Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 06:14 PM EST

PDB ID	:	1CNT
Title	:	CILIARY NEUROTROPHIC FACTOR
Authors	:	Mcdonald, N.Q.; Panayotatos, N.; Hendrickson, W.A.
Deposited on	:	1996-06-06
Resolution	:	2.40 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 (i)) were used in the production of this report:

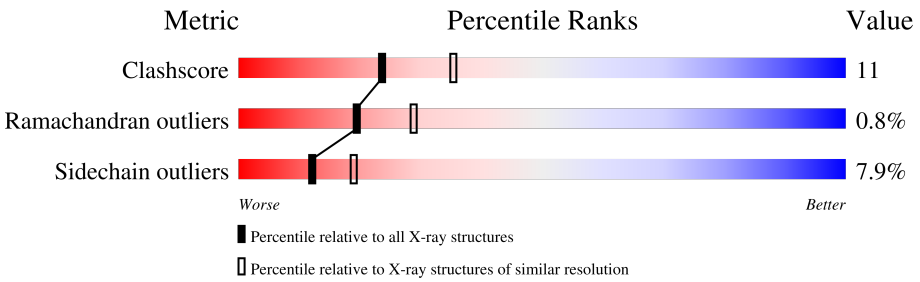
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	187	57% 21% • 20%
1	2	187	44% 25% • 30%
1	3	187	55% 22% •• 22%
1	4	187	44% 21% • 33%

2 Entry composition (i)

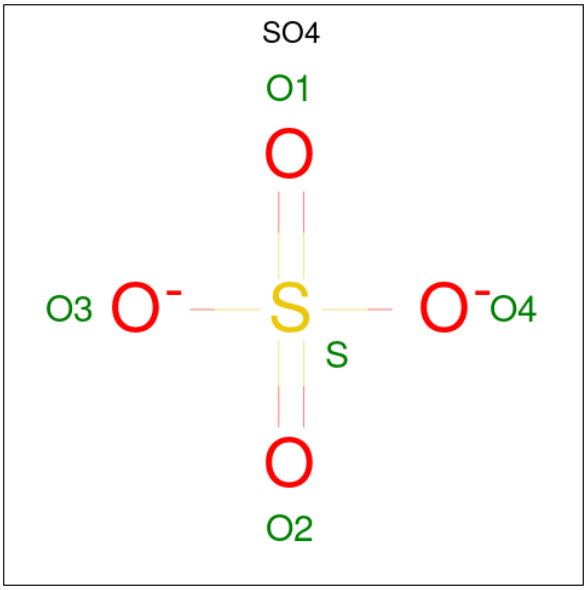
There are 4 unique types of molecules in this entry. The entry contains 4756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CILIARY NEUROTROPHIC FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	150	1243	797	219	224	3	0	0	0
			Total	C	N	O	S			
1	2	130	1081	696	194	189	2	0	0	0
			Total	C	N	O	S			
1	3	146	1209	775	217	215	2	0	0	0
			Total	C	N	O	S			
1	4	126	1053	675	189	187	2	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	1	1	5	4	1	0	0
			Total	O	S		
2	1	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	3	1	Total O S 5 4 1	0	0
2	3	1	Total O S 5 4 1	0	0

- Molecule 3 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	3	1	Total Yb 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1	49	Total O 49 49	0	0
4	2	28	Total O 28 28	0	0
4	3	40	Total O 40 40	0	0
4	4	32	Total O 32 32	0	0

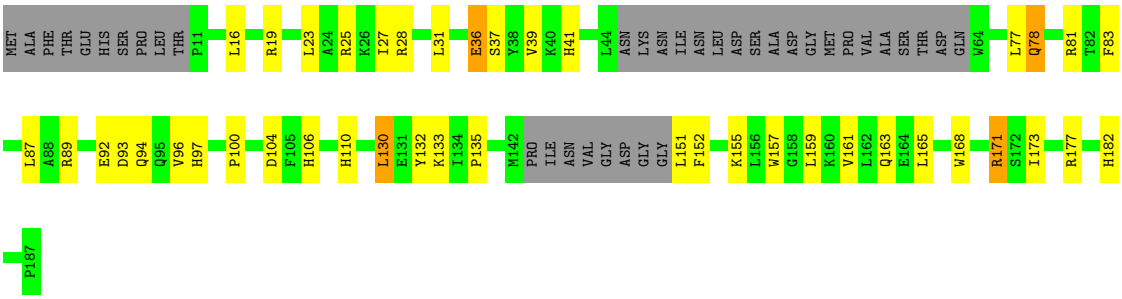
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

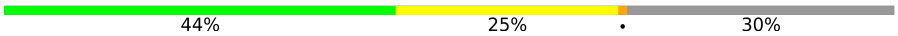
• Molecule 1: CILIARY NEUROTROPHIC FACTOR

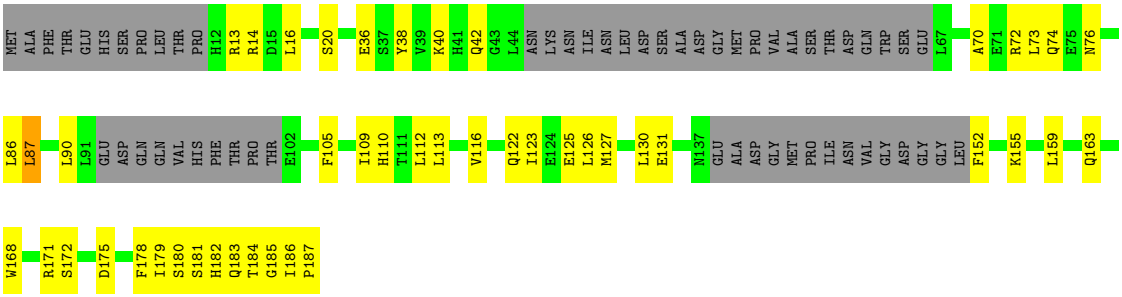
Chain 1:



• Molecule 1: CILIARY NEUROTROPHIC FACTOR

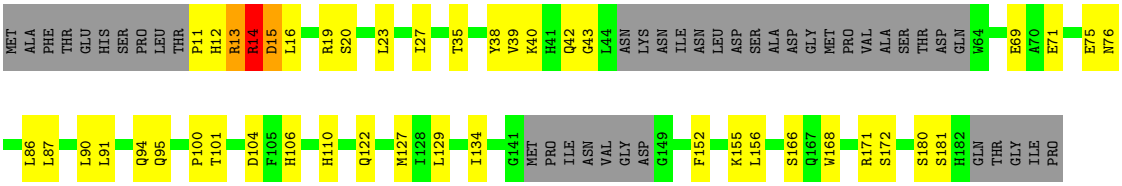
Chain 2:





• Molecule 1: CILIARY NEUROTROPHIC FACTOR

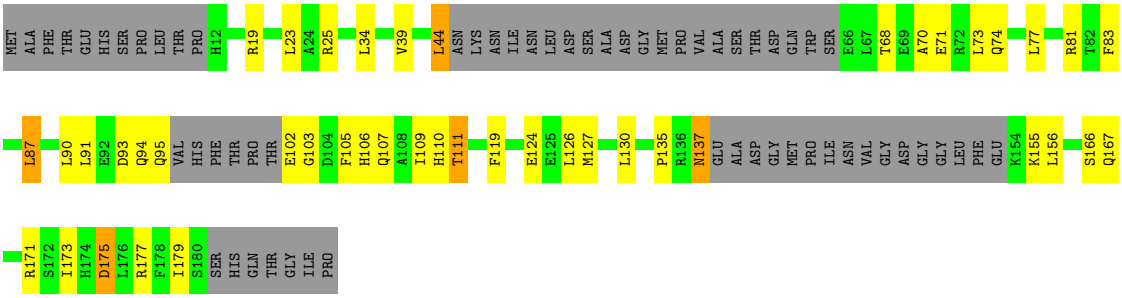
Chain 3:



• Molecule 1: CILIARY NEUROTROPHIC FACTOR

Chain 4:

44%
21%
•
33%


MET
ALA
PHE
THR
GLU
HIS
SER
PRO
LEU
THR
PRO
H12
R19
L23
A24
R25
L34
V39
L44
ASN
LYS
ASN
ILE
ASN
LEU
ASP
SER
ALA
ASP
GLY
MET
PRO
VAL
ALA
SER
THR
ASP
GLN
TRP
SER
E66
L67
T68
E69
A70
E71
R72
L73
Q74
L77
R81
T82
F83
L87
L90
L91
E92
D93
Q94
Q95
VAL
HIS
PHE
THR
PRO
THR
E102
G103
D104
F105
H106
Q107
A108
I109
H110
T111
F119
E124
E125
L126
M127
L130
P135
R136
N137
GLU
ALA
ASP
GLY
MET
PRO
ILE
ASN
VAL
GLY
ASP
GLY
GLY
LEU
PHE
GLU
K154
K155
L156
S166
Q167
R171
S172
I173
H174
D175
L176
R177
F178
I179
S180
SER
HIS
GLN
THR
GLY
ILE
PRO

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.95Å 62.09Å 208.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

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: SO4, YB

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	1	0.33	0/1270	0.55	0/1715
1	2	0.33	0/1101	0.53	0/1482
1	3	0.33	0/1235	0.56	0/1667
1	4	0.35	0/1070	0.55	0/1440
All	All	0.33	0/4676	0.55	0/6304

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	1243	0	1237	25	0
1	2	1081	0	1097	30	0
1	3	1209	0	1205	26	0
1	4	1053	0	1066	24	0
2	1	10	0	0	0	0
2	3	10	0	0	0	0
3	3	1	0	0	0	0
4	1	49	0	0	0	0
4	2	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	40	0	0	3	0
4	4	32	0	0	3	0
All	All	4756	0	4605	103	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 11.

All (103) 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)
1:2:14:ARG:HH21	1:2:187:PRO:HD3	1.47	0.80
1:1:25:ARG:HH21	1:1:177:ARG:HH21	1.36	0.74
1:1:78:GLN:HE22	1:1:81:ARG:HH11	1.38	0.70
1:2:181:SER:HB3	1:2:187:PRO:HD2	1.74	0.69
1:2:178:PHE:O	1:2:182:HIS:HB2	1.94	0.68
1:3:152:PHE:HA	1:3:155:LYS:HD2	1.78	0.65
1:4:81:ARG:HD3	1:4:137:ASN:HB3	1.79	0.64
1:3:13:ARG:HG2	1:3:180:SER:OG	1.98	0.64
1:1:173:ILE:O	1:1:177:ARG:HG3	1.97	0.64
1:2:20:SER:HA	1:2:122:GLN:HE22	1.62	0.64
1:3:35:THR:O	1:3:39:VAL:HG23	1.98	0.63
1:4:83:PHE:O	1:4:87:LEU:HD22	1.99	0.63
1:3:71:GLU:O	1:3:75:GLU:HG3	2.01	0.61
1:1:25:ARG:HH21	1:1:177:ARG:NH2	2.00	0.60
1:4:34:LEU:HD21	1:4:109:ILE:HD13	1.83	0.60
1:4:23:LEU:HD23	1:4:119:PHE:HA	1.85	0.58
1:3:43:GLY:HA2	4:3:958:HOH:O	2.03	0.58
1:4:107:GLN:O	1:4:111:THR:HG23	2.04	0.57
1:1:25:ARG:NH2	1:1:177:ARG:NH2	2.54	0.56
1:2:152:PHE:HD1	1:2:155:LYS:HD3	1.70	0.56
1:1:168:TRP:CZ3	1:1:171:ARG:HG2	2.41	0.55
1:3:168:TRP:CZ3	1:3:171:ARG:HG2	2.42	0.54
1:2:159:LEU:O	1:2:163:GLN:HG3	2.07	0.54
1:2:181:SER:CB	1:2:187:PRO:HD2	2.36	0.54
1:1:159:LEU:O	1:1:163:GLN:HG3	2.08	0.54
1:4:25:ARG:HH22	1:4:177:ARG:HH21	1.56	0.54
1:4:175:ASP:O	1:4:179:ILE:HG13	2.08	0.54
1:4:73:LEU:HD21	1:4:126:LEU:HD23	1.90	0.53
1:2:184:THR:HB	1:2:186:ILE:HG13	1.91	0.53
1:2:87:LEU:HB3	1:2:113:LEU:HD21	1.90	0.53
1:4:77:LEU:HD21	1:4:81:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:77:LEU:HD23	1:1:135:PRO:HD2	1.90	0.53
1:2:73:LEU:HD21	1:2:126:LEU:HD23	1.90	0.52
1:3:20:SER:HA	1:3:122:GLN:NE2	2.23	0.52
1:1:93:ASP:O	1:1:97:HIS:HB3	2.09	0.52
1:1:96:VAL:HG12	1:1:96:VAL:O	2.10	0.52
1:2:20:SER:HA	1:2:122:GLN:NE2	2.26	0.51
1:1:23:LEU:O	1:1:27:ILE:HG13	2.11	0.51
1:2:112:LEU:O	1:2:116:VAL:HG23	2.11	0.50
1:3:95:GLN:HG2	1:3:106:HIS:CE1	2.46	0.50
1:3:13:ARG:NH2	1:3:181:SER:HA	2.27	0.50
1:3:127:MET:HB2	1:3:134:ILE:HD11	1.92	0.49
1:4:103:GLY:HA2	4:4:832:HOH:O	2.12	0.49
1:3:20:SER:HA	1:3:122:GLN:HE22	1.78	0.49
1:4:68:THR:OG1	1:4:71:GLU:HB2	2.14	0.48
1:2:72:ARG:HH11	1:2:175:ASP:HA	1.78	0.48
1:3:91:LEU:HD21	1:3:110:HIS:CE1	2.49	0.48
1:4:91:LEU:HD21	1:4:110:HIS:HE1	1.79	0.48
1:2:13:ARG:HD3	1:2:179:ILE:O	2.14	0.47
1:3:13:ARG:HH21	1:3:181:SER:HA	1.78	0.47
1:4:95:GLN:HA	1:4:106:HIS:HE1	1.80	0.47
1:1:110:HIS:HE1	1:4:124:GLU:OE1	1.98	0.47
1:2:123:ILE:O	1:2:127:MET:HG3	2.15	0.47
1:2:38:TYR:O	1:2:42:GLN:HG2	2.15	0.46
1:4:25:ARG:HG2	1:4:173:ILE:HD11	1.97	0.46
1:2:152:PHE:HA	1:2:155:LYS:HD3	1.98	0.46
1:3:100:PRO:HD2	4:3:977:HOH:O	2.16	0.45
1:2:16:LEU:HB3	1:2:126:LEU:HD13	1.98	0.45
1:2:186:ILE:HB	1:2:187:PRO:HD3	1.98	0.45
1:3:14:ARG:O	1:3:16:LEU:N	2.49	0.45
1:2:14:ARG:HG2	1:2:180:SER:HB2	1.99	0.44
1:4:91:LEU:HD21	1:4:110:HIS:CE1	2.52	0.44
1:2:181:SER:O	1:2:185:GLY:HA2	2.17	0.44
1:1:152:PHE:HA	1:1:155:LYS:HD2	2.00	0.44
1:4:105:PHE:O	1:4:109:ILE:HG12	2.18	0.44
1:3:38:TYR:O	1:3:42:GLN:HG2	2.18	0.44
1:1:31:LEU:HD11	1:1:165:LEU:HG	1.99	0.44
1:4:90:LEU:O	1:4:94:GLN:HG2	2.17	0.44
1:4:70:ALA:HB3	4:4:851:HOH:O	2.18	0.44
1:1:37:SER:O	1:1:41:HIS:CD2	2.70	0.43
1:2:14:ARG:NH2	1:2:187:PRO:HD3	2.26	0.43
1:1:182:HIS:CD2	1:1:182:HIS:N	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:70:ALA:O	1:2:74:GLN:HG2	2.19	0.43
1:3:19:ARG:NH2	1:3:122:GLN:HG2	2.34	0.43
1:3:11:PRO:HB2	1:3:129:LEU:HD21	2.00	0.43
1:3:23:LEU:O	1:3:27:ILE:HG13	2.19	0.43
1:1:16:LEU:HD13	1:1:19:ARG:NH2	2.33	0.43
1:2:87:LEU:O	1:2:90:LEU:HB2	2.19	0.42
1:2:125:GLU:OE2	1:3:110:HIS:HD2	2.02	0.42
1:2:76:ASN:HD21	1:2:172:SER:HA	1.84	0.42
1:2:110:HIS:HB3	4:3:817:HOH:O	2.19	0.42
1:1:151:LEU:O	1:1:155:LYS:HG3	2.19	0.42
1:3:42:GLN:NE2	1:3:94:GLN:OE1	2.52	0.42
1:3:152:PHE:CE2	1:3:156:LEU:HD11	2.54	0.42
1:3:14:ARG:HB3	1:3:15:ASP:H	1.48	0.42
1:4:155:LYS:HB2	1:4:155:LYS:NZ	2.34	0.42
1:2:175:ASP:O	1:2:179:ILE:HG13	2.20	0.41
1:4:74:GLN:HA	1:4:127:MET:HE1	2.02	0.41
1:1:37:SER:O	1:1:41:HIS:HD2	2.04	0.41
1:2:14:ARG:HH21	1:2:187:PRO:CD	2.24	0.41
1:4:74:GLN:HB3	4:4:824:HOH:O	2.20	0.41
1:1:83:PHE:CZ	1:1:165:LEU:HA	2.55	0.41
1:1:157:TRP:O	1:1:161:VAL:HG23	2.21	0.41
1:1:36:GLU:O	1:1:39:VAL:HG22	2.21	0.41
1:1:133:LYS:HA	1:1:133:LYS:HD2	1.93	0.41
1:2:105:PHE:O	1:2:109:ILE:HG12	2.20	0.41
1:3:12:HIS:HE1	1:3:69:GLU:OE1	2.04	0.41
1:4:19:ARG:O	1:4:23:LEU:HB2	2.21	0.40
1:1:94:GLN:HB3	1:1:106:HIS:HE1	1.86	0.40
1:1:130:LEU:HB3	1:1:132:TYR:CE2	2.56	0.40
1:3:76:ASN:ND2	1:3:172:SER:OG	2.54	0.40
1:4:39:VAL:HA	1:4:44:LEU:CD1	2.51	0.40
1:3:127:MET:HB2	1:3:134:ILE:CD1	2.52	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	1	144/187 (77%)	138 (96%)	5 (4%)	1 (1%)	22	32
1	2	122/187 (65%)	120 (98%)	2 (2%)	0	100	100
1	3	140/187 (75%)	134 (96%)	4 (3%)	2 (1%)	11	15
1	4	118/187 (63%)	114 (97%)	3 (2%)	1 (1%)	19	29
All	All	524/748 (70%)	506 (97%)	14 (3%)	4 (1%)	19	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	15	ASP
1	1	100	PRO
1	3	14	ARG
1	4	135	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	1	134/165 (81%)	125 (93%)	9 (7%)	16	26
1	2	116/165 (70%)	107 (92%)	9 (8%)	12	19
1	3	129/165 (78%)	120 (93%)	9 (7%)	15	24
1	4	113/165 (68%)	101 (89%)	12 (11%)	6	9
All	All	492/660 (74%)	453 (92%)	39 (8%)	12	19

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	28	ARG
1	1	36	GLU
1	1	78	GLN
1	1	87	LEU

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Mol	Chain	Res	Type
1	1	89	ARG
1	1	92	GLU
1	1	104	ASP
1	1	130	LEU
1	1	171	ARG
1	2	36	GLU
1	2	40	LYS
1	2	86	LEU
1	2	87	LEU
1	2	130	LEU
1	2	131	GLU
1	2	168	TRP
1	2	171	ARG
1	2	183	GLN
1	3	13	ARG
1	3	14	ARG
1	3	40	LYS
1	3	86	LEU
1	3	87	LEU
1	3	90	LEU
1	3	101	THR
1	3	104	ASP
1	3	166	SER
1	4	44	LEU
1	4	87	LEU
1	4	93	ASP
1	4	102	GLU
1	4	111	THR
1	4	130	LEU
1	4	137	ASN
1	4	156	LEU
1	4	166	SER
1	4	167	GLN
1	4	171	ARG
1	4	175	ASP

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

Mol	Chain	Res	Type
1	1	41	HIS
1	1	42	GLN
1	1	74	GLN

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Mol	Chain	Res	Type
1	1	76	ASN
1	1	78	GLN
1	1	94	GLN
1	1	110	HIS
1	1	115	GLN
1	1	122	GLN
1	2	76	ASN
1	2	122	GLN
1	3	12	HIS
1	3	42	GLN
1	3	76	ASN
1	3	94	GLN
1	3	95	GLN
1	3	110	HIS
1	3	122	GLN
1	3	163	GLN
1	4	76	ASN
1	4	106	HIS
1	4	110	HIS
1	4	115	GLN
1	4	137	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	SO4	3	192	-	4,4,4	0.62	0	6,6,6	0.09	0
2	SO4	1	191	-	4,4,4	0.65	0	6,6,6	0.07	0
2	SO4	1	190	-	4,4,4	0.56	0	6,6,6	0.16	0
2	SO4	3	189	3	4,4,4	0.53	0	6,6,6	0.21	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.