



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 02:50 AM EDT

PDB ID : 5BQB
Title : Crystal structure of Norrin, a Wnt signalling activator, Crystal Form III
Authors : Chang, T.-H.; Hsieh, F.-L.; Harlos, K.; Jones, E.Y.
Deposited on : 2015-05-28
Resolution : 2.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) 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

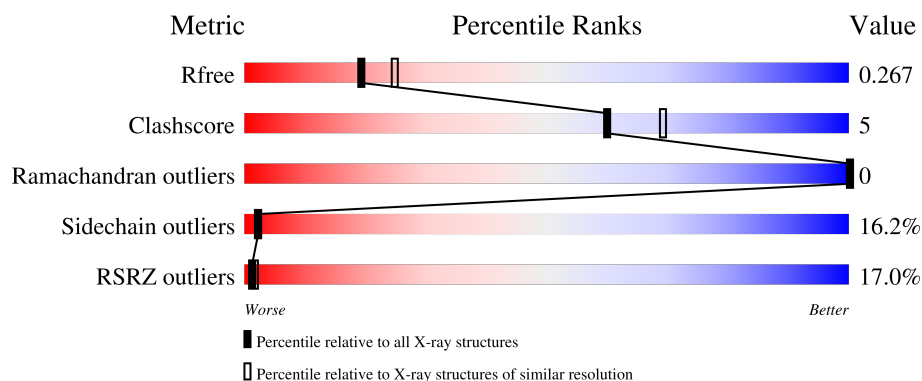
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	122	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>11%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	122	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>15%</div> <div>•</div> <div>20%</div> </div> </div>
1	C	122	<div> <div>14%</div> <div> <div></div> <div>65%</div> <div>15%</div> <div>•</div> <div>20%</div> </div> </div>
1	D	122	<div> <div>33%</div> <div> <div></div> <div>57%</div> <div>21%</div> <div>•</div> <div>20%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	203	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3230 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 Norrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			782	477	153	138	14			
1	B	98	Total	C	N	O	S	0	0	0
			774	473	152	135	14			
1	C	98	Total	C	N	O	S	0	0	0
			774	473	152	135	14			
1	D	98	Total	C	N	O	S	0	0	0
			774	473	152	135	14			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q00604
A	23	PRO	-	expression tag	UNP Q00604
A	24	GLY	-	expression tag	UNP Q00604
A	134	GLY	-	expression tag	UNP Q00604
A	135	THR	-	expression tag	UNP Q00604
A	136	GLU	-	expression tag	UNP Q00604
A	137	THR	-	expression tag	UNP Q00604
A	138	SER	-	expression tag	UNP Q00604
A	139	GLN	-	expression tag	UNP Q00604
A	140	VAL	-	expression tag	UNP Q00604
A	141	ALA	-	expression tag	UNP Q00604
A	142	PRO	-	expression tag	UNP Q00604
A	143	ALA	-	expression tag	UNP Q00604
B	22	GLY	-	expression tag	UNP Q00604
B	23	PRO	-	expression tag	UNP Q00604
B	24	GLY	-	expression tag	UNP Q00604
B	134	GLY	-	expression tag	UNP Q00604
B	135	THR	-	expression tag	UNP Q00604
B	136	GLU	-	expression tag	UNP Q00604
B	137	THR	-	expression tag	UNP Q00604
B	138	SER	-	expression tag	UNP Q00604

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	139	GLN	-	expression tag	UNP Q00604
B	140	VAL	-	expression tag	UNP Q00604
B	141	ALA	-	expression tag	UNP Q00604
B	142	PRO	-	expression tag	UNP Q00604
B	143	ALA	-	expression tag	UNP Q00604
C	22	GLY	-	expression tag	UNP Q00604
C	23	PRO	-	expression tag	UNP Q00604
C	24	GLY	-	expression tag	UNP Q00604
C	134	GLY	-	expression tag	UNP Q00604
C	135	THR	-	expression tag	UNP Q00604
C	136	GLU	-	expression tag	UNP Q00604
C	137	THR	-	expression tag	UNP Q00604
C	138	SER	-	expression tag	UNP Q00604
C	139	GLN	-	expression tag	UNP Q00604
C	140	VAL	-	expression tag	UNP Q00604
C	141	ALA	-	expression tag	UNP Q00604
C	142	PRO	-	expression tag	UNP Q00604
C	143	ALA	-	expression tag	UNP Q00604
D	22	GLY	-	expression tag	UNP Q00604
D	23	PRO	-	expression tag	UNP Q00604
D	24	GLY	-	expression tag	UNP Q00604
D	134	GLY	-	expression tag	UNP Q00604
D	135	THR	-	expression tag	UNP Q00604
D	136	GLU	-	expression tag	UNP Q00604
D	137	THR	-	expression tag	UNP Q00604
D	138	SER	-	expression tag	UNP Q00604
D	139	GLN	-	expression tag	UNP Q00604
D	140	VAL	-	expression tag	UNP Q00604
D	141	ALA	-	expression tag	UNP Q00604
D	142	PRO	-	expression tag	UNP Q00604
D	143	ALA	-	expression tag	UNP Q00604

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	25	Total	O	0	0
			25	25		
4	C	7	Total	O	0	0
			7	7		

Continued on next page...

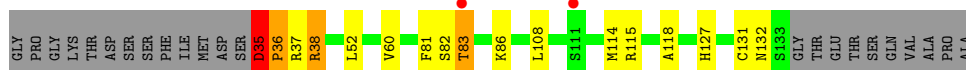
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O	0	0
			1	1		

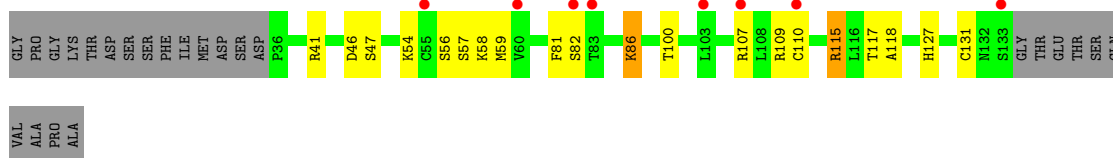
3 Residue-property plots [i](#)

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.

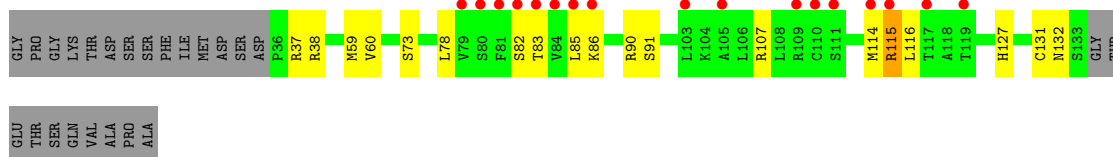
• Molecule 1: Norrin



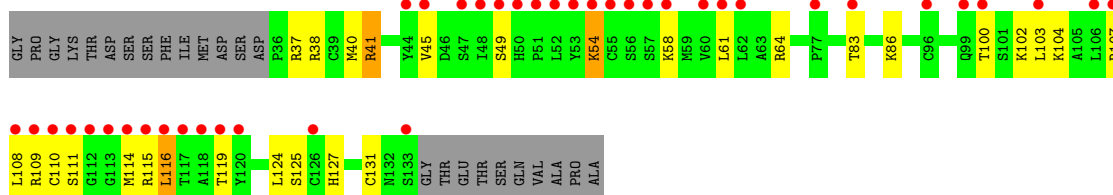
• Molecule 1: Norrin



• Molecule 1: Norrin



• Molecule 1: Norrin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.76Å 38.09Å 177.20Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	44.19 – 2.30 44.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.19-2.30) 99.1 (44.19-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.251 0.250 , 0.267	Depositor DCC
R_{free} test set	1354 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3230	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, CL

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	0.44	0/798	0.72	2/1070 (0.2%)
1	B	0.31	0/790	0.50	0/1058
1	C	0.36	0/790	0.48	0/1058
1	D	0.25	0/790	0.47	0/1058
All	All	0.35	0/3168	0.55	2/4244 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	38	ARG	N-CA-CB	-12.92	87.34	110.60
1	A	35	ASP	C-N-CD	6.02	141.04	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	PRO	Mainchain

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	782	0	771	8	0
1	B	774	0	768	9	0
1	C	774	0	768	3	0
1	D	774	0	768	9	0
2	A	26	0	10	1	0
2	C	26	0	10	2	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	39	0	0	0	0
4	B	25	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
All	All	3230	0	3095	29	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 5.

All (29) 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:82:SER:OG	1:A:83:THR:N	2.26	0.67
1:A:35:ASP:N	1:A:35:ASP:OD1	2.32	0.62
1:D:110:CYS:N	1:D:114:MET:O	2.34	0.60
1:B:41:ARG:NH1	2:C:201:CIT:O5	2.35	0.60
1:D:108:LEU:O	1:D:116:LEU:N	2.38	0.56
1:C:82:SER:OG	1:C:83:THR:N	2.39	0.56
1:D:41:ARG:NE	1:D:124:LEU:O	2.41	0.53
2:A:202:CIT:O4	2:A:202:CIT:O7	2.18	0.53
1:D:100:THR:OG1	1:D:125:SER:N	2.42	0.52
2:C:202:CIT:O3	2:C:202:CIT:O7	2.24	0.52
1:D:41:ARG:HD2	1:D:125:SER:HA	1.90	0.52
1:A:35:ASP:N	1:A:36:PRO:CD	2.72	0.52
1:B:46:ASP:OD1	1:B:47:SER:N	2.45	0.49
1:B:86:LYS:H	1:B:86:LYS:CD	2.24	0.49
1:C:38:ARG:HH11	1:C:38:ARG:HG2	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PHE:CE2	1:B:118:ALA:HB2	2.50	0.47
1:D:54:LYS:O	1:D:111:SER:OG	2.16	0.47
1:A:35:ASP:HA	1:A:38:ARG:NH1	2.29	0.47
1:D:45:VAL:HG12	1:D:61:LEU:HA	1.97	0.46
1:D:103:LEU:HD12	1:D:104:LYS:N	2.31	0.45
1:D:110:CYS:SG	1:D:111:SER:N	2.92	0.43
1:A:81:PHE:CD1	1:A:81:PHE:N	2.87	0.42
1:C:115:ARG:N	1:C:115:ARG:HD2	2.35	0.42
1:A:35:ASP:N	1:A:36:PRO:HD2	2.34	0.41
1:B:107:ARG:N	1:B:107:ARG:CD	2.83	0.41
1:B:86:LYS:H	1:B:86:LYS:HD3	1.85	0.41
1:B:47:SER:HA	1:B:59:MET:HA	2.03	0.41
1:A:118:ALA:HB2	1:B:81:PHE:CE2	2.56	0.41
1:B:115:ARG:H	1:B:115:ARG:HG3	1.79	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	97/122 (80%)	96 (99%)	1 (1%)	0	100	100
1	B	96/122 (79%)	93 (97%)	3 (3%)	0	100	100
1	C	96/122 (79%)	92 (96%)	4 (4%)	0	100	100
1	D	96/122 (79%)	88 (92%)	8 (8%)	0	100	100
All	All	385/488 (79%)	369 (96%)	16 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	92/110 (84%)	80 (87%)	12 (13%)	4	4
1	B	91/110 (83%)	78 (86%)	13 (14%)	3	3
1	C	91/110 (83%)	75 (82%)	16 (18%)	2	1
1	D	91/110 (83%)	73 (80%)	18 (20%)	1	1
All	All	365/440 (83%)	306 (84%)	59 (16%)	2	2

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	37	ARG
1	A	52	LEU
1	A	60	VAL
1	A	83	THR
1	A	86	LYS
1	A	108	LEU
1	A	114	MET
1	A	115	ARG
1	A	127	HIS
1	A	131	CYS
1	A	132	ASN
1	B	54	LYS
1	B	56	SER
1	B	57	SER
1	B	58	LYS
1	B	82	SER
1	B	86	LYS
1	B	100	THR
1	B	109	ARG
1	B	110	CYS
1	B	115	ARG
1	B	117	THR
1	B	127	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	131	CYS
1	C	37	ARG
1	C	59	MET
1	C	60	VAL
1	C	73	SER
1	C	78	LEU
1	C	85	LEU
1	C	86	LYS
1	C	90	ARG
1	C	91	SER
1	C	107	ARG
1	C	114	MET
1	C	115	ARG
1	C	116	LEU
1	C	127	HIS
1	C	131	CYS
1	C	132	ASN
1	D	37	ARG
1	D	38	ARG
1	D	40	MET
1	D	41	ARG
1	D	49	SER
1	D	54	LYS
1	D	58	LYS
1	D	64	ARG
1	D	83	THR
1	D	86	LYS
1	D	102	LYS
1	D	107	ARG
1	D	109	ARG
1	D	115	ARG
1	D	116	LEU
1	D	119	THR
1	D	127	HIS
1	D	131	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	94	HIS
1	D	99	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are 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	CIT	C	202	-	12,12,12	0.98	0	17,17,17	1.64	1 (5%)
2	CIT	C	201	-	12,12,12	1.12	0	17,17,17	1.68	3 (17%)
2	CIT	A	201	-	12,12,12	1.01	0	17,17,17	1.65	4 (23%)
2	CIT	A	202	-	12,12,12	1.17	0	17,17,17	1.61	4 (23%)

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
2	CIT	C	202	-	-	10/16/16/16	-
2	CIT	C	201	-	-	7/16/16/16	-
2	CIT	A	201	-	-	2/16/16/16	-
2	CIT	A	202	-	-	11/16/16/16	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	202	CIT	O6-C6-C3	4.60	121.03	113.05
2	A	201	CIT	O6-C6-C3	4.57	120.98	113.05
2	A	202	CIT	O6-C6-C3	4.40	120.69	113.05
2	C	201	CIT	O6-C6-C3	4.32	120.55	113.05
2	A	201	CIT	O2-C1-C2	2.40	122.04	114.35
2	A	202	CIT	O2-C1-C2	2.27	121.64	114.35
2	C	201	CIT	O2-C1-C2	2.10	121.11	114.35
2	A	201	CIT	O2-C1-O1	-2.09	118.08	123.30
2	A	201	CIT	O4-C5-C4	2.08	121.02	114.35
2	A	202	CIT	O2-C1-O1	-2.06	118.16	123.30
2	C	201	CIT	C3-C4-C5	-2.01	108.94	113.81
2	A	202	CIT	O5-C6-C3	-2.00	119.42	122.25

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	CIT	O7-C3-C4-C5
2	C	202	CIT	O7-C3-C4-C5
2	C	202	CIT	O7-C3-C6-O5
2	C	202	CIT	O7-C3-C6-O6
2	C	202	CIT	C4-C3-C6-O5
2	C	202	CIT	C4-C3-C6-O6
2	C	201	CIT	C1-C2-C3-O7
2	C	201	CIT	C1-C2-C3-C6
2	C	201	CIT	C2-C3-C4-C5
2	C	201	CIT	C6-C3-C4-C5
2	C	202	CIT	C6-C3-C4-C5
2	C	201	CIT	C1-C2-C3-C4
2	C	202	CIT	C2-C3-C4-C5
2	A	202	CIT	O7-C3-C4-C5
2	A	202	CIT	C6-C3-C4-C5
2	A	202	CIT	C4-C3-C6-O5
2	A	202	CIT	C2-C3-C4-C5
2	C	202	CIT	C1-C2-C3-O7
2	A	202	CIT	C3-C4-C5-O3
2	A	202	CIT	C3-C4-C5-O4
2	A	202	CIT	C4-C3-C6-O6
2	C	201	CIT	C2-C3-C6-O6
2	C	202	CIT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	202	CIT	C1-C2-C3-C6
2	A	202	CIT	C2-C3-C6-O5
2	A	202	CIT	C2-C3-C6-O6
2	A	202	CIT	O2-C1-C2-C3
2	A	201	CIT	O2-C1-C2-C3
2	A	202	CIT	O1-C1-C2-C3
2	A	201	CIT	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	202	CIT	1	0
2	C	201	CIT	1	0
2	A	202	CIT	1	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

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, 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	99/122 (81%)	0.60	2 (2%) 65 71	34, 59, 123, 175	0
1	B	98/122 (80%)	0.85	8 (8%) 11 15	37, 71, 118, 141	0
1	C	98/122 (80%)	1.45	17 (17%) 1 1	56, 85, 157, 185	0
1	D	98/122 (80%)	2.51	40 (40%) 0 0	62, 121, 183, 223	0
All	All	393/488 (80%)	1.35	67 (17%) 1 2	34, 82, 163, 223	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	MET	12.2
1	D	110	CYS	10.1
1	D	115	ARG	10.0
1	D	55	CYS	9.6
1	C	81	PHE	9.3
1	C	85	LEU	8.9
1	D	112	GLY	8.2
1	C	79	VAL	8.2
1	D	61	LEU	7.9
1	D	60	VAL	7.1
1	D	118	ALA	7.0
1	D	107	ARG	6.9
1	C	82	SER	6.5
1	D	58	LYS	6.0
1	D	49	SER	5.9
1	D	56	SER	5.6
1	D	45	VAL	5.5
1	D	116	LEU	5.3
1	D	111	SER	5.2
1	C	83	THR	5.2
1	D	106	LEU	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	83	THR	5.2
1	D	120	TYR	4.8
1	C	80	SER	4.8
1	C	84	VAL	4.8
1	D	50	HIS	4.4
1	C	109	ARG	4.1
1	C	110	CYS	4.1
1	D	99	GLN	4.1
1	D	48	ILE	3.8
1	D	109	ARG	3.8
1	D	51	PRO	3.7
1	D	119	THR	3.5
1	B	107	ARG	3.5
1	B	110	CYS	3.5
1	D	44	TYR	3.5
1	D	100	THR	3.4
1	D	47	SER	3.3
1	D	108	LEU	3.3
1	D	113	GLY	3.2
1	D	133	SER	3.2
1	C	111	SER	3.1
1	D	57	SER	3.1
1	C	86	LYS	2.9
1	C	114	MET	2.9
1	A	83	THR	2.8
1	B	133	SER	2.7
1	B	60	VAL	2.7
1	D	52	LEU	2.7
1	D	53	TYR	2.6
1	C	117	THR	2.6
1	C	115	ARG	2.5
1	C	119	THR	2.5
1	A	111	SER	2.5
1	C	103	LEU	2.4
1	B	55	CYS	2.4
1	D	126	CYS	2.4
1	B	82	SER	2.4
1	C	105	ALA	2.3
1	D	96	CYS	2.2
1	D	54	LYS	2.2
1	D	117	THR	2.2
1	B	83	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	77	PRO	2.1
1	B	103	LEU	2.1
1	D	103	LEU	2.1
1	D	62	LEU	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(\AA^2)	Q<0.9
3	CL	A	203	1/1	0.40	0.72	198,198,198,198	0
2	CIT	A	202	13/13	0.52	0.31	132,160,200,200	0
2	CIT	C	202	13/13	0.56	0.32	111,177,221,228	0
2	CIT	C	201	13/13	0.57	0.28	94,149,161,164	0
3	CL	D	201	1/1	0.76	0.27	101,101,101,101	0
2	CIT	A	201	13/13	0.86	0.21	53,74,97,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.