Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:03 pm BST

PDB ID	:	6E7O
Title	:	Crystal structure of deglycosylated human EPDR1
Authors	:	Wei, Y.; Prive, G.G.
Deposited on	:	2018-07-27
Resolution	:	3.00 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:

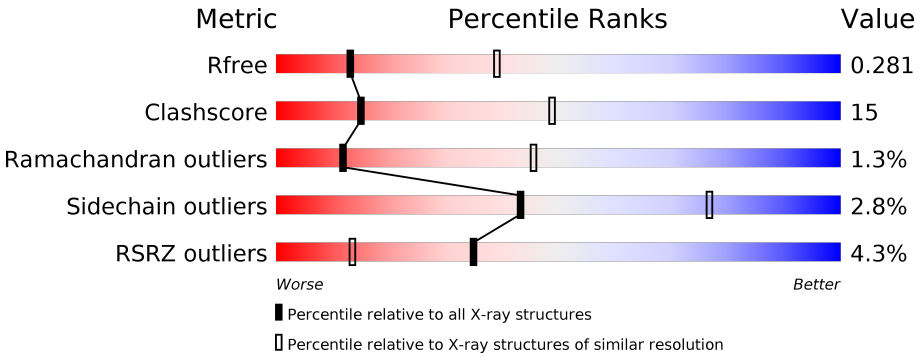
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	194	55% 29% • 14%
1	B	194	52% 29% • 17%
1	C	194	8% 54% 24% • 21%
1	D	194	6% 58% 25% • 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5040 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 Mammalian ependymin-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1327	842	218	259	8			
1	B	161	Total	C	N	O	S	0	0	0
			1280	812	207	254	7			
1	C	154	Total	C	N	O	S	0	0	0
			1158	736	182	235	5			
1	D	163	Total	C	N	O	S	0	0	0
			1275	813	206	248	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	-	expression tag	UNP Q9UM22
A	225	HIS	-	expression tag	UNP Q9UM22
A	226	HIS	-	expression tag	UNP Q9UM22
A	227	HIS	-	expression tag	UNP Q9UM22
A	228	HIS	-	expression tag	UNP Q9UM22
A	229	HIS	-	expression tag	UNP Q9UM22
A	230	HIS	-	expression tag	UNP Q9UM22
B	37	SER	-	expression tag	UNP Q9UM22
B	225	HIS	-	expression tag	UNP Q9UM22
B	226	HIS	-	expression tag	UNP Q9UM22
B	227	HIS	-	expression tag	UNP Q9UM22
B	228	HIS	-	expression tag	UNP Q9UM22
B	229	HIS	-	expression tag	UNP Q9UM22
B	230	HIS	-	expression tag	UNP Q9UM22
C	37	SER	-	expression tag	UNP Q9UM22
C	225	HIS	-	expression tag	UNP Q9UM22
C	226	HIS	-	expression tag	UNP Q9UM22
C	227	HIS	-	expression tag	UNP Q9UM22
C	228	HIS	-	expression tag	UNP Q9UM22
C	229	HIS	-	expression tag	UNP Q9UM22
C	230	HIS	-	expression tag	UNP Q9UM22

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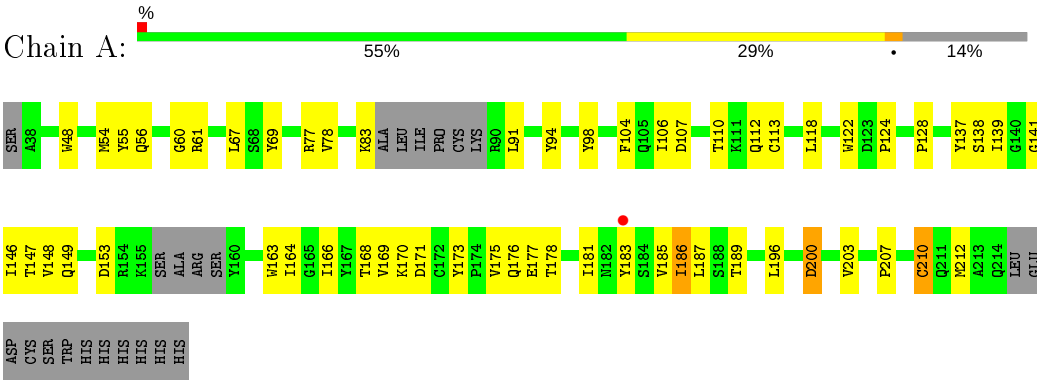
Chain	Residue	Modelled	Actual	Comment	Reference
D	37	SER	-	expression tag	UNP Q9UM22
D	225	HIS	-	expression tag	UNP Q9UM22
D	226	HIS	-	expression tag	UNP Q9UM22
D	227	HIS	-	expression tag	UNP Q9UM22
D	228	HIS	-	expression tag	UNP Q9UM22
D	229	HIS	-	expression tag	UNP Q9UM22
D	230	HIS	-	expression tag	UNP Q9UM22

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.

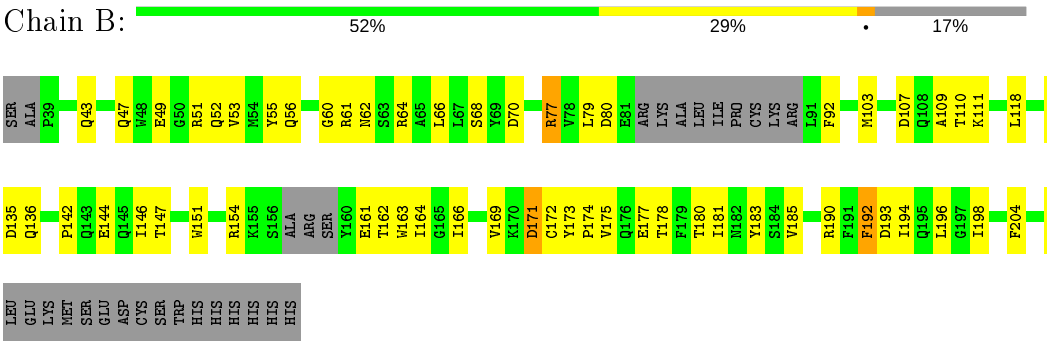
- Molecule 1: Mammalian ependymin-related protein 1

Chain A:



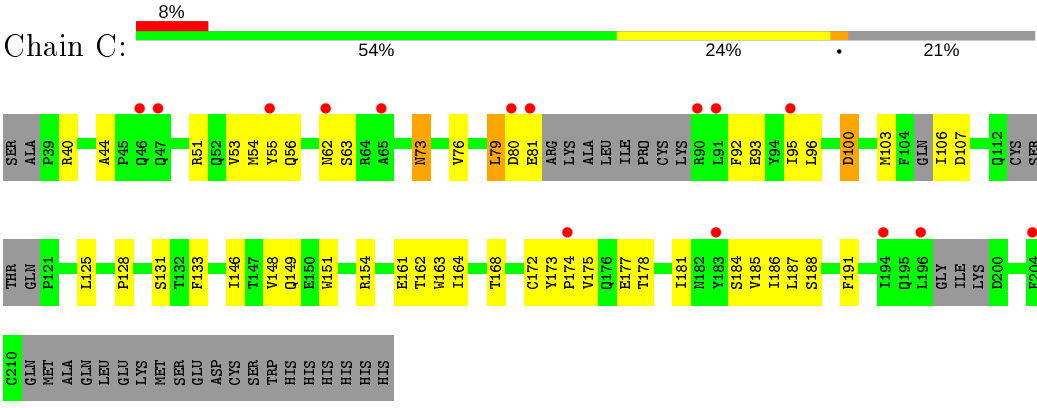
- Molecule 1: Mammalian ependymin-related protein 1

Chain B:



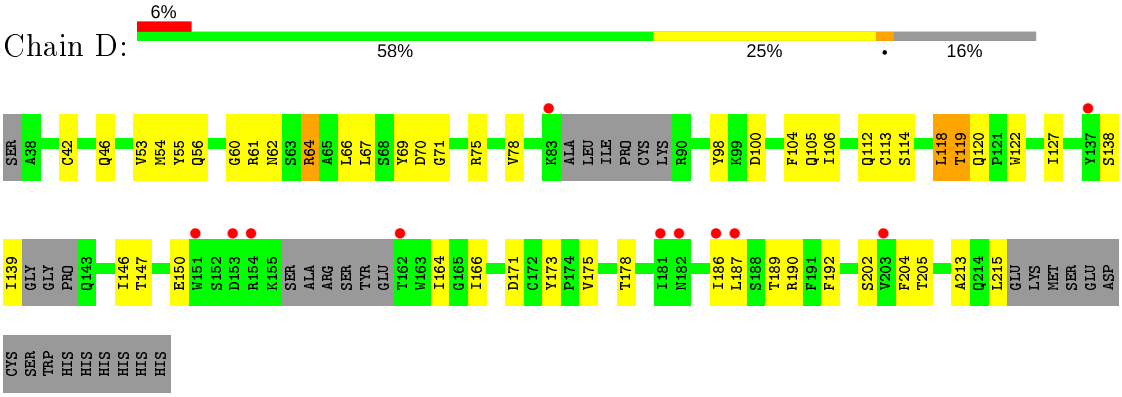
- Molecule 1: Mammalian ependymin-related protein 1

Chain C:



• Molecule 1: Mammalian ependymin-related protein 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	87.81Å 97.48Å 189.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.69 – 3.00 65.24 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.69-3.00) 91.6 (65.24-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.14_3211)	Depositor
R, R_{free}	0.255 , 0.278 0.257 , 0.281	Depositor DCC
R_{free} test set	863 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5040	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

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

[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

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	0.29	0/1358	0.57	0/1849
1	B	0.36	0/1311	0.61	1/1788 (0.1%)
1	C	0.26	0/1184	0.52	1/1621 (0.1%)
1	D	0.29	0/1304	0.55	0/1780
All	All	0.30	0/5157	0.56	2/7038 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	172	CYS	CA-CB-SG	-5.38	104.32	114.00
1	C	79	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1327	0	1240	38	0
1	B	1280	0	1184	42	0
1	C	1158	0	1007	34	0
1	D	1275	0	1172	45	0
All	All	5040	0	4603	146	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 15.

All (146) 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:C:79:LEU:HD23	1:C:93:GLU:HB3	1.56	0.85
1:D:53:VAL:HG12	1:D:64:ARG:HB3	1.60	0.84
1:A:137:TYR:OH	1:B:64:ARG:NH2	2.18	0.76
1:C:96:LEU:HD23	1:C:103:MET:HB3	1.68	0.76
1:D:114:SER:HB2	1:D:215:LEU:HD12	1.69	0.75
1:B:103:MET:HB3	1:B:118:LEU:HD13	1.67	0.75
1:A:138:SER:OG	1:A:145:GLN:OE1	2.03	0.73
1:B:47:GLN:NE2	1:B:70:ASP:OD1	2.22	0.73
1:B:161:GLU:HG2	1:B:181:ILE:HD12	1.70	0.72
1:B:127:ILE:HG22	1:B:163:TRP:HH2	1.54	0.72
1:C:185:VAL:O	1:C:187:LEU:N	2.23	0.72
1:B:109:ALA:O	1:B:111:LYS:NZ	2.22	0.72
1:A:185:VAL:O	1:A:187:LEU:N	2.22	0.71
1:B:162:THR:HG23	1:B:180:THR:HG23	1.74	0.69
1:C:154:ARG:HA	1:C:162:THR:HA	1.75	0.69
1:D:55:TYR:HB2	1:D:62:ASN:ND2	2.08	0.67
1:B:51:ARG:NH2	1:B:193:ASP:OD1	2.28	0.66
1:D:55:TYR:HB2	1:D:62:ASN:HD22	1.58	0.66
1:D:56:GLN:O	1:D:60:GLY:N	2.30	0.64
1:D:75:ARG:HH21	1:D:204:PHE:HB2	1.63	0.63
1:B:174:PRO:HD2	1:B:194:ILE:HD13	1.81	0.63
1:C:149:GLN:HG3	1:C:151:TRP:HE1	1.63	0.62
1:C:92:PHE:CB	1:C:107:ASP:HA	2.30	0.62
1:C:51:ARG:NH1	1:C:81:GLU:OE2	2.28	0.62
1:A:55:TYR:HA	1:A:61:ARG:O	1.99	0.62
1:D:104:PHE:HA	1:D:114:SER:O	2.00	0.62
1:C:161:GLU:HG2	1:C:181:ILE:HG22	1.81	0.62
1:B:154:ARG:HA	1:B:162:THR:HA	1.82	0.60
1:A:146:ILE:HG13	1:B:146:ILE:HG13	1.83	0.59
1:A:181:ILE:HG12	1:A:186:ILE:HG13	1.84	0.59
1:D:67:LEU:HD21	1:D:69:TYR:HB2	1.84	0.59
1:A:54:MET:HG3	1:A:189:THR:HG22	1.84	0.59
1:A:164:ILE:HG23	1:A:178:THR:HB	1.84	0.59
1:C:148:VAL:HG12	1:C:168:THR:HA	1.85	0.58
1:A:149:GLN:NE2	1:A:169:VAL:HG23	2.18	0.58
1:D:98:TYR:HD2	1:D:122:TRP:HB2	1.68	0.58
1:C:106:ILE:HD13	1:C:207:PRO:HD2	1.86	0.57
1:B:49:GLU:OE2	1:B:68:SER:OG	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:VAL:HG11	1:C:175:VAL:HG21	1.86	0.57
1:D:55:TYR:HA	1:D:61:ARG:O	2.05	0.56
1:C:146:ILE:HG23	1:D:146:ILE:HG12	1.87	0.56
1:C:53:VAL:HA	1:C:63:SER:O	2.06	0.56
1:D:113:CYS:O	1:D:213:ALA:HB1	2.05	0.56
1:D:56:GLN:O	1:D:60:GLY:CA	2.54	0.56
1:B:53:VAL:HG23	1:B:192:PHE:HZ	1.72	0.55
1:B:55:TYR:HA	1:B:61:ARG:O	2.07	0.55
1:D:98:TYR:CD2	1:D:122:TRP:HE3	2.25	0.54
1:A:77:ARG:HD2	1:A:203:VAL:HG12	1.89	0.54
1:C:44:ALA:HA	1:C:172:CYS:HB3	1.90	0.54
1:D:106:ILE:HA	1:D:112:GLN:O	2.09	0.53
1:B:164:ILE:HG23	1:B:178:THR:HB	1.89	0.53
1:C:178:THR:HG22	1:C:188:SER:HB2	1.90	0.53
1:A:48:TRP:HB3	1:A:196:LEU:HD23	1.90	0.53
1:B:161:GLU:HG2	1:B:181:ILE:CD1	2.39	0.53
1:C:73:ASN:ND2	1:C:73:ASN:O	2.39	0.52
1:B:111:LYS:HD3	1:B:111:LYS:N	2.24	0.52
1:D:186:ILE:O	1:D:187:LEU:HB2	2.10	0.52
1:C:163:TRP:HE1	1:C:177:GLU:CD	2.14	0.51
1:C:174:PRO:HB2	1:C:191:PHE:HD1	1.74	0.51
1:A:106:ILE:HG12	1:A:113:CYS:SG	2.51	0.51
1:A:144:GLU:OE2	1:B:171:ASP:N	2.43	0.51
1:C:76:VAL:HG13	1:C:96:LEU:HD12	1.91	0.51
1:A:168:THR:HB	1:A:173:TYR:H	1.75	0.51
1:D:53:VAL:HG21	1:D:190:ARG:CZ	2.41	0.51
1:A:200:ASP:O	1:A:203:VAL:HG23	2.11	0.50
1:D:138:SER:HA	1:D:147:THR:HA	1.94	0.50
1:A:148:VAL:HG21	1:A:166:ILE:HD11	1.93	0.50
1:B:77:ARG:NH2	1:B:79:LEU:HD22	2.26	0.50
1:D:118:LEU:O	1:D:119:THR:HG22	2.11	0.50
1:B:133:PHE:HB2	1:B:151:TRP:CZ3	2.47	0.50
1:C:128:PRO:HG2	1:C:131:SER:HB3	1.93	0.50
1:C:175:VAL:HG13	1:D:139:ILE:HD11	1.93	0.50
1:D:164:ILE:HG23	1:D:178:THR:OG1	2.10	0.50
1:C:164:ILE:HG23	1:C:178:THR:OG1	2.12	0.50
1:D:118:LEU:O	1:D:120:GLN:N	2.43	0.50
1:A:61:ARG:HG2	1:B:183:TYR:O	2.12	0.49
1:D:42:CYS:SG	1:D:127:ILE:HD12	2.52	0.49
1:D:113:CYS:HB3	1:D:213:ALA:CB	2.42	0.49
1:B:163:TRP:HE1	1:B:177:GLU:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:O	1:A:60:GLY:N	2.46	0.49
1:B:163:TRP:NE1	1:B:177:GLU:HG3	2.28	0.49
1:D:171:ASP:HB2	1:D:173:TYR:CE1	2.48	0.49
1:A:183:TYR:O	1:B:61:ARG:HG2	2.13	0.48
1:B:56:GLN:O	1:B:60:GLY:N	2.45	0.48
1:A:147:THR:O	1:A:169:VAL:HG12	2.13	0.48
1:C:56:GLN:HG2	1:C:187:LEU:HD13	1.95	0.48
1:D:150:GLU:HG2	1:D:166:ILE:HG12	1.96	0.47
1:D:105:GLN:HB2	1:D:114:SER:HB3	1.96	0.47
1:C:95:ILE:O	1:C:103:MET:HA	2.15	0.47
1:D:54:MET:HG3	1:D:189:THR:HG22	1.97	0.47
1:A:141:GLY:HA3	1:B:173:TYR:CZ	2.50	0.47
1:B:51:ARG:HG3	1:B:192:PHE:CE1	2.49	0.46
1:B:55:TYR:HB2	1:B:62:ASN:OD1	2.15	0.46
1:B:66:LEU:HD13	1:B:79:LEU:HD23	1.98	0.46
1:A:142:PRO:HD2	1:B:173:TYR:OH	2.15	0.46
1:D:215:LEU:HA	1:D:215:LEU:HD23	1.81	0.46
1:C:54:MET:O	1:C:62:ASN:HA	2.16	0.46
1:D:75:ARG:NH2	1:D:204:PHE:HB2	2.30	0.46
1:C:151:TRP:O	1:C:164:ILE:HA	2.17	0.45
1:B:107:ASP:HB3	1:B:110:THR:HB	1.98	0.45
1:B:166:ILE:O	1:B:175:VAL:HG22	2.16	0.45
1:C:55:TYR:OH	1:D:55:TYR:OH	2.31	0.45
1:A:106:ILE:HG21	1:A:207:PRO:HG2	1.97	0.45
1:B:135:ASP:OD1	1:B:136:GLN:N	2.50	0.45
1:A:128:PRO:HG2	1:A:153:ASP:OD2	2.18	0.44
1:A:166:ILE:CG2	1:A:176:GLN:HB3	2.47	0.44
1:B:147:THR:HB	1:B:169:VAL:HG11	2.00	0.44
1:A:163:TRP:HE1	1:A:177:GLU:HG2	1.82	0.44
1:D:46:GLN:HA	1:D:69:TYR:HE2	1.83	0.43
1:A:170:LYS:HB3	1:B:144:GLU:OE1	2.19	0.43
1:A:110:THR:CG2	1:A:112:GLN:HG2	2.48	0.43
1:A:78:VAL:HG13	1:A:94:TYR:HD1	1.84	0.43
1:C:133:PHE:HB2	1:C:151:TRP:CZ3	2.54	0.43
1:C:55:TYR:HB2	1:C:62:ASN:OD1	2.19	0.43
1:B:151:TRP:O	1:B:164:ILE:HA	2.18	0.43
1:D:113:CYS:HB3	1:D:213:ALA:HB2	2.00	0.43
1:D:53:VAL:HG13	1:D:192:PHE:HZ	1.84	0.43
1:D:166:ILE:O	1:D:175:VAL:HG22	2.19	0.43
1:D:118:LEU:C	1:D:120:GLN:H	2.21	0.42
1:A:122:TRP:HE1	1:A:124:PRO:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:CYS:HB3	1:A:210:CYS:HA	2.02	0.42
1:B:196:LEU:HD12	1:B:196:LEU:H	1.85	0.42
1:C:163:TRP:NE1	1:C:177:GLU:OE1	2.45	0.42
1:B:162:THR:HG23	1:B:180:THR:CG2	2.47	0.42
1:D:150:GLU:CG	1:D:166:ILE:HG12	2.49	0.42
1:A:141:GLY:O	1:A:145:GLN:HB3	2.20	0.42
1:C:168:THR:HB	1:C:173:TYR:H	1.85	0.42
1:A:166:ILE:O	1:A:175:VAL:HG22	2.20	0.42
1:C:100:ASP:OD1	1:C:100:ASP:N	2.52	0.41
1:A:104:PHE:CD2	1:A:210:CYS:SG	3.13	0.41
1:D:66:LEU:O	1:D:78:VAL:HA	2.21	0.41
1:D:114:SER:CB	1:D:215:LEU:HD12	2.46	0.41
1:C:184:SER:HA	1:D:60:GLY:O	2.21	0.41
1:A:83:LYS:HD3	1:A:83:LYS:HA	1.82	0.41
1:B:52:GLN:HA	1:B:190:ARG:O	2.21	0.41
1:D:46:GLN:O	1:D:71:GLY:N	2.48	0.41
1:D:202:SER:O	1:D:205:THR:HG22	2.20	0.41
1:D:70:ASP:HB3	1:D:75:ARG:CG	2.51	0.41
1:D:67:LEU:HD12	1:D:78:VAL:HG12	2.03	0.41
1:A:67:LEU:HD21	1:A:69:TYR:HB2	2.02	0.40
1:A:139:ILE:HD13	1:B:192:PHE:HB3	2.02	0.40
1:B:80:ASP:HB2	1:B:92:PHE:O	2.22	0.40
1:B:198:ILE:HG12	1:B:204:PHE:HE2	1.86	0.40
1:C:125:LEU:HA	1:C:125:LEU:HD23	1.93	0.40
1:D:70:ASP:HB3	1:D:75:ARG:HG2	2.03	0.40
1:A:98:TYR:HA	1:A:118:LEU:HD23	2.03	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	161/194 (83%)	153 (95%)	4 (2%)	4 (2%)	5 28
1	B	155/194 (80%)	148 (96%)	5 (3%)	2 (1%)	12 45
1	C	142/194 (73%)	132 (93%)	9 (6%)	1 (1%)	22 60
1	D	155/194 (80%)	148 (96%)	6 (4%)	1 (1%)	25 64
All	All	613/776 (79%)	581 (95%)	24 (4%)	8 (1%)	12 45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ILE
1	B	185	VAL
1	C	186	ILE
1	D	119	THR
1	A	107	ASP
1	A	200	ASP
1	A	91	LEU
1	B	142	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	145/179 (81%)	142 (98%)	3 (2%)	53 82
1	B	142/179 (79%)	137 (96%)	5 (4%)	36 71
1	C	119/179 (66%)	115 (97%)	4 (3%)	37 72
1	D	137/179 (76%)	134 (98%)	3 (2%)	52 81
All	All	543/716 (76%)	528 (97%)	15 (3%)	43 77

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	A	210	CYS
1	A	212	MET

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Mol	Chain	Res	Type
1	B	43	GLN
1	B	77	ARG
1	B	171	ASP
1	B	192	PHE
1	B	211	GLN
1	C	40	ARG
1	C	73	ASN
1	C	80	ASP
1	C	100	ASP
1	D	64	ARG
1	D	100	ASP
1	D	118	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	62	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	167/194 (86%)	-0.00	1 (0%) 89 72	51, 82, 126, 149	0
1	B	161/194 (82%)	-0.08	0 100 100	42, 74, 108, 152	0
1	C	154/194 (79%)	0.58	16 (10%) 6 2	81, 114, 176, 185	0
1	D	163/194 (84%)	0.32	11 (6%) 17 5	75, 104, 144, 152	0
All	All	645/776 (83%)	0.20	28 (4%) 35 13	42, 94, 149, 185	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	162	THR	7.1
1	C	196	LEU	4.7
1	C	205	THR	4.0
1	D	182	ASN	3.9
1	C	194	ILE	3.8
1	C	62	ASN	3.7
1	C	80	ASP	3.6
1	D	181	ILE	3.4
1	C	204	PHE	3.3
1	C	90	ARG	3.2
1	C	91	LEU	3.1
1	C	174	PRO	3.0
1	D	151	TRP	2.7
1	D	154	ARG	2.4
1	D	137	TYR	2.4
1	C	81	GLU	2.4
1	C	65	ALA	2.3
1	C	183	TYR	2.3
1	C	46	GLN	2.3
1	C	55	TYR	2.3
1	D	203	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	47	GLN	2.2
1	D	83	LYS	2.2
1	D	186	ILE	2.2
1	D	187	LEU	2.1
1	D	153	ASP	2.1
1	C	95	ILE	2.1
1	A	183	TYR	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.