



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:16 AM UTC

PDB ID : 4Y2S / pdb_00004y2s
Title : Structure of soluble epoxide hydrolase in complex with 1-[3-(trifluoromethyl)phenyl]-1H-pyrazol-4-ol
Authors : Amano, Y.; Yamaguchi, T.
Deposited on : 2015-02-10
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	:	4-5-2 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

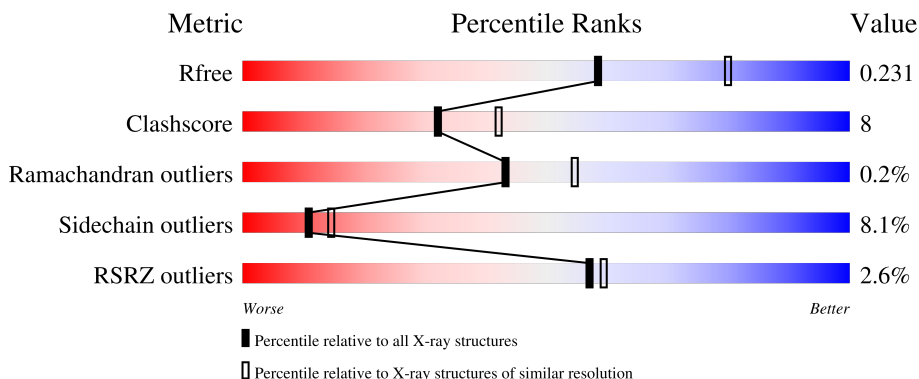
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

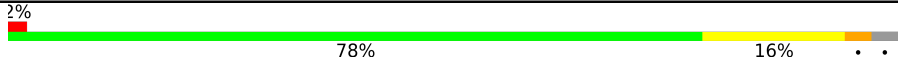
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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	561	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4411 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 Bifunctional epoxide hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4323	2771	728	788	36			

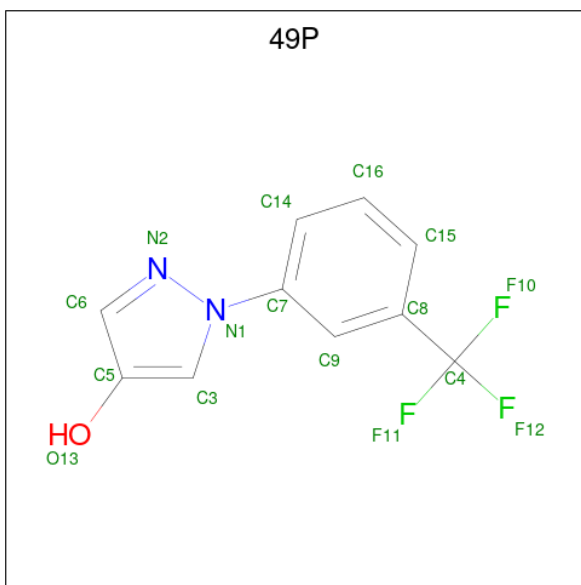
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	556	HIS	-	expression tag	UNP P34913
A	557	HIS	-	expression tag	UNP P34913
A	558	HIS	-	expression tag	UNP P34913
A	559	HIS	-	expression tag	UNP P34913
A	560	HIS	-	expression tag	UNP P34913
A	561	HIS	-	expression tag	UNP P34913

- 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		

- Molecule 3 is 1-[3-(trifluoromethyl)phenyl]-1H-pyrazol-4-ol (CCD ID: 49P) (formula: C₁₀H₇F₃N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			16	10	3	2	1		

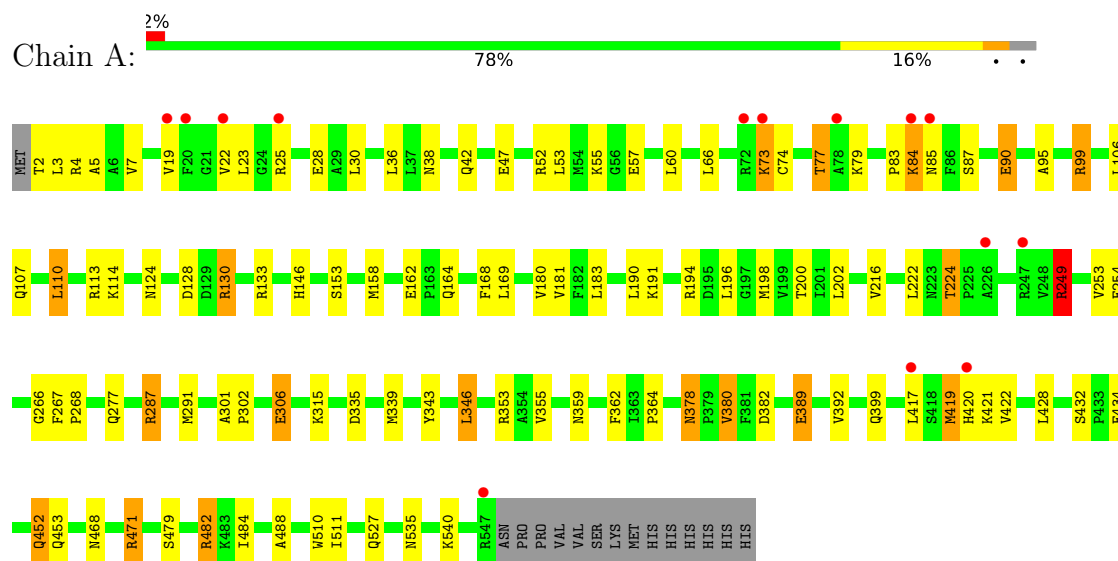
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		

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: Bifunctional epoxide hydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.74Å 92.74Å 244.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.29 – 2.30 76.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (76.29-2.30) 99.5 (76.29-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.195 , 0.233 0.193 , 0.231	Depositor DCC
R_{free} test set	1436 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4411	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: 49P, 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	1.09	3/4428 (0.1%)	1.22	20/6000 (0.3%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	ALA	C-O	-6.36	1.16	1.24
1	A	540	LYS	CA-C	5.15	1.59	1.52
1	A	249	ARG	C-O	5.06	1.30	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	THR	CA-C-N	-9.72	109.52	119.92
1	A	224	THR	C-N-CA	-9.72	109.52	119.92
1	A	389	GLU	CA-C-N	-8.41	110.74	119.83
1	A	389	GLU	C-N-CA	-8.41	110.74	119.83
1	A	287	ARG	NE-CZ-NH2	7.80	126.22	119.20
1	A	302	PRO	O-C-N	6.63	124.27	121.15
1	A	419	MET	N-CA-C	-6.56	106.02	112.97
1	A	130	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	A	346	LEU	N-CA-C	5.98	118.75	111.82
1	A	19	VAL	N-CA-C	5.81	116.59	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ARG	CB-CG-CD	5.79	124.61	111.30
1	A	130	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	A	315	LYS	N-CA-C	-5.39	105.41	111.28
1	A	191	LYS	CA-C-N	-5.33	113.41	119.28
1	A	191	LYS	C-N-CA	-5.33	113.41	119.28
1	A	302	PRO	CA-C-N	5.26	124.76	119.19
1	A	302	PRO	C-N-CA	5.26	124.76	119.19
1	A	471	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	287	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	133	ARG	N-CA-C	5.05	118.21	111.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide

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	4323	0	4329	69	0
2	A	1	0	0	0	0
3	A	16	0	6	0	0
4	A	71	0	0	1	0
All	All	4411	0	4335	69	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 8.

All (69) 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:60:LEU:HD23	1:A:130:ARG:HD2	1.49	0.93
1:A:180:VAL:HG11	1:A:198:MET:HE3	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD22	1:A:200:THR:HB	1.51	0.92
1:A:158:MET:SD	1:A:164:GLN:HG3	2.12	0.89
1:A:180:VAL:HG11	1:A:198:MET:CE	2.06	0.86
1:A:60:LEU:CD2	1:A:130:ARG:HD2	2.07	0.84
1:A:60:LEU:HD23	1:A:130:ARG:CD	2.08	0.83
1:A:128:ASP:OD1	1:A:130:ARG:HD3	1.83	0.79
1:A:22:VAL:HG22	1:A:25:ARG:HH22	1.48	0.78
1:A:249:ARG:O	1:A:249:ARG:HG2	1.82	0.76
1:A:73:LYS:O	1:A:77:THR:HG22	1.87	0.73
1:A:180:VAL:CG1	1:A:198:MET:CE	2.69	0.71
1:A:180:VAL:CG1	1:A:198:MET:HE3	2.21	0.68
1:A:378:ASN:C	1:A:378:ASN:HD22	2.02	0.67
1:A:87:SER:HB3	1:A:90:GLU:HB2	1.77	0.67
1:A:277:GLN:HE22	1:A:527:GLN:HB3	1.62	0.62
1:A:23:LEU:HD12	1:A:38:ASN:ND2	2.14	0.62
1:A:277:GLN:HG3	1:A:535:ASN:ND2	2.14	0.62
1:A:22:VAL:HG11	1:A:95:ALA:HB2	1.82	0.61
1:A:306:GLU:H	1:A:306:GLU:CD	2.09	0.61
1:A:452:GLN:HE21	1:A:453:GLN:HE21	1.50	0.59
1:A:468:ASN:OD1	1:A:471:ARG:NH2	2.36	0.59
1:A:277:GLN:NE2	1:A:527:GLN:HB3	2.18	0.58
1:A:22:VAL:HG21	1:A:95:ALA:CB	2.33	0.58
1:A:378:ASN:ND2	1:A:380:VAL:HG12	2.19	0.57
1:A:87:SER:CB	1:A:90:GLU:HB2	2.34	0.56
1:A:158:MET:HE1	1:A:168:PHE:HB2	1.89	0.55
1:A:84:LYS:O	1:A:85:ASN:HB2	2.07	0.55
1:A:110:LEU:CD1	1:A:146:HIS:HB3	2.38	0.54
1:A:180:VAL:CG1	1:A:198:MET:HE2	2.38	0.54
1:A:419:MET:HA	1:A:419:MET:HE2	1.90	0.53
1:A:55:LYS:NZ	1:A:162:GLU:OE1	2.29	0.53
1:A:378:ASN:HD21	1:A:380:VAL:HG12	1.71	0.52
1:A:378:ASN:HD22	1:A:380:VAL:H	1.59	0.51
1:A:158:MET:HE1	1:A:168:PHE:CB	2.41	0.50
1:A:22:VAL:HG21	1:A:95:ALA:HB2	1.94	0.49
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.95	0.49
1:A:52:ARG:HD2	1:A:57:GLU:OE2	2.11	0.49
1:A:339:MET:HE2	1:A:343:TYR:CE2	2.47	0.49
1:A:484:ILE:HB	1:A:511:ILE:HG12	1.95	0.48
1:A:99:ARG:HD2	4:A:757:HOH:O	2.13	0.48
1:A:339:MET:HE2	1:A:343:TYR:HE2	1.79	0.48
1:A:355:VAL:O	1:A:488:ALA:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLN:NE2	1:A:453:GLN:HE21	2.13	0.47
1:A:180:VAL:HG12	1:A:198:MET:HE2	1.96	0.47
1:A:60:LEU:HD21	1:A:130:ARG:HD2	1.93	0.47
1:A:22:VAL:CG2	1:A:25:ARG:HH22	2.24	0.46
1:A:2:THR:HG23	1:A:3:LEU:H	1.79	0.46
1:A:22:VAL:HG22	1:A:25:ARG:NH2	2.23	0.46
1:A:420:HIS:O	1:A:421:LYS:C	2.60	0.45
1:A:22:VAL:HG23	1:A:25:ARG:HH12	1.82	0.45
1:A:5:ALA:HB3	1:A:180:VAL:HG22	1.99	0.44
1:A:479:SER:O	1:A:482:ARG:HG3	2.17	0.44
1:A:389:GLU:HG3	1:A:392:VAL:HG23	1.99	0.44
1:A:84:LYS:HE3	1:A:84:LYS:HB2	1.85	0.44
1:A:382:ASP:OD2	1:A:422:VAL:N	2.50	0.43
1:A:7:VAL:HG21	1:A:169:LEU:HD21	2.01	0.42
1:A:339:MET:HE3	1:A:339:MET:HA	2.02	0.42
1:A:124:ASN:HA	1:A:153:SER:HB3	2.02	0.42
1:A:254:GLU:OE2	1:A:287:ARG:HD3	2.20	0.42
1:A:267:PHE:CD1	1:A:267:PHE:C	2.97	0.42
1:A:30:LEU:HD13	1:A:83:PRO:HG3	2.02	0.42
1:A:277:GLN:HG3	1:A:535:ASN:HD21	1.81	0.42
1:A:364:PRO:HG3	1:A:510:TRP:CE2	2.55	0.41
1:A:346:LEU:HD11	1:A:362:PHE:CZ	2.55	0.41
1:A:36:LEU:HD22	1:A:74:CYS:HB3	2.03	0.41
1:A:378:ASN:ND2	1:A:380:VAL:H	2.19	0.41
1:A:346:LEU:HD11	1:A:362:PHE:CE1	2.57	0.40
1:A:114:LYS:HB3	1:A:114:LYS:HE3	1.92	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	544/561 (97%)	529 (97%)	14 (3%)	1 (0%)	43 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	PRO

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	472/487 (97%)	434 (92%)	38 (8%)	11 14

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	28	GLU
1	A	42	GLN
1	A	47	GLU
1	A	53	LEU
1	A	66	LEU
1	A	73	LYS
1	A	77	THR
1	A	79	LYS
1	A	84	LYS
1	A	90	GLU
1	A	99	ARG
1	A	106	LEU
1	A	107	GLN
1	A	110	LEU
1	A	113	ARG
1	A	181	VAL
1	A	183	LEU
1	A	194	ARG
1	A	196	LEU

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Mol	Chain	Res	Type
1	A	202	LEU
1	A	216	VAL
1	A	222	LEU
1	A	224	THR
1	A	249	ARG
1	A	253	VAL
1	A	306	GLU
1	A	353	ARG
1	A	359	ASN
1	A	378	ASN
1	A	380	VAL
1	A	399	GLN
1	A	417	LEU
1	A	428	LEU
1	A	432	SER
1	A	434	GLU
1	A	452	GLN
1	A	482	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	42	GLN
1	A	107	GLN
1	A	204	GLN
1	A	277	GLN
1	A	378	ASN
1	A	384	GLN
1	A	453	GLN
1	A	506	HIS
1	A	535	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	49P	A	602	-	17,17,17	0.90	0	21,25,25	1.21	2 (9%)

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	49P	A	602	-	-	0/10/10/10	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	49P	C7-N1-C3	-2.83	125.03	129.12
3	A	602	49P	C15-C8-C9	2.06	121.83	117.86

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](#)

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	546/561 (97%)	-0.27	14 (2%) 57 59	13, 26, 53, 92	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	PHE	5.9
1	A	85	ASN	3.3
1	A	72	ARG	3.1
1	A	73	LYS	2.8
1	A	22	VAL	2.6
1	A	417	LEU	2.5
1	A	19	VAL	2.5
1	A	547	ARG	2.3
1	A	78	ALA	2.3
1	A	226	ALA	2.2
1	A	247	ARG	2.2
1	A	420	HIS	2.1
1	A	84	LYS	2.0
1	A	25	ARG	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 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	A	601	1/1	0.85	0.11	40,40,40,40	0
3	49P	A	602	16/16	0.91	0.11	39,43,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.