2:D:10[B]:TRP:CD1	2:D:152:HIS:CE1	3.03	0.46
2:D:128:PRO:HG3	2:D:141:LEU:HD23	1.98	0.46
1:C:199:PRO:O	1:C:202:THR:CG2	2.59	0.46
1:C:44:LEU:HD21	2:D:44:LEU:CD1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:PRO:HA	1:C:114:VAL:HB	1.97	0.46
1:E:197:ILE:N	1:E:197:ILE:HD12	2.31	0.46
1:A:82:PRO:HA	1:A:114:VAL:HB	1.98	0.46
2:B:73[B]:ASP:OD1	2:B:74:THR:HG23	2.16	0.46
2:D:10[B]:TRP:CD2	2:D:10[B]:TRP:C	2.87	0.46
1:C:53:ASN:CB	1:C:54:VAL:HG13	2.44	0.45
2:H:37:GLN:OE1	2:H:87:ARG:NH1	2.47	0.45
1:A:159:TYR:O	1:A:180:ALA:HA	2.16	0.45
1:C:198:ILE:CG1	1:C:202:THR:HG21	2.46	0.45
1:G:82:PRO:HA	1:G:114:VAL:HB	1.98	0.45
1:E:50:ILE:HD11	1:E:54:VAL:HG23	1.99	0.45
2:B:128:PRO:HD2	2:B:199:TRP:CZ2	2.51	0.45
2:F:83:MET:HB3	2:F:83:MET:HE2	1.82	0.45
2:B:133:ILE:HG23	2:B:196:ALA:CB	2.45	0.45
1:C:159:TYR:O	1:C:180:ALA:HA	2.17	0.45
2:H:13:VAL:HG11	2:H:19:VAL:HG21	1.98	0.45
1:C:184:LYS:CB	1:C:186:ASP:OD1	2.65	0.44
1:G:159:TYR:O	1:G:180:ALA:HA	2.17	0.44
1:C:133:SER:HB2	1:C:134:SER:CA	2.40	0.44
2:D:10[B]:TRP:CG	2:D:11:ARG:N	2.84	0.44
2:F:98:GLY:N	5:F:309:HOH:O	2.49	0.44
1:A:196:SER:O	1:A:198:ILE:HG22	2.17	0.44
2:D:128:PRO:HD2	2:D:199:TRP:CZ2	2.53	0.44
1:G:47:VAL:HG23	1:G:48:ILE:N	2.31	0.44
2:H:215:LEU:HD22	2:H:219:ASP:CB	2.47	0.44
2:F:13:VAL:HG22	2:F:19:VAL:CG2	2.47	0.44
1:E:66:LEU:HG	1:E:68:LYS:HE3	2.00	0.44
2:F:98:GLY:CA	5:F:309:HOH:O	2.66	0.44
1:A:188:ALA:HB1	1:A:191:ASN:O	2.17	0.44
1:A:190:ALA:H	1:A:191:ASN:C	2.21	0.44
2:B:100:GLU:H	2:B:100:GLU:HG2	1.51	0.44
2:D:226:ALA:O	2:D:227:LYS:CB	2.65	0.44
1:C:133:SER:CB	1:C:134:SER:CA	2.86	0.44
2:B:99:TYR:CD1	2:B:101:GLN:HG2	2.52	0.44
2:H:50:LEU:O	2:H:70:ARG:NH1	2.51	0.43
1:E:72:ARG:NE	5:E:301:HOH:O	2.35	0.43
2:H:110:THR:OG1	2:H:152:HIS:NE2	2.45	0.43
1:G:47:VAL:CG2	1:G:48:ILE:N	2.81	0.43
1:C:103:LYS:HD3	2:D:46:TRP:CE3	2.53	0.43
2:F:50:LEU:O	2:F:70:ARG:NH1	2.51	0.43
2:F:125:VAL:HG23	2:F:235:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:HB3	2:D:169:CYS:HB3	1.99	0.43
1:G:155:ASP:C	1:G:157:ASP:N	2.72	0.43
2:H:20:ASN:O	2:H:21:LEU:HD23	2.18	0.43
2:D:110:THR:OG1	2:D:152:HIS:NE2	2.44	0.43
1:G:160:ILE:HD12	1:G:180:ALA:CB	2.44	0.43
2:H:125:VAL:HG23	2:H:235:ALA:HB3	2.01	0.43
2:B:152:HIS:CD2	2:B:213:TYR:CD2	3.07	0.43
2:D:4:LEU:HD23	2:D:25:LEU:HA	2.01	0.43
1:E:101:ASN:ND2	1:E:103:LYS:HE2	2.34	0.43
2:F:5:GLU:OE1	2:F:5:GLU:HA	2.19	0.43
2:B:83:MET:HB3	2:B:83:MET:HE2	1.88	0.43
1:G:179:VAL:HG21	2:H:142:VAL:HG11	2.01	0.43
1:E:203:PHE:CD2	2:F:135:HIS:CD2	3.07	0.42
1:E:181:TRP:CZ2	2:F:187:CYS:SG	3.11	0.42
2:D:10[B]:TRP:CZ2	2:D:214:GLY:O	2.70	0.42
1:G:165:VAL:O	1:G:165:VAL:HG13	2.19	0.42
2:F:36:TYR:CE2	2:F:46:TRP:HB2	2.54	0.42
2:H:83:MET:HE2	2:H:83:MET:HB3	1.85	0.42
2:H:170:THR:HG23	2:H:190:SER:OG	2.20	0.42
2:F:15:ARG:NE	2:F:113:GLU:OE1	2.50	0.42
2:B:50:LEU:O	2:B:70:ARG:NH1	2.51	0.42
2:H:36:TYR:CE2	2:H:46:TRP:HB2	2.54	0.42
2:F:112:LEU:HD22	2:F:149:TYR:HE1	1.84	0.42
2:D:13:VAL:HG22	2:D:19:VAL:CG2	2.46	0.42
2:H:99:TYR:O	2:H:101:GLN:HG2	2.20	0.42
2:F:20:ASN:O	2:F:21:LEU:HD23	2.20	0.42
2:B:142:VAL:HG12	2:B:144:LEU:HD23	2.00	0.42
1:C:28:THR:O	1:C:29:ALA:HB3	2.20	0.42
2:D:229:VAL:O	2:D:231:GLN:HG2	2.19	0.42
2:F:60:SER:C	2:F:61:LEU:HD22	2.40	0.42
2:F:229:VAL:O	2:F:231:GLN:HG2	2.19	0.42
1:C:181:TRP:HD1	1:C:182:SER:HB2	1.84	0.42
2:D:10[B]:TRP:CE2	2:D:213:TYR:HB3	2.55	0.42
1:A:72:ARG:NE	5:A:302:HOH:O	2.16	0.42
2:B:2:THR:O	2:B:3:LEU:HB3	2.20	0.42
2:D:5:GLU:HA	2:D:5:GLU:OE1	2.20	0.42
2:D:36:TYR:CE2	2:D:46:TRP:HB2	2.55	0.42
2:B:36:TYR:CE2	2:B:46:TRP:HB2	2.55	0.41
2:H:110:THR:HG1	2:H:152:HIS:CE1	2.36	0.41
1:E:138:VAL:HG22	1:E:181:TRP:HB3	2.02	0.41
1:G:119:GLN:HG2	1:G:120:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:LYS:HA	1:E:133:SER:OG	2.19	0.41
1:G:6:GLN:CG	1:G:90:CYS:SG	3.05	0.41
1:A:102:TYR:HE1	2:B:94:SER:HG	1.67	0.41
2:D:50:LEU:O	2:D:70:ARG:NH1	2.52	0.41
1:G:155:ASP:O	1:G:157:ASP:N	2.53	0.41
1:E:198:ILE:HG23	1:E:198:ILE:O	2.21	0.41
1:A:138:VAL:HG22	1:A:181:TRP:HB3	2.03	0.41
2:D:56:LYS:HG2	2:D:69:THR:HG23	2.01	0.41
1:C:152:GLN:CA	1:C:153:SER:HB2	2.50	0.41
1:E:181:TRP:CD2	2:F:144:LEU:HD21	2.56	0.41
1:G:59:SER:C	1:G:60:GLN:HG3	2.41	0.41
2:H:229:VAL:O	2:H:231:GLN:HG2	2.21	0.41
2:B:99:TYR:CB	2:B:100:GLU:CA	2.82	0.41
2:B:125:VAL:HG23	2:B:235:ALA:HB3	2.02	0.41
2:D:12:LEU:CD2	2:D:112:LEU:HD22	2.38	0.41
2:H:4:LEU:HD23	2:H:25:LEU:HA	2.03	0.41
2:H:152:HIS:HB3	2:H:213:TYR:HB2	2.02	0.41
1:C:134:SER:N	1:C:135:ASP:CA	2.79	0.40
2:B:20:ASN:O	2:B:21:LEU:HD23	2.22	0.40
2:D:20:ASN:O	2:D:21:LEU:HD23	2.21	0.40
1:G:28:THR:HA	1:G:29:ALA:HA	1.92	0.40
1:G:152:GLN:HA	1:G:160:ILE:HG21	2.03	0.40
2:F:4:LEU:HD23	2:F:25:LEU:HA	2.03	0.40
2:F:144:LEU:HD12	2:F:144:LEU:HA	1.94	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	187/210 (89%)	169 (90%)	11 (6%)	7 (4%)	3 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	196/210 (93%)	179 (91%)	13 (7%)	4 (2%)	7	14
1	E	195/210 (93%)	179 (92%)	12 (6%)	4 (2%)	7	13
1	G	162/210 (77%)	146 (90%)	13 (8%)	3 (2%)	8	15
2	B	237/242 (98%)	227 (96%)	9 (4%)	1 (0%)	34	57
2	D	235/242 (97%)	224 (95%)	9 (4%)	2 (1%)	17	35
2	F	234/242 (97%)	224 (96%)	9 (4%)	1 (0%)	34	57
2	H	228/242 (94%)	217 (95%)	9 (4%)	2 (1%)	17	35
All	All	1674/1808 (93%)	1565 (94%)	85 (5%)	24 (1%)	11	22

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	132	LYS
1	E	134	SER
1	A	171	MET
1	A	188	ALA
1	C	153	SER
1	C	188	ALA
1	G	153	SER
2	H	224	ASP
1	E	186	ASP
1	E	198	ILE
1	A	153	SER
1	A	192	ALA
1	C	182	SER
2	D	100	GLU
2	D	227	LYS
2	H	185	ARG
1	C	183	ASN
1	G	156	SER
1	A	199	PRO
2	B	3	LEU
1	G	157	ASP
2	F	4	LEU
1	A	190	ALA
1	A	94	PRO

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	166/189 (88%)	150 (90%)	16 (10%)	8 16
1	C	174/189 (92%)	157 (90%)	17 (10%)	8 15
1	E	172/189 (91%)	155 (90%)	17 (10%)	8 15
1	G	145/189 (77%)	130 (90%)	15 (10%)	7 13
2	B	205/214 (96%)	191 (93%)	14 (7%)	16 32
2	D	205/214 (96%)	193 (94%)	12 (6%)	19 39
2	F	207/214 (97%)	193 (93%)	14 (7%)	16 32
2	H	192/214 (90%)	174 (91%)	18 (9%)	8 17
All	All	1466/1612 (91%)	1343 (92%)	123 (8%)	11 21

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5	GLU
1	E	9	SER
1	E	10	THR
1	E	13	VAL
1	E	20	VAL
1	E	28	THR
1	E	52	SER
1	E	53	ASN
1	E	55	ASP
1	E	68	LYS
1	E	93	SER
1	E	116	PRO
1	E	138	VAL
1	E	142	THR
1	E	157	ASP
1	E	177	SER
1	E	200	GLU
2	F	7	ASN
2	F	40	LEU

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Mol	Chain	Res	Type
2	F	69	THR
2	F	73	ASP
2	F	84	SER
2	F	99	TYR
2	F	109	LEU
2	F	114	ASP
2	F	169	CYS
2	F	191	ARG
2	F	217	GLU
2	F	225	ARG
2	F	229	VAL
2	F	240	ARG
1	A	10	THR
1	A	20	VAL
1	A	52	SER
1	A	55	ASP
1	A	93	SER
1	A	100	SER
1	A	102	TYR
1	A	138	VAL
1	A	157	ASP
1	A	177	SER
1	A	189	CYS
1	A	191	ASN
1	A	198	ILE
1	A	199	PRO
1	A	200	GLU
1	A	201	ASP
2	B	7	ASN
2	B	10	TRP
2	B	11	ARG
2	B	69	THR
2	B	84	SER
2	B	89	LEU
2	B	100	GLU
2	B	114	ASP
2	B	130	GLU
2	B	144	LEU
2	B	191	ARG
2	B	217	GLU
2	B	220	GLU
2	B	240	ARG

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Mol	Chain	Res	Type
1	C	13	VAL
1	C	20	VAL
1	C	28	THR
1	C	55	ASP
1	C	93	SER
1	C	102	TYR
1	C	129	ARG
1	C	134	SER
1	C	138	VAL
1	C	142	THR
1	C	171	MET
1	C	177	SER
1	C	182	SER
1	C	189	CYS
1	C	194	ASN
1	C	198	ILE
1	C	202	THR
2	D	3	LEU
2	D	7	ASN
2	D	73	ASP
2	D	84	SER
2	D	99	TYR
2	D	112	LEU
2	D	113	GLU
2	D	114	ASP
2	D	117	ASN
2	D	169	CYS
2	D	191	ARG
2	D	222	THR
1	G	9	SER
1	G	20	VAL
1	G	52	SER
1	G	55	ASP
1	G	73	PHE
1	G	93	SER
1	G	95	SER
1	G	101	ASN
1	G	119	GLN
1	G	128	LEU
1	G	145	ASP
1	G	151	SER
1	G	155	ASP

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Mol	Chain	Res	Type
1	G	156	SER
1	G	177	SER
2	H	7	ASN
2	H	10	TRP
2	H	12	LEU
2	H	69	THR
2	H	84	SER
2	H	89	LEU
2	H	113	GLU
2	H	114	ASP
2	H	115	LEU
2	H	130	GLU
2	H	132	GLU
2	H	150	PRO
2	H	162	LYS
2	H	169	CYS
2	H	170	THR
2	H	184	SER
2	H	191	ARG
2	H	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
2	B	29	GLN
1	C	127	GLN
1	C	194	ASN
2	D	29	GLN
1	G	38	GLN
2	H	38	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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	EDO	G	301	-	3,3,3	0.65	0	2,2,2	0.32	0
4	EDO	G	302	-	3,3,3	0.52	0	2,2,2	0.31	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
4	EDO	G	301	-	-	0/1/1/1	-
4	EDO	G	302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	302	EDO	O1-C1-C2-O2

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	195/210 (92%)	0.00	2 (1%) 82 80	30, 65, 120, 148	0
1	C	200/210 (95%)	-0.06	4 (2%) 65 60	34, 58, 115, 131	0
1	E	199/210 (94%)	0.04	7 (3%) 44 36	32, 62, 113, 145	0
1	G	167/210 (79%)	0.30	18 (10%) 5 3	34, 68, 130, 168	0
2	B	239/242 (98%)	0.15	14 (5%) 22 17	40, 71, 118, 145	0
2	D	237/242 (97%)	0.03	6 (2%) 57 51	43, 76, 122, 137	0
2	F	238/242 (98%)	-0.11	4 (1%) 70 66	37, 62, 106, 139	0
2	H	234/242 (96%)	0.30	15 (6%) 19 14	44, 93, 128, 167	0
All	All	1709/1808 (94%)	0.08	70 (4%) 37 30	30, 70, 121, 168	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	115	LEU	5.3
1	G	125	VAL	5.2
1	G	155	ASP	4.4
1	A	102	TYR	4.3
2	B	114	ASP	3.9
2	B	99	TYR	3.9
2	B	113	GLU	3.8
1	G	156	SER	3.7
2	H	180	ALA	3.6
1	C	153	SER	3.5
2	H	182	ASN	3.4
2	B	112	LEU	3.4
1	E	186	ASP	3.3
1	G	126	TYR	3.3
2	H	141	LEU	3.3
2	B	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	98	GLY	3.2
1	G	95	SER	3.2
1	E	187	PHE	3.1
2	H	183	ASP	3.1
1	G	158	VAL	3.1
2	B	13	VAL	3.1
2	B	187	CYS	3.0
2	H	196	ALA	3.0
2	F	24	ILE	2.9
2	H	179	PRO	2.9
2	H	30	TYR	2.9
1	E	185	SER	2.9
1	E	198	ILE	2.8
1	G	124	ALA	2.8
1	G	141	PHE	2.8
1	G	137	SER	2.7
2	H	181	LEU	2.7
1	G	157	ASP	2.7
2	B	221	TRP	2.6
1	G	179	VAL	2.6
2	H	198	PHE	2.6
1	C	186	ASP	2.5
2	B	118	VAL	2.5
1	G	159	TYR	2.5
2	D	10[A]	TRP	2.5
1	C	152	GLN	2.4
2	H	184	SER	2.4
1	G	173	PHE	2.4
2	F	99	TYR	2.4
1	G	151	SER	2.4
2	H	139	ALA	2.4
2	F	31	PRO	2.3
1	C	187	PHE	2.3
2	H	77	ARG	2.3
2	H	114	ASP	2.3
1	G	139	CYS	2.3
2	B	182	ASN	2.3
1	A	99	GLY	2.2
2	B	180	ALA	2.2
2	D	152	HIS	2.2
2	D	221	TRP	2.2
1	G	127	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	180	ALA	2.2
2	D	112	LEU	2.1
2	D	114	ASP	2.1
1	G	181	TRP	2.1
1	E	190	ALA	2.1
1	E	204	PHE	2.1
2	H	112	LEU	2.1
2	B	179	PRO	2.1
2	D	180	ALA	2.1
1	E	193	PHE	2.0
2	F	187	CYS	2.0
2	H	140	THR	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)

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
4	EDO	G	302	4/4	0.82	0.13	69,79,83,83	0
4	EDO	G	301	4/4	0.95	0.17	56,57,64,65	0
3	CA	C	301	1/1	0.95	0.15	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.