



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:18 PM UTC

PDB ID : 3SY8 / pdb_00003sy8
Title : Crystal structure of the response regulator RocR
Authors : Chen, M.W.; Kotaka, M.; Vonrhein, C.; Bricogne, G.; Lescar, J.
Deposited on : 2011-07-16
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

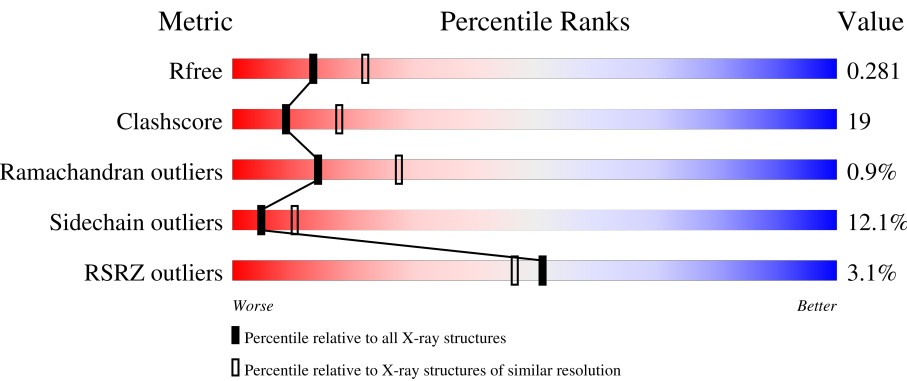
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	400	9% 65% 27% 5%
1	B	400	69% 24%
1	C	400	61% 29% 5% 5%
1	D	400	9% 56% 30% 7% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11886 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 RocR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2979	1899	509	554	17			
1	B	392	Total	C	N	O	S	0	0	0
			3007	1918	513	558	18			
1	C	380	Total	C	N	O	S	0	0	0
			2906	1856	493	540	17			
1	D	371	Total	C	N	O	S	0	0	0
			2807	1792	477	522	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	TRP	ARG	conflict	UNP Q9HX69
A	393	LEU	-	expression tag	UNP Q9HX69
A	394	GLU	-	expression tag	UNP Q9HX69
A	395	HIS	-	expression tag	UNP Q9HX69
A	396	HIS	-	expression tag	UNP Q9HX69
A	397	HIS	-	expression tag	UNP Q9HX69
A	398	HIS	-	expression tag	UNP Q9HX69
A	399	HIS	-	expression tag	UNP Q9HX69
A	400	HIS	-	expression tag	UNP Q9HX69
B	286	TRP	ARG	conflict	UNP Q9HX69
B	393	LEU	-	expression tag	UNP Q9HX69
B	394	GLU	-	expression tag	UNP Q9HX69
B	395	HIS	-	expression tag	UNP Q9HX69
B	396	HIS	-	expression tag	UNP Q9HX69
B	397	HIS	-	expression tag	UNP Q9HX69
B	398	HIS	-	expression tag	UNP Q9HX69
B	399	HIS	-	expression tag	UNP Q9HX69
B	400	HIS	-	expression tag	UNP Q9HX69
C	286	TRP	ARG	conflict	UNP Q9HX69
C	393	LEU	-	expression tag	UNP Q9HX69
C	394	GLU	-	expression tag	UNP Q9HX69

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Chain	Residue	Modelled	Actual	Comment	Reference
C	395	HIS	-	expression tag	UNP Q9HX69
C	396	HIS	-	expression tag	UNP Q9HX69
C	397	HIS	-	expression tag	UNP Q9HX69
C	398	HIS	-	expression tag	UNP Q9HX69
C	399	HIS	-	expression tag	UNP Q9HX69
C	400	HIS	-	expression tag	UNP Q9HX69
D	286	TRP	ARG	conflict	UNP Q9HX69
D	393	LEU	-	expression tag	UNP Q9HX69
D	394	GLU	-	expression tag	UNP Q9HX69
D	395	HIS	-	expression tag	UNP Q9HX69
D	396	HIS	-	expression tag	UNP Q9HX69
D	397	HIS	-	expression tag	UNP Q9HX69
D	398	HIS	-	expression tag	UNP Q9HX69
D	399	HIS	-	expression tag	UNP Q9HX69
D	400	HIS	-	expression tag	UNP Q9HX69

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

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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

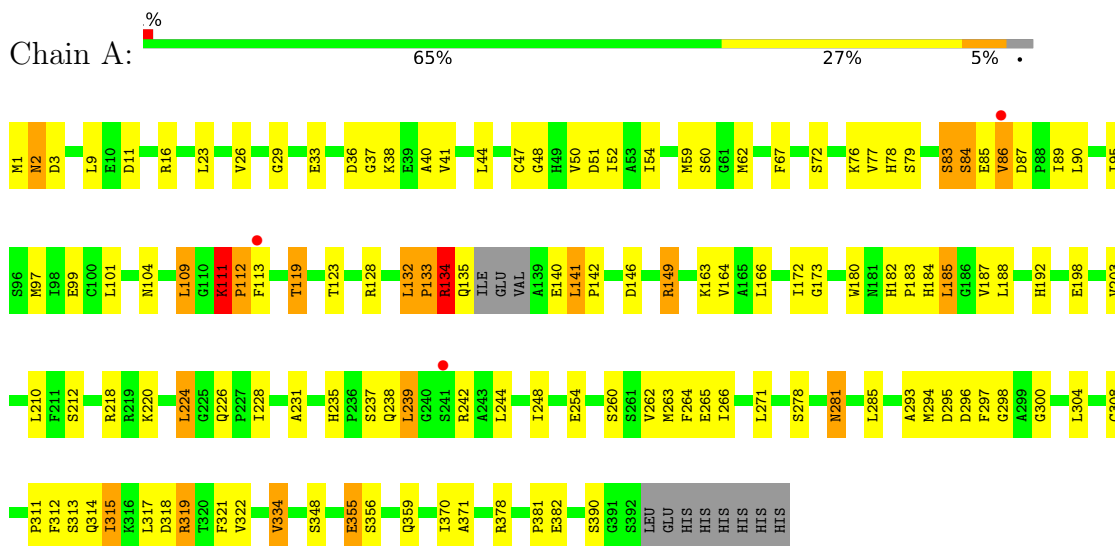
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	53	Total	O	0	0
			53	53		
4	C	33	Total	O	0	0
			33	33		
4	D	47	Total	O	0	0
			47	47		

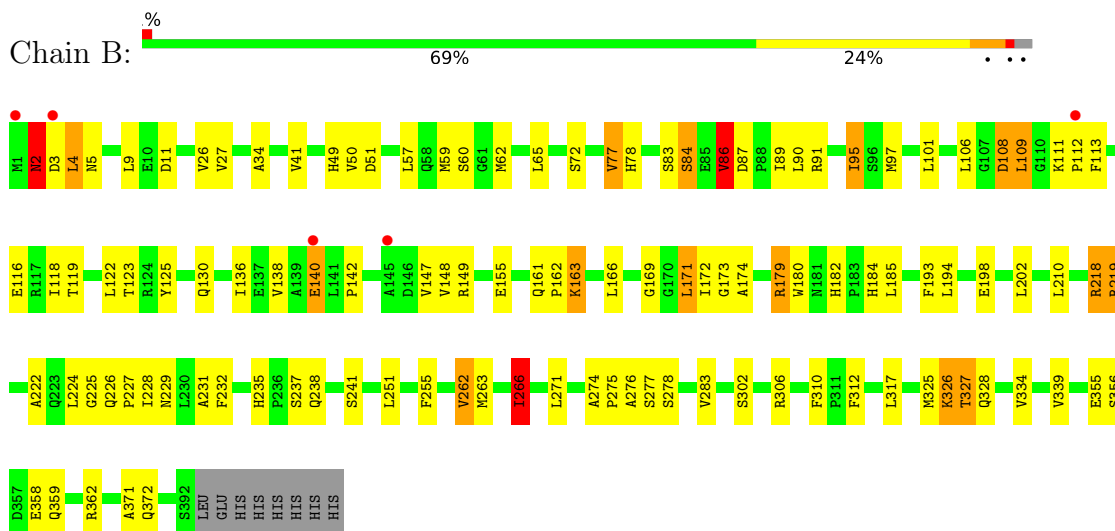
3 Residue-property plots [i](#)

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: RocR

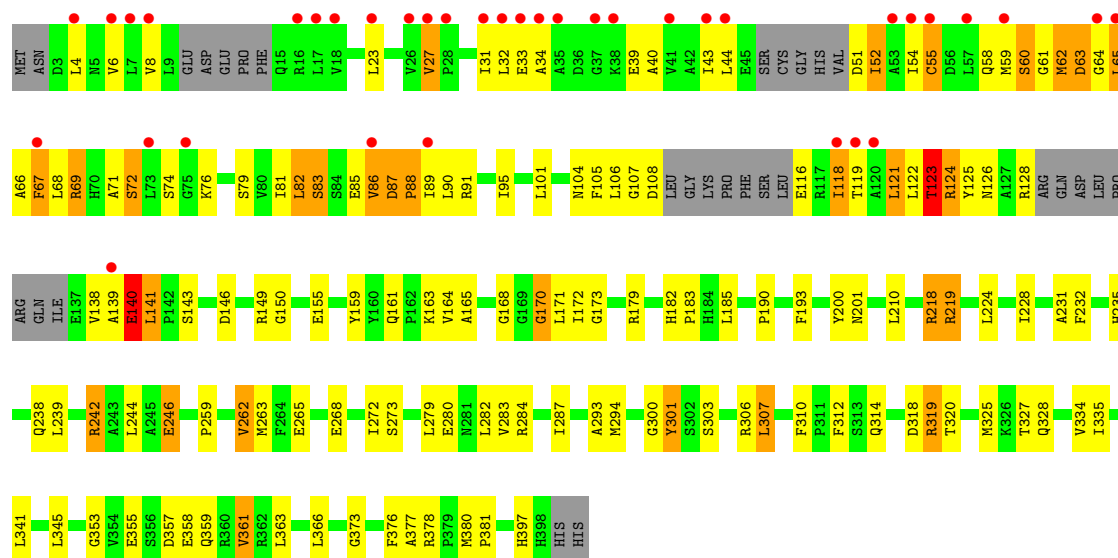


• Molecule 1: RocR



• Molecule 1: RocR





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.80Å 118.80Å 495.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.50 19.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-2.50) 83.1 (19.96-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.216 , 0.285 0.211 , 0.281	Depositor DCC
R_{free} test set	3045 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.7	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	0.95	EDS
Total number of atoms	11886	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 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	0.88	1/3036 (0.0%)	1.10	8/4118 (0.2%)
1	B	1.01	1/3065 (0.0%)	1.13	9/4158 (0.2%)
1	C	0.78	0/2962	1.05	5/4018 (0.1%)
1	D	0.93	1/2855 (0.0%)	1.12	13/3871 (0.3%)
All	All	0.91	3/11918 (0.0%)	1.10	35/16165 (0.2%)

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
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	300	GLY	N-CA	7.05	1.52	1.45
1	B	339	VAL	CA-CB	5.67	1.61	1.54
1	A	334	VAL	CA-CB	5.61	1.60	1.54

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315	ILE	CB-CA-C	-8.71	97.64	110.62
1	A	111	LYS	CA-C-N	7.29	128.96	119.84
1	A	111	LYS	C-N-CA	7.29	128.96	119.84
1	D	27	VAL	N-CA-C	6.62	114.45	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ASN	N-CA-C	6.56	118.11	108.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	LYS	Peptide
1	C	141	LEU	Peptide

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	2979	0	3002	93	0
1	B	3007	0	3040	90	0
1	C	2906	0	2930	112	0
1	D	2807	0	2811	164	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	D	15	0	17	2	0
4	A	35	0	0	7	0
4	B	53	0	0	5	0
4	C	33	0	0	2	0
4	D	47	0	0	4	0
All	All	11886	0	11800	438	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 19.

The worst 5 of 438 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:9:LEU:HD22	1:B:62:MET:HE1	1.24	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ALA:HB1	1:D:283:VAL:HG21	1.23	1.15
1:D:68:LEU:HG	1:D:69:ARG:NH1	1.70	1.07
1:D:66:ALA:N	1:D:69:ARG:HE	1.53	1.06
4:A:421:HOH:O	1:B:277:SER:HB3	1.50	1.06

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	385/400 (96%)	356 (92%)	24 (6%)	5 (1%)	9	18
1	B	390/400 (98%)	370 (95%)	18 (5%)	2 (0%)	24	43
1	C	376/400 (94%)	349 (93%)	25 (7%)	2 (0%)	24	43
1	D	361/400 (90%)	338 (94%)	18 (5%)	5 (1%)	9	17
All	All	1512/1600 (94%)	1413 (94%)	85 (6%)	14 (1%)	14	27

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	112	PRO
1	A	133	PRO
1	A	134	ARG
1	D	67	PHE

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	324/337 (96%)	282 (87%)	42 (13%)	4	8
1	B	328/337 (97%)	294 (90%)	34 (10%)	7	14
1	C	317/337 (94%)	278 (88%)	39 (12%)	4	10
1	D	300/337 (89%)	261 (87%)	39 (13%)	4	8
All	All	1269/1348 (94%)	1115 (88%)	154 (12%)	5	10

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	31	ILE
1	D	246	GLU
1	D	52	ILE
1	D	124	ARG
1	D	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	104	ASN
1	C	314	GLN
1	C	182	HIS
1	C	233	ASN
1	C	372	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 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
3	EPE	D	3380	2	15,15,15	0.72	1 (6%)	19,20,20	2.43	7 (36%)

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	EPE	D	3380	2	-	3/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3380	EPE	C10-S	2.15	1.80	1.77

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3380	EPE	C5-N4-C3	5.35	120.36	108.84
3	D	3380	EPE	O2S-S-C10	4.03	112.81	106.73
3	D	3380	EPE	C6-N1-C2	3.76	116.93	108.84
3	D	3380	EPE	C6-C5-N4	3.73	118.18	110.65
3	D	3380	EPE	C9-N1-C6	-3.72	101.33	111.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3380	EPE	C10-C9-N1-C2
3	D	3380	EPE	C10-C9-N1-C6

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Mol	Chain	Res	Type	Atoms
3	D	3380	EPE	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3380	EPE	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	389/400 (97%)	-0.24	3 (0%) 82 80	37, 63, 85, 98	0
1	B	392/400 (98%)	-0.28	5 (1%) 75 71	34, 54, 79, 96	0
1	C	380/400 (95%)	-0.02	2 (0%) 87 85	53, 74, 100, 109	0
1	D	371/400 (92%)	0.13	37 (9%) 12 10	35, 60, 141, 146	0
All	All	1532/1600 (95%)	-0.11	47 (3%) 51 47	34, 63, 104, 146	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	LEU	4.4
1	D	53	ALA	4.3
1	B	112	PRO	4.1
1	D	86	VAL	3.9
1	B	145	ALA	3.8

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	MG	C	401	1/1	0.79	0.11	90,90,90,90	0
3	EPE	D	3380	15/15	0.87	0.12	56,61,69,70	0
2	MG	D	401	1/1	0.89	0.05	50,50,50,50	0
2	MG	A	401	1/1	0.89	0.05	49,49,49,49	0
2	MG	B	401	1/1	0.97	0.05	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.