



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 07:12 PM EDT

PDB ID : 9BY5 / pdb_00009by5
Title : Crystal Structure of RT-PhyR (ruthe_01174)
Authors : Swingle, D.; Isiorho, E.A.; Gardner, K.H.
Deposited on : 2024-05-23
Resolution : 1.99 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 : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

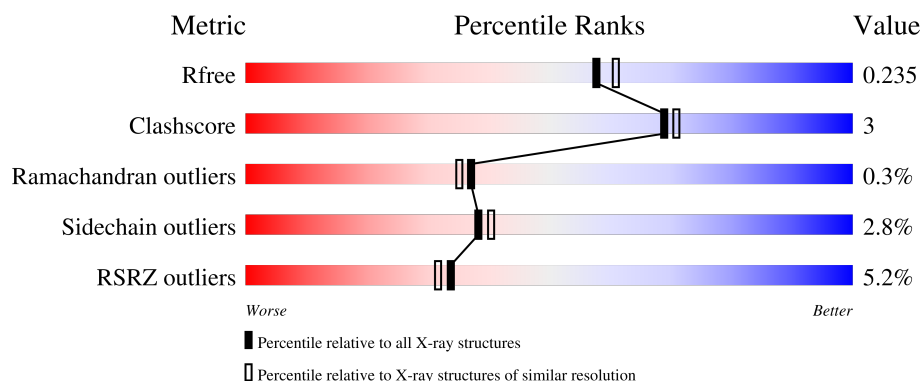
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


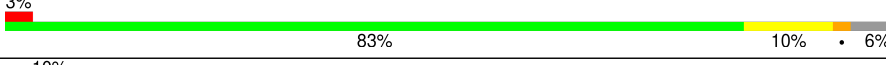

The reported resolution of this entry is 1.99 Å.

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 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	271	
1	B	271	
1	C	271	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11765 atoms, of which 5790 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 Response regulator receiver protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	248	Total	C	H	N	O	S	0	0	0
			3818	1194	1914	336	369	5			
1	B	256	Total	C	H	N	O	S	0	0	0
			3919	1225	1961	344	384	5			
1	C	245	Total	C	H	N	O	S	0	0	0
			3793	1187	1903	333	365	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP S9SJ09
A	2	PHE	-	expression tag	UNP S9SJ09
B	1	GLU	-	expression tag	UNP S9SJ09
B	2	PHE	-	expression tag	UNP S9SJ09
C	1	GLU	-	expression tag	UNP S9SJ09
C	2	PHE	-	expression tag	UNP S9SJ09

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

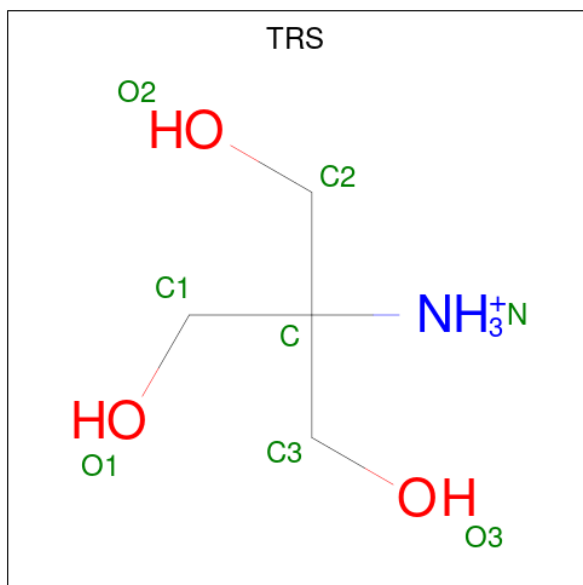
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		

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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

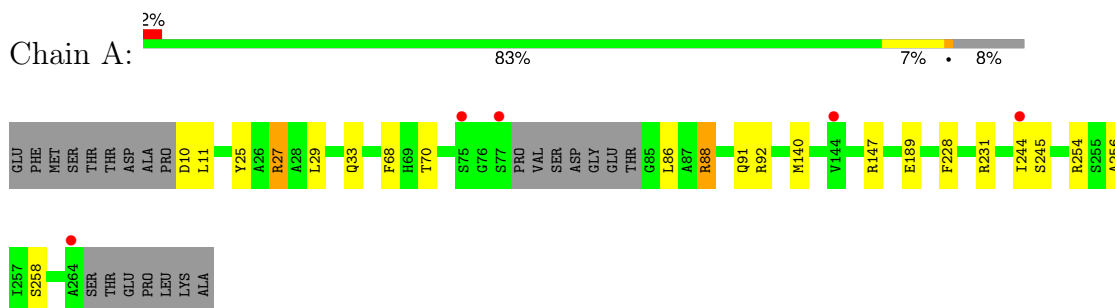
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	0	0
			103	103		
5	B	58	Total	O	0	0
			58	58		
5	C	47	Total	O	0	0
			47	47		

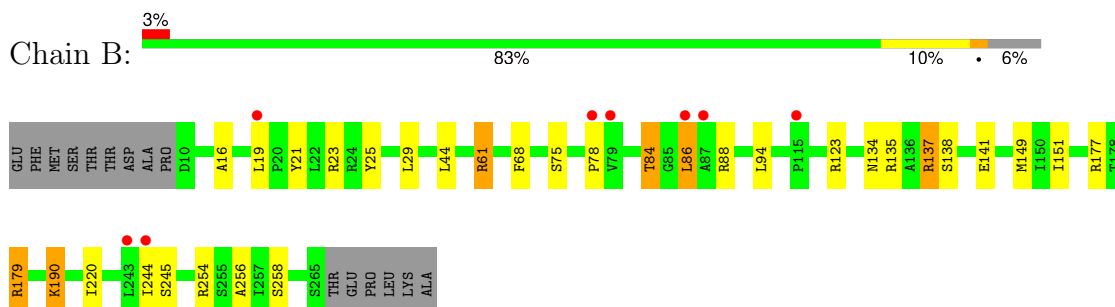
3 Residue-property plots [i](#)

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.

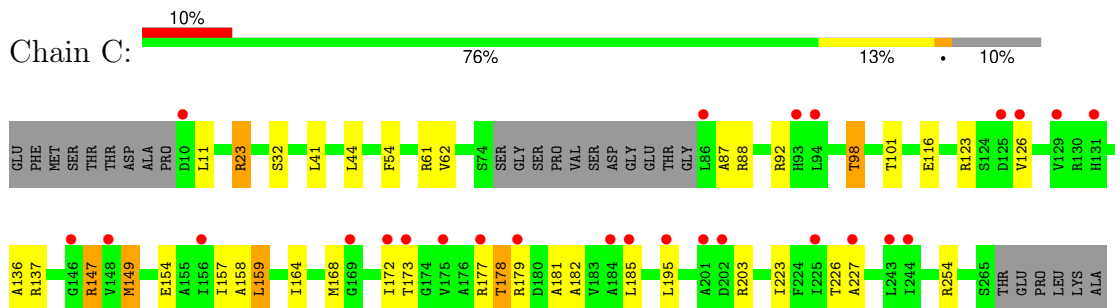
- Molecule 1: Response regulator receiver protein



- Molecule 1: Response regulator receiver protein



- Molecule 1: Response regulator receiver protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.91Å 118.64Å 121.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 – 1.99 34.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.00-1.99) 99.9 (34.00-1.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.209 , 0.237 0.207 , 0.235	Depositor DCC
R_{free} test set	2657 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11765	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: TRS, NA, MG

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	0.58	1/1932 (0.1%)	0.83	2/2624 (0.1%)
1	B	0.66	0/1988	0.98	2/2703 (0.1%)
1	C	0.69	1/1918 (0.1%)	1.05	7/2606 (0.3%)
All	All	0.64	2/5838 (0.0%)	0.96	11/7933 (0.1%)

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	4
1	B	0	9
1	C	0	9
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	PHE	C-O	-6.96	1.16	1.24
1	C	23	ARG	C-O	-6.58	1.16	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	PHE	CA-C-O	-8.57	111.47	120.55
1	A	70	THR	CA-CB-OG1	-7.51	98.34	109.60
1	B	68	PHE	CA-C-O	-7.24	112.88	120.55
1	B	134	ASN	CA-C-O	-6.89	113.25	120.55
1	C	227	ALA	N-CA-C	-6.16	100.47	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ALA	O-C-N	6.03	128.51	122.12
1	C	158	ALA	CA-C-O	-5.91	114.29	120.55
1	C	62	VAL	CA-C-O	-5.91	114.91	121.17
1	C	159	LEU	CA-C-O	-5.89	114.63	120.82
1	C	227	ALA	CA-C-O	-5.59	114.68	121.05
1	C	98	THR	CA-CB-OG1	-5.35	101.57	109.60

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ARG	Sidechain
1	A	27	ARG	Sidechain
1	A	88	ARG	Sidechain
1	A	92	ARG	Sidechain
1	B	123	ARG	Sidechain
1	B	135	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	179	ARG	Sidechain
1	B	23	ARG	Sidechain
1	B	254	ARG	Sidechain
1	B	61	ARG	Sidechain
1	B	88	ARG	Sidechain
1	C	147	ARG	Sidechain
1	C	177	ARG	Sidechain
1	C	179	ARG	Sidechain
1	C	203	ARG	Sidechain
1	C	23	ARG	Sidechain
1	C	254	ARG	Sidechain
1	C	61	ARG	Sidechain
1	C	88	ARG	Sidechain
1	C	92	ARG	Sidechain

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	1904	1914	1914	10	0
1	B	1958	1961	1961	13	0
1	C	1890	1903	1903	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
4	B	8	12	12	0	0
5	A	103	0	0	0	0
5	B	58	0	0	0	0
5	C	47	0	0	0	0
All	All	5975	5790	5790	39	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 (39) 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:B:138:SER:O	1:B:141:GLU:HG2	1.79	0.81
1:C:123:ARG:HG2	1:C:123:ARG:HH11	1.44	0.81
1:A:147:ARG:HD2	1:A:189:GLU:OE2	1.84	0.78
1:A:228:PHE:HB3	1:A:231:ARG:HD2	1.72	0.70
1:C:164:ILE:HG22	1:C:168:MET:HE2	1.74	0.69
1:B:244:ILE:HD11	1:B:256:ALA:HB2	1.78	0.64
1:B:78:PRO:HB2	1:B:84:THR:HG21	1.79	0.64
1:C:149:MET:HE3	1:C:185:LEU:HD12	1.80	0.63
1:B:19:LEU:HD11	1:B:44:LEU:HD22	1.80	0.62
1:B:25:TYR:CZ	1:B:29:LEU:HD11	2.35	0.61
1:C:123:ARG:HH11	1:C:123:ARG:CG	2.13	0.61
1:B:21:TYR:CB	1:B:61:ARG:HH12	2.17	0.57
1:B:21:TYR:HB2	1:B:61:ARG:HH12	1.70	0.57
1:C:116:GLU:HA	1:C:126:VAL:HG22	1.87	0.56
1:C:154:GLU:HB2	1:C:157:ILE:HD12	1.88	0.54
1:A:25:TYR:CZ	1:A:29:LEU:HD11	2.43	0.54
1:C:101:THR:HB	1:C:136:ALA:HB2	1.90	0.53
1:A:140:MET:HE3	1:A:258:SER:HB3	1.93	0.50
1:C:147:ARG:HB3	1:C:173:THR:CG2	2.44	0.47
1:B:86:LEU:CD2	1:B:94:LEU:HD21	2.45	0.47
1:C:123:ARG:CG	1:C:123:ARG:NH1	2.76	0.47
1:A:86:LEU:HB3	1:A:91:GLN:HE21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:HG23	1:C:181:ALA:CB	2.46	0.46
1:B:16:ALA:HA	1:B:19:LEU:HD12	1.98	0.46
1:A:27:ARG:HG2	1:A:33:GLN:HA	1.98	0.45
1:B:244:ILE:HD13	1:B:244:ILE:HA	1.88	0.45
1:C:149:MET:CE	1:C:185:LEU:HD12	2.45	0.44
1:A:88:ARG:HD3	1:B:245:SER:HB3	2.01	0.43
1:C:98:THR:HB	1:C:101:THR:HG21	2.00	0.43
1:B:149:MET:HE2	1:B:151:ILE:HG12	2.01	0.43
1:A:244:ILE:HD11	1:A:256:ALA:HB2	2.01	0.43
1:C:195:LEU:HD23	1:C:223:ILE:HB	2.02	0.41
1:C:178:THR:HG23	1:C:181:ALA:HB2	2.01	0.41
1:A:244:ILE:HD13	1:A:244:ILE:HA	1.95	0.41
1:C:149:MET:HE1	1:C:182:ALA:HA	2.03	0.40
1:C:226:THR:O	1:C:226:THR:HG23	2.20	0.40
1:A:88:ARG:HD2	1:A:88:ARG:HA	1.94	0.40
1:B:190:LYS:HE3	1:B:220:ILE:HD11	2.04	0.40
1:C:11:LEU:HD21	1:C:54:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	244/271 (90%)	241 (99%)	3 (1%)	0	100	100
1	B	254/271 (94%)	246 (97%)	7 (3%)	1 (0%)	30	27
1	C	241/271 (89%)	235 (98%)	5 (2%)	1 (0%)	30	27
All	All	739/813 (91%)	722 (98%)	15 (2%)	2 (0%)	37	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	LEU
1	C	87	ALA

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	200/220 (91%)	197 (98%)	3 (2%)	60	66
1	B	207/220 (94%)	201 (97%)	6 (3%)	37	39
1	C	199/220 (90%)	191 (96%)	8 (4%)	27	26
All	All	606/660 (92%)	589 (97%)	17 (3%)	38	40

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	11	LEU
1	A	245	SER
1	B	75	SER
1	B	84	THR
1	B	137	ARG
1	B	179	ARG
1	B	190	LYS
1	B	258	SER
1	C	32	SER
1	C	41	LEU
1	C	44	LEU
1	C	137	ARG
1	C	149	MET
1	C	159	LEU
1	C	172	ILE
1	C	178	THR

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

Mol	Chain	Res	Type
1	A	69	HIS
1	C	69	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	TRS	B	301	-	7,7,7	0.16	0	9,9,9	0.27	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	TRS	B	301	-	-	7/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	TRS	N-C-C1-O1
4	B	301	TRS	C1-C-C2-O2
4	B	301	TRS	C3-C-C2-O2
4	B	301	TRS	N-C-C2-O2
4	B	301	TRS	C1-C-C3-O3
4	B	301	TRS	C3-C-C1-O1
4	B	301	TRS	N-C-C3-O3

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, 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	248/271 (91%)	0.07	5 (2%) 64 63	33, 49, 74, 126	0
1	B	256/271 (94%)	0.33	8 (3%) 51 49	36, 57, 93, 123	0
1	C	245/271 (90%)	0.84	26 (10%) 13 12	36, 67, 95, 132	0
All	All	749/813 (92%)	0.41	39 (5%) 34 32	33, 58, 93, 132	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	VAL	3.5
1	B	244	ILE	3.5
1	C	243	LEU	3.3
1	B	79	VAL	2.9
1	C	86	LEU	2.8
1	C	179	ARG	2.8
1	C	185	LEU	2.8
1	C	126	VAL	2.8
1	C	227	ALA	2.7
1	C	93	HIS	2.7
1	A	264	ALA	2.7
1	C	94	LEU	2.7
1	B	86	LEU	2.6
1	C	202	ASP	2.6
1	A	77	SER	2.5
1	B	87	ALA	2.5
1	A	244	ILE	2.4
1	C	156	ILE	2.3
1	C	173	THR	2.3
1	C	131	HIS	2.3
1	C	201	ALA	2.3
1	C	225	ILE	2.3
1	C	195	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	172	ILE	2.2
1	C	125	ASP	2.2
1	B	243	LEU	2.2
1	C	146	GLY	2.2
1	C	184	ALA	2.2
1	B	115	PRO	2.2
1	C	129	VAL	2.2
1	C	175	VAL	2.2
1	B	78	PRO	2.2
1	B	19	LEU	2.1
1	C	10	ASP	2.1
1	C	244	ILE	2.1
1	A	75	SER	2.1
1	C	177	ARG	2.0
1	C	169	GLY	2.0
1	C	148	VAL	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
4	TRS	B	301	8/8	0.78	0.17	43,62,76,82	0
3	NA	C	302	1/1	0.92	0.09	50,50,50,50	0
2	MG	C	301	1/1	0.93	0.10	67,67,67,67	0
2	MG	B	302	1/1	0.95	0.06	47,47,47,47	0
3	NA	A	304	1/1	0.97	0.09	46,46,46,46	0
3	NA	A	303	1/1	0.98	0.05	45,45,45,45	0
2	MG	A	301	1/1	0.98	0.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	A	302	1/1	0.99	0.10	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.