Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 03:09 pm GMT

PDB ID	:	5NNB
Title	:	Isatin hydrolase A (IHA) from Labrenzia aggregata with isatinate bound
Authors	:	Sommer, T.; Bjerregaard-Andersen, K.; Morth, J.P.
Deposited on	:	2017-04-08
Resolution	:	1.80 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:

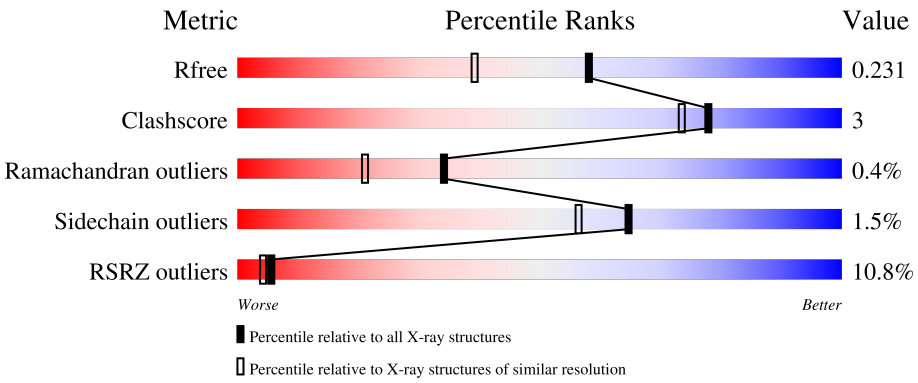
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	257	8% 92% 7% •
1	B	257	3% 89% 9% ••
1	C	257	26% 94% 5% •
1	D	257	6% 89% 9% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8278 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.

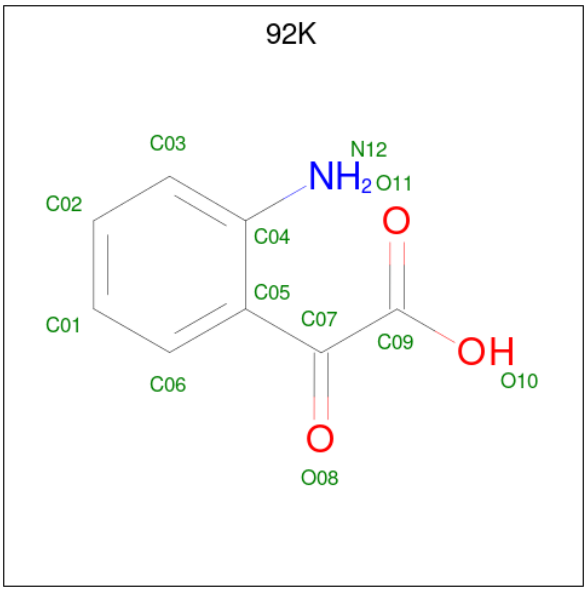
- Molecule 1 is a protein called isatin hydrolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	1951	1235	342	366	8	0	0	0
1	B	255	1951	1235	342	366	8	0	0	0
1	C	255	1955	1239	342	366	8	0	1	0
1	D	255	1951	1235	342	366	8	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is Isatinic acid (three-letter code: 92K) (formula: $C_8H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	8	1	3	0	0
			Total	C	N	O		
3	B	1	12	8	1	3	0	0
			Total	C	N	O		
3	D	1	12	8	1	3	0	0

- Molecule 4 is water.

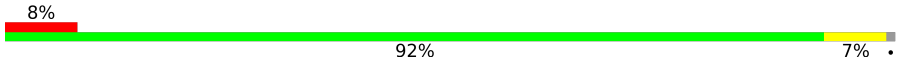
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	104	104	104	0	0
			Total	O		
4	B	144	144	144	0	0
			Total	O		
4	C	73	73	73	0	0
			Total	O		
4	D	109	109	109	0	0

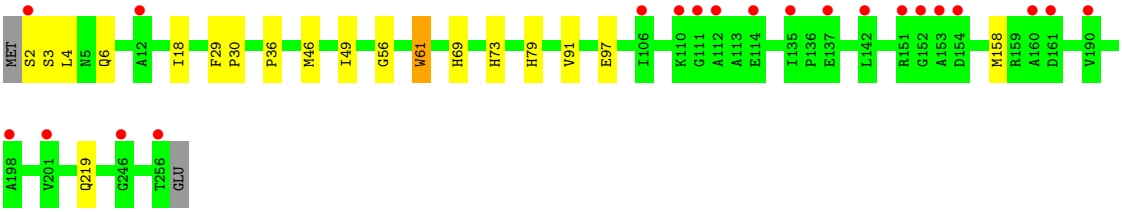
3 Residue-property plots (i)

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: isatin hydrolase A

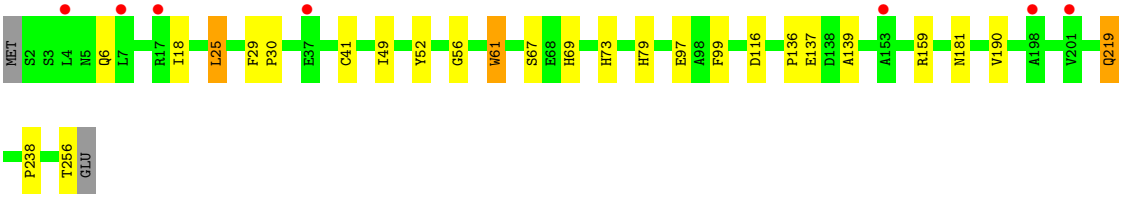
Chain A:





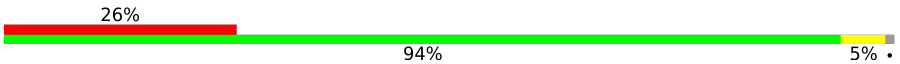
• Molecule 1: isatin hydrolase A

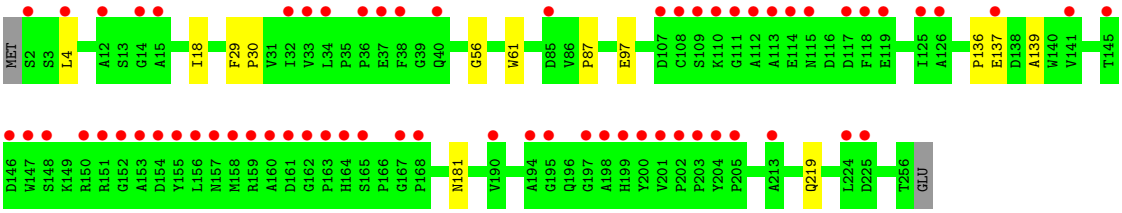
Chain B:



• Molecule 1: isatin hydrolase A

Chain C:





• Molecule 1: isatin hydrolase A

Chain D:

MET
S2
A12
I18
P36
R45
M46
E47
E48
I49
G56
P57
A58
W61
H69
H73
H79
E97
A98
F99
K110
E114
E119
P136
E137
D138
A139
W140
K149
D154
M158
R159
A160
D161
I177
A198
H199
Y200
V201
P202
L210
K215
L218
Q219
P238
T256
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.35Å 69.92Å 93.54Å 108.23° 95.26° 103.76°	Depositor
Resolution (Å)	19.50 – 1.80 19.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.7 (19.50-1.80) 94.0 (19.50-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.188 , 0.228 0.194 , 0.231	Depositor DCC
R_{free} test set	3842 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8278	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 92K

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	0.37	0/2008	0.50	0/2742
1	B	0.38	0/2008	0.54	1/2742 (0.0%)
1	C	0.34	0/2015	0.50	0/2752
1	D	0.35	0/2008	0.49	0/2742
All	All	0.36	0/8039	0.51	1/10978 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	25	LEU	CA-CB-CG	5.68	128.36	115.30

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	A	1951	0	1881	13	0
1	B	1951	0	1881	17	0
1	C	1955	0	1890	7	0
1	D	1951	0	1881	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	0	1	0
3	B	12	0	0	3	0
3	D	12	0	0	2	0
4	A	104	0	0	0	0
4	B	144	0	0	1	0
4	C	73	0	0	1	0
4	D	109	0	0	3	0
All	All	8278	0	7533	44	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 3.

All (44) 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:D:79:HIS:NE2	3:D:302:92K:O10	2.04	0.90
1:B:79:HIS:NE2	3:B:302:92K:O11	2.12	0.83
1:A:79:HIS:NE2	3:A:302:92K:O11	2.11	0.83
1:A:18:ILE:HD12	1:B:97:GLU:HA	1.73	0.69
1:C:97:GLU:HA	1:D:18:ILE:HD12	1.81	0.62
1:C:18:ILE:HD12	1:D:97:GLU:HA	1.80	0.61
1:C:4:LEU:HD12	1:D:256:THR:HG23	1.85	0.58
1:A:97:GLU:HA	1:B:18:ILE:HD12	1.84	0.57
1:C:137:GLU:HG3	1:C:181:ASN:HB3	1.87	0.56
1:B:137:GLU:HG3	1:B:181:ASN:HB3	1.88	0.55
1:B:116:ASP:OD2	1:B:159:ARG:NH2	2.42	0.52
1:D:136:PRO:HG2	1:D:139:ALA:HB2	1.92	0.52
1:D:49:ILE:HB	1:D:61:TRP:CD1	2.45	0.51
1:D:45:ARG:NH1	4:D:406:HOH:O	2.43	0.51
1:D:149:LYS:NZ	4:D:404:HOH:O	2.40	0.51
1:D:119:GLU:OE2	1:D:200:TYR:OH	2.25	0.50
1:A:6:GLN:HE22	1:B:6:GLN:NE2	2.09	0.49
1:D:79:HIS:CD2	3:D:302:92K:O10	2.64	0.49
1:A:49:ILE:HB	1:A:61:TRP:CD1	2.48	0.48
1:B:79:HIS:HE2	3:B:302:92K:C09	2.22	0.48
1:A:2:SER:OG	1:A:3:SER:N	2.45	0.48
1:C:136:PRO:HG2	1:C:139:ALA:HB2	1.97	0.47
1:D:69:HIS:HA	1:D:73:HIS:CD2	2.50	0.47
1:A:158:MET:HG2	1:D:36:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:HIS:CD2	3:B:302:92K:O11	2.66	0.47
1:B:219:GLN:OE1	4:B:401:HOH:O	2.20	0.47
1:A:69:HIS:HA	1:A:73:HIS:CD2	2.50	0.46
1:D:140:TRP:CH2	1:D:218:LEU:HG	2.50	0.46
1:C:29:PHE:HA	1:C:30:PRO:HD3	1.79	0.46
1:B:136:PRO:HG2	1:B:139:ALA:HB2	1.98	0.46
1:A:4:LEU:HD12	1:B:256:THR:HG23	2.00	0.44
1:B:41:CYS:HG	1:B:67:SER:HG	1.60	0.44
1:A:6:GLN:HE22	1:B:6:GLN:HE22	1.66	0.44
1:B:99:PHE:CE1	1:B:238:PRO:HD2	2.53	0.43
1:A:36:PRO:HG3	1:D:158:MET:HG2	2.00	0.43
1:B:69:HIS:HA	1:B:73:HIS:CD2	2.54	0.43
1:B:29:PHE:HA	1:B:30:PRO:HD3	1.86	0.42
1:B:49:ILE:HB	1:B:61:TRP:CD1	2.55	0.42
1:A:29:PHE:HA	1:A:30:PRO:HD3	1.93	0.42
1:C:87:PRO:HD3	4:C:451:HOH:O	2.20	0.42
1:D:99:PHE:CE1	1:D:238:PRO:HD2	2.55	0.41
1:D:177:ILE:HD11	1:D:210:LEU:HA	2.02	0.41
1:A:46:MET:HB2	1:A:46:MET:HE3	1.98	0.40
1:D:215:LYS:NZ	4:D:415:HOH:O	2.55	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	253/257 (98%)	247 (98%)	5 (2%)	1 (0%)	34	21
1	B	253/257 (98%)	247 (98%)	5 (2%)	1 (0%)	34	21
1	C	254/257 (99%)	248 (98%)	5 (2%)	1 (0%)	34	21
1	D	253/257 (98%)	246 (97%)	6 (2%)	1 (0%)	34	21
All	All	1013/1028 (98%)	988 (98%)	21 (2%)	4 (0%)	34	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLY
1	B	56	GLY
1	C	56	GLY
1	D	56	GLY

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	205/207 (99%)	202 (98%)	3 (2%)	65	56
1	B	205/207 (99%)	200 (98%)	5 (2%)	49	36
1	C	206/207 (100%)	204 (99%)	2 (1%)	76	71
1	D	205/207 (99%)	203 (99%)	2 (1%)	76	71
All	All	821/828 (99%)	809 (98%)	12 (2%)	65	56

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	TRP
1	A	91	VAL
1	A	219	GLN
1	B	25	LEU
1	B	52	TYR
1	B	61	TRP
1	B	190	VAL
1	B	219	GLN
1	C	61	TRP
1	C	219	GLN
1	D	61	TRP
1	D	219	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	B	6	GLN
1	D	6	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	92K	B	302	2	12,12,12	1.09	1 (8%)	15,16,16	1.59	4 (26%)
3	92K	A	302	2	12,12,12	1.19	1 (8%)	15,16,16	1.54	3 (20%)
3	92K	D	302	2	12,12,12	1.40	3 (25%)	15,16,16	1.31	2 (13%)

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	92K	B	302	2	-	3/8/8/8	0/1/1/1
3	92K	A	302	2	-	3/8/8/8	0/1/1/1
3	92K	D	302	2	-	6/8/8/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	92K	C09-C07	-2.60	1.52	1.54
3	A	302	92K	C09-C07	-2.58	1.52	1.54
3	D	302	92K	O11-C09	2.31	1.28	1.22
3	B	302	92K	C05-C07	2.20	1.53	1.49
3	D	302	92K	C05-C07	2.09	1.53	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	92K	O10-C09-C07	3.65	123.72	113.22
3	A	302	92K	O10-C09-C07	3.27	122.64	113.22
3	D	302	92K	C03-C04-C05	3.12	121.12	118.10
3	A	302	92K	C03-C04-C05	2.64	120.66	118.10
3	B	302	92K	C04-C05-C07	2.43	125.36	121.52
3	B	302	92K	O10-C09-O11	-2.38	118.17	123.61
3	A	302	92K	C04-C05-C07	2.34	125.22	121.52
3	B	302	92K	C03-C04-C05	2.31	120.33	118.10
3	D	302	92K	C04-C05-C07	2.02	124.71	121.52

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	92K	C04-C05-C07-C09
3	B	302	92K	C04-C05-C07-C09
3	D	302	92K	C04-C05-C07-C09
3	D	302	92K	O08-C07-C09-O10
3	A	302	92K	C04-C05-C07-O08
3	B	302	92K	C04-C05-C07-O08
3	D	302	92K	C05-C07-C09-O10
3	D	302	92K	C06-C05-C07-C09
3	D	302	92K	C04-C05-C07-O08
3	D	302	92K	C06-C05-C07-O08
3	A	302	92K	C06-C05-C07-O08
3	B	302	92K	C06-C05-C07-O08

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	92K	3	0
3	A	302	92K	1	0
3	D	302	92K	2	0

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	255/257 (99%)	0.56	21 (8%) 11 9	22, 34, 57, 85	0
1	B	255/257 (99%)	0.40	7 (2%) 54 49	22, 31, 50, 75	0
1	C	255/257 (99%)	1.34	66 (25%) 0 0	23, 46, 94, 121	0
1	D	255/257 (99%)	0.57	16 (6%) 20 15	22, 34, 56, 76	0
All	All	1020/1028 (99%)	0.72	110 (10%) 5 4	22, 35, 69, 121	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	VAL	9.7
1	C	152	GLY	8.3
1	C	198	ALA	7.7
1	C	201	VAL	7.6
1	C	113	ALA	6.9
1	C	162	GLY	6.8
1	C	194	ALA	6.4
1	D	202	PRO	6.1
1	D	161	ASP	5.8
1	C	118	PHE	5.5
1	C	147	TRP	5.3
1	C	204	TYR	5.0
1	C	157	ASN	5.0
1	C	203	PRO	4.9
1	C	151	ARG	4.8
1	C	165	SER	4.7
1	C	202	PRO	4.7
1	C	150	ARG	4.7
1	C	153	ALA	4.5
1	C	200	TYR	4.4
1	C	114	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	154	ASP	4.4
1	C	110	LYS	4.3
1	C	158	MET	4.2
1	D	47	GLU	4.1
1	C	159	ARG	3.9
1	D	160	ALA	3.9
1	A	161	ASP	3.8
1	C	155	TYR	3.8
1	C	119	GLU	3.8
1	C	117	ASP	3.6
1	A	201	VAL	3.5
1	C	109	SER	3.5
1	C	36	PRO	3.5
1	C	161	ASP	3.4
1	A	110	LYS	3.4
1	C	190	VAL	3.4
1	C	156	LEU	3.4
1	D	57	PRO	3.3
1	A	114	GLU	3.3
1	C	195	GLY	3.2
1	C	213	ALA	3.2
1	D	110	LYS	3.1
1	C	163	PRO	3.1
1	D	12	ALA	3.1
1	C	160	ALA	3.1
1	C	167	GLY	3.1
1	C	225	ASP	3.1
1	C	148	SER	3.0
1	D	149	LYS	3.0
1	A	160	ALA	3.0
1	A	151	ARG	3.0
1	C	37	GLU	3.0
1	A	256	THR	2.9
1	D	154	ASP	2.9
1	C	112	ALA	2.9
1	C	34	LEU	2.9
1	A	152	GLY	2.9
1	C	2	SER	2.8
1	C	168	PRO	2.8
1	B	201	VAL	2.8
1	C	199	HIS	2.8
1	A	112	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	198	ALA	2.7
1	A	2	SER	2.7
1	C	15	ALA	2.7
1	C	197	GLY	2.7
1	A	137	GLU	2.7
1	B	7	LEU	2.7
1	C	146	ASP	2.6
1	B	37	GLU	2.6
1	B	198	ALA	2.6
1	A	106	ILE	2.6
1	D	45	ARG	2.6
1	C	33	VAL	2.6
1	A	142	LEU	2.5
1	C	126	ALA	2.5
1	A	154	ASP	2.4
1	C	145	THR	2.4
1	C	164	HIS	2.4
1	D	114	GLU	2.4
1	C	111	GLY	2.4
1	C	115	ASN	2.4
1	C	40	GLN	2.4
1	C	224	LEU	2.3
1	A	12	ALA	2.3
1	C	107	ASP	2.3
1	C	12	ALA	2.3
1	C	4	LEU	2.3
1	B	17	ARG	2.3
1	C	14	GLY	2.2
1	B	153	ALA	2.2
1	C	125	ILE	2.2
1	C	85	ASP	2.2
1	A	190	VAL	2.2
1	C	38	PHE	2.2
1	D	58	ALA	2.2
1	A	246	GLY	2.2
1	C	32	ILE	2.1
1	A	153	ALA	2.1
1	C	141	VAL	2.1
1	B	4	LEU	2.1
1	D	199	HIS	2.1
1	D	198	ALA	2.1
1	C	205	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	137	GLU	2.1
1	A	111	GLY	2.1
1	A	135	ILE	2.1
1	C	108	CYS	2.0
1	C	137	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	92K	B	302	12/12	0.80	0.19	40,43,50,51	0
3	92K	D	302	12/12	0.88	0.22	25,33,46,49	0
3	92K	A	302	12/12	0.91	0.19	32,37,51,55	0
2	MN	B	301	1/1	0.99	0.10	27,27,27,27	0
2	MN	C	301	1/1	0.99	0.05	32,32,32,32	0
2	MN	D	301	1/1	0.99	0.08	25,25,25,25	0
2	MN	A	301	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.