



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 AM UTC

PDB ID : 5Y9W / pdb_00005y9w
Title : Crystal 1 for AtLURE1.2-AtPRK6LRR
Authors : Chai, J.; Zhang, X.
Deposited on : 2017-08-28
Resolution : 1.85 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

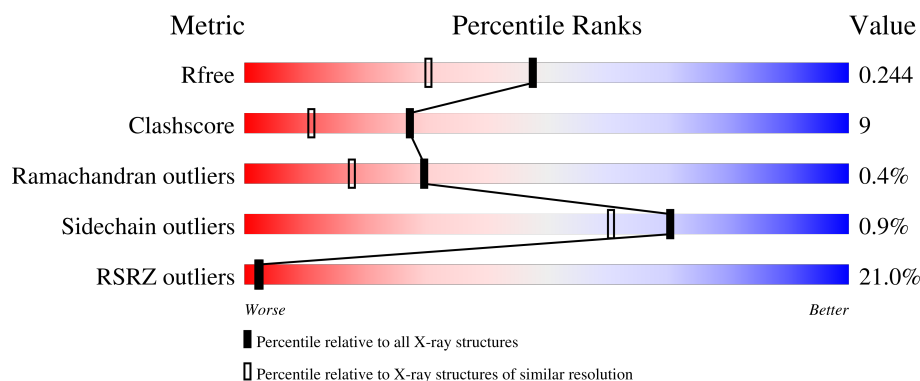
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	242	36% 68% 18% 12%
1	B	242	3% 79% 10% 11%
2	C	71	3% 49% 48%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4062 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 Pollen receptor-like kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	216	Total	C	N	O	S	0	0	0
			1688	1069	285	326	8			
1	A	213	Total	C	N	O	S	0	0	0
			1663	1052	282	321	8			

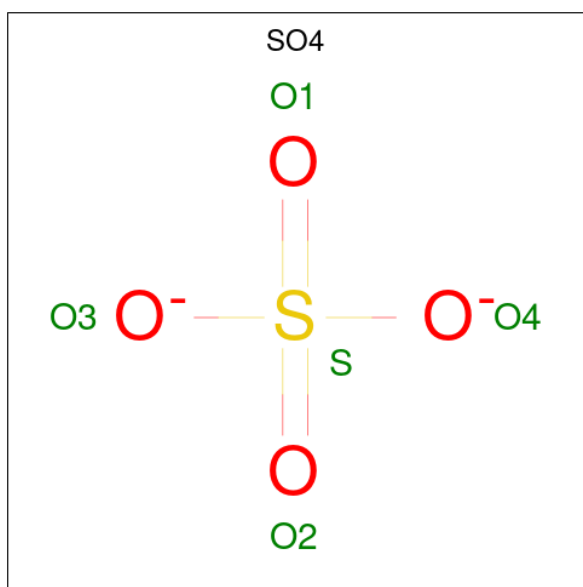
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	263	HIS	-	expression tag	UNP Q3E991
B	264	HIS	-	expression tag	UNP Q3E991
B	265	HIS	-	expression tag	UNP Q3E991
B	266	HIS	-	expression tag	UNP Q3E991
B	267	HIS	-	expression tag	UNP Q3E991
B	268	HIS	-	expression tag	UNP Q3E991
A	263	HIS	-	expression tag	UNP Q3E991
A	264	HIS	-	expression tag	UNP Q3E991
A	265	HIS	-	expression tag	UNP Q3E991
A	266	HIS	-	expression tag	UNP Q3E991
A	267	HIS	-	expression tag	UNP Q3E991
A	268	HIS	-	expression tag	UNP Q3E991

- Molecule 2 is a protein called Protein LURE 1.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	37	Total	C	N	O	S	0	0	0
			294	178	60	49	7			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

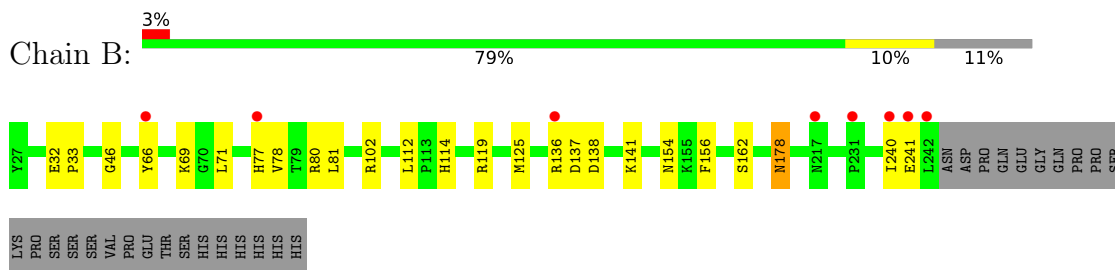
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	273	Total	O	0	0
			273	273		
4	C	23	Total	O	0	0
			23	23		
4	A	86	Total	O	0	0
			86	86		

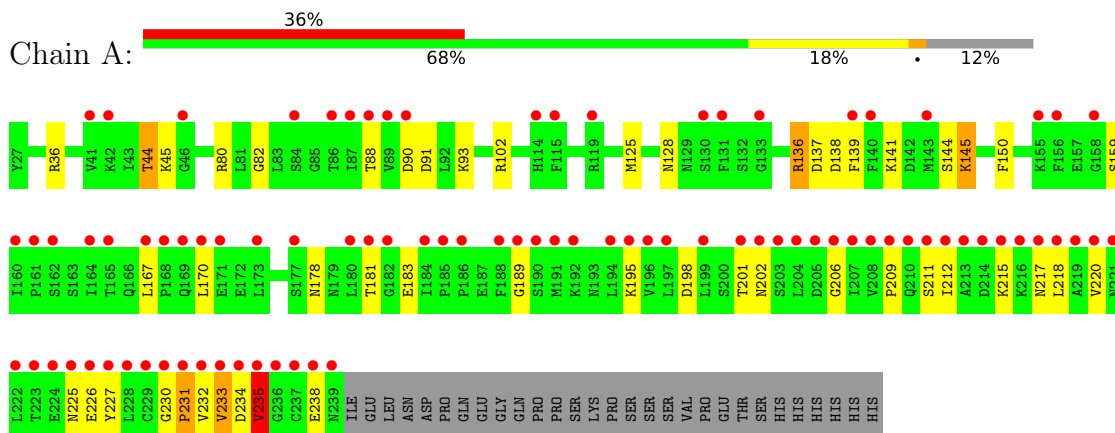
3 Residue-property plots

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.

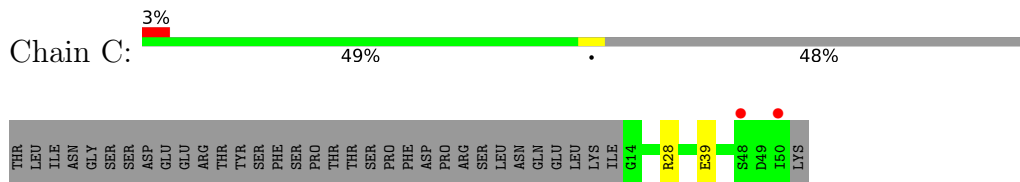
- Molecule 1: Pollen receptor-like kinase 6



- Molecule 1: Pollen receptor-like kinase 6



- Molecule 2: Protein LURE 1.2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.69Å 48.51Å 146.31Å 90.00° 102.67° 90.00°	Depositor
Resolution (Å)	35.38 – 1.85 35.38 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.38-1.85) 97.8 (35.38-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.204 , 0.241 0.209 , 0.244	Depositor DCC
R_{free} test set	2845 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	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	4062	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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: SO4

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	0.77	1/1694 (0.1%)	0.78	5/2288 (0.2%)
1	B	0.72	5/1719 (0.3%)	0.62	0/2322
2	C	0.28	0/297	0.52	0/391
All	All	0.72	6/3710 (0.2%)	0.69	5/5001 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	PRO	CA-C	-6.09	1.47	1.52
1	B	141	LYS	C-O	-5.97	1.17	1.24
1	B	178	ASN	C-O	-5.92	1.18	1.24
1	B	114	HIS	CG-ND1	-5.55	1.32	1.38
1	B	46	GLY	C-O	-5.32	1.18	1.24
1	B	112	LEU	C-O	-5.08	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLU	N-CA-C	8.11	121.04	111.71
1	A	44	THR	N-CA-C	5.46	117.31	111.36
1	A	231	PRO	CB-CA-C	-5.17	106.69	111.40
1	A	144	SER	N-CA-C	5.16	116.90	111.28
1	A	45	LYS	N-CA-C	5.02	116.77	108.49

There are no chirality outliers.

There are no planarity outliers.

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	1663	0	1673	50	0
1	B	1688	0	1699	15	1
2	C	294	0	286	2	0
3	A	5	0	0	1	0
3	B	25	0	0	1	0
3	C	5	0	0	1	0
4	A	86	0	0	3	1
4	B	273	0	0	4	1
4	C	23	0	0	1	0
All	All	4062	0	3658	67	2

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 9.

All (67) 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:235:VAL:CG2	1:A:238:GLU:OE1	1.88	1.20
1:A:235:VAL:HG23	1:A:238:GLU:OE1	1.48	1.08
1:A:235:VAL:HG21	1:A:238:GLU:OE1	1.63	0.96
1:B:125:MET:SD	4:B:1027:HOH:O	2.29	0.91
1:A:183:GLU:HG2	1:A:206:GLY:HA3	1.55	0.87
1:A:201:THR:HG22	1:A:201:THR:O	1.77	0.84
1:A:136:ARG:HD2	1:A:138:ASP:OD1	1.78	0.83
1:A:136:ARG:CD	1:A:138:ASP:OD1	2.29	0.80
1:A:189:GLY:HA3	1:A:211:SER:O	1.82	0.79
1:A:136:ARG:CZ	1:A:138:ASP:OD1	2.32	0.78
1:B:119:ARG:NH2	4:B:803:HOH:O	2.25	0.70
1:A:90:ASP:O	1:A:93:LYS:NZ	2.22	0.68
1:A:102:ARG:HB2	1:A:125:MET:HE3	1.75	0.68
1:A:128:ASN:ND2	4:A:804:HOH:O	2.28	0.66
1:B:80:ARG:NE	3:B:703:SO4:O3	2.25	0.65
1:A:136:ARG:NH1	1:A:138:ASP:OD1	2.29	0.65
1:A:136:ARG:NE	1:A:138:ASP:OD1	2.29	0.64
1:A:202:ASN:H	1:A:225:ASN:HD21	1.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:NH1	1:A:91:ASP:OD1	2.25	0.64
1:A:136:ARG:CZ	1:A:138:ASP:CG	2.71	0.64
1:A:80:ARG:NH2	4:A:805:HOH:O	2.33	0.61
1:B:102:ARG:HB2	1:B:125:MET:HE3	1.83	0.60
1:A:232:VAL:O	1:A:232:VAL:HG23	2.01	0.60
1:A:202:ASN:H	1:A:225:ASN:ND2	1.99	0.60
1:A:235:VAL:HG23	1:A:235:VAL:O	2.02	0.59
1:A:136:ARG:CZ	1:A:138:ASP:OD2	2.52	0.58
1:A:167:LEU:HD12	1:A:170:LEU:HD22	1.86	0.57
1:A:145:LYS:HA	1:A:145:LYS:HE2	1.86	0.56
1:A:44:THR:HG23	1:A:82:GLY:O	2.05	0.56
1:A:178:ASN:HB2	1:A:202:ASN:HD21	1.69	0.56
1:A:235:VAL:HG21	1:A:238:GLU:CD	2.29	0.56
1:A:195:LYS:NZ	1:A:217:ASN:HB2	2.21	0.56
1:B:154:ASN:HB2	1:B:178:ASN:HD21	1.72	0.54
1:B:137:ASP:OD2	1:B:162:SER:OG	2.14	0.54
1:B:78:VAL:HG13	1:B:81:LEU:HD22	1.89	0.53
1:B:136:ARG:NE	1:B:138:ASP:OD1	2.42	0.53
1:A:227:TYR:N	1:A:227:TYR:CD1	2.76	0.53
1:A:215:LYS:HZ2	1:A:217:ASN:H	1.57	0.52
1:A:136:ARG:NH1	1:A:138:ASP:CG	2.71	0.49
1:A:231:PRO:O	1:A:231:PRO:HG2	2.14	0.47
1:B:156:PHE:H	1:B:178:ASN:HD22	1.61	0.47
1:A:145:LYS:HE2	1:A:145:LYS:CA	2.43	0.47
1:A:88:THR:OG1	3:A:701:SO4:O4	2.32	0.47
1:A:159:SER:HA	1:A:181:THR:O	2.15	0.46
1:A:195:LYS:HZ3	1:A:217:ASN:HB2	1.80	0.46
2:C:28:ARG:NH2	4:C:201:HOH:O	2.29	0.45
2:C:39:GLU:HG2	3:C:101:SO4:O2	2.16	0.45
1:A:141:LYS:HA	1:A:141:LYS:HD2	1.54	0.45
1:A:88:THR:O	4:A:801:HOH:O	2.21	0.45
1:A:125:MET:HA	1:A:150:PHE:HB2	1.98	0.45
1:A:211:SER:O	1:A:211:SER:OG	2.34	0.44
1:A:215:LYS:CD	1:A:217:ASN:H	2.29	0.44
1:B:66:TYR:HE2	1:B:77:HIS:CE1	2.36	0.44
1:A:211:SER:C	1:A:212:ILE:HD12	2.42	0.44
1:B:156:PHE:H	1:B:178:ASN:ND2	2.16	0.43
1:A:235:VAL:CG2	1:A:238:GLU:CD	2.81	0.42
1:B:69:LYS:O	1:B:71:LEU:HD13	2.19	0.42
1:A:139:PHE:CD1	1:A:139:PHE:C	2.96	0.42
1:B:136:ARG:NH1	4:B:819:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:OD1	1:A:198:ASP:C	2.63	0.42
1:A:218:LEU:HG	1:A:220:VAL:HG22	2.00	0.42
1:A:230:GLY:N	1:A:231:PRO:HD2	2.35	0.41
1:B:240:ILE:O	4:B:802:HOH:O	2.22	0.41
1:A:209:PRO:HB2	1:A:212:ILE:HD13	2.02	0.41
1:A:215:LYS:HD3	1:A:217:ASN:N	2.37	0.40
1:B:32:GLU:HB2	1:B:33:PRO:HD3	2.03	0.40
1:A:233:VAL:HB	1:A:234:ASP:H	1.63	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:TYR:OH	1:B:241:GLU:OE1[3_545]	1.96	0.24
4:B:983:HOH:O	4:A:866:HOH:O[3_555]	2.01	0.19

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	211/242 (87%)	200 (95%)	9 (4%)	2 (1%)	14	4
1	B	214/242 (88%)	205 (96%)	9 (4%)	0	100	100
2	C	35/71 (49%)	35 (100%)	0	0	100	100
All	All	460/555 (83%)	440 (96%)	18 (4%)	2 (0%)	30	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	VAL
1	A	235	VAL

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	194/222 (87%)	190 (98%)	4 (2%)	47	30
1	B	197/222 (89%)	197 (100%)	0	100	100
2	C	31/65 (48%)	31 (100%)	0	100	100
All	All	422/509 (83%)	418 (99%)	4 (1%)	70	60

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ARG
1	A	137	ASP
1	A	145	LYS
1	A	235	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	GLN
1	B	77	HIS
1	B	178	ASN
1	A	202	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](#)

7 ligands are modelled in this entry.

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	SO4	B	703	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	B	704	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	B	701	-	4,4,4	0.27	0	6,6,6	0.30	0
3	SO4	C	101	-	4,4,4	0.19	0	6,6,6	0.22	0
3	SO4	A	701	-	4,4,4	0.27	0	6,6,6	0.06	0
3	SO4	B	705	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	B	702	-	4,4,4	0.25	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	SO4	1	0
3	C	101	SO4	1	0
3	A	701	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	213/242 (88%)	1.95	88 (41%) 0 1	25, 58, 89, 96	0
1	B	216/242 (89%)	-0.01	8 (3%) 45 48	18, 25, 38, 52	0
2	C	37/71 (52%)	0.69	2 (5%) 31 34	24, 36, 49, 55	0
All	All	466/555 (83%)	0.94	98 (21%) 2 2	18, 34, 82, 96	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	PRO	8.7
1	A	233	VAL	8.1
1	A	230	GLY	8.0
1	A	208	VAL	7.6
1	A	232	VAL	7.1
1	A	207	ILE	6.3
1	A	229	CYS	5.6
1	A	212	ILE	5.2
1	A	219	ALA	5.2
1	B	242	LEU	5.1
1	A	218	LEU	5.0
1	A	204	LEU	4.9
1	A	239	ASN	4.7
1	A	213	ALA	4.7
1	A	228	LEU	4.7
1	A	237	CYS	4.6
1	A	188	PHE	4.5
1	A	184	ILE	4.5
1	A	203	SER	4.5
1	A	227	TYR	4.4
1	A	225	ASN	4.4
1	A	235	VAL	4.3
1	A	173	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	206	GLY	3.9
1	A	160	ILE	3.9
1	A	236	GLY	3.7
1	A	209	PRO	3.7
1	A	220	VAL	3.7
1	A	196	VAL	3.6
1	A	168	PRO	3.6
1	A	182	GLY	3.6
1	A	143	MET	3.6
1	A	181	THR	3.6
1	A	194	LEU	3.5
1	A	197	LEU	3.5
1	B	66	TYR	3.5
1	A	86	THR	3.4
2	C	50	ILE	3.4
1	B	217	ASN	3.3
1	A	210	GLN	3.3
1	A	84	SER	3.3
1	A	226	GLU	3.2
1	A	164	ILE	3.2
1	A	41	VAL	3.2
1	A	89	VAL	3.2
1	A	170	LEU	3.2
1	A	180	LEU	3.1
1	A	215	LYS	3.1
1	A	156	PHE	3.1
1	A	165	THR	3.0
1	A	192	LYS	3.0
1	A	222	LEU	3.0
1	A	217	ASN	3.0
1	A	189	GLY	2.9
1	A	185	PRO	2.9
1	A	140	PHE	2.9
1	A	216	LYS	2.9
1	A	224	GLU	2.9
1	A	202	ASN	2.9
1	A	238	GLU	2.8
1	A	214	ASP	2.8
1	A	158	GLY	2.8
1	A	167	LEU	2.8
1	A	171	GLU	2.7
1	A	186	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	199	LEU	2.6
1	A	195	LYS	2.6
1	A	191	MET	2.6
1	B	77	HIS	2.6
1	A	139	PHE	2.6
1	A	201	THR	2.6
1	B	231	PRO	2.5
1	A	130	SER	2.5
1	A	223	THR	2.5
1	A	42	LYS	2.5
1	A	162	SER	2.5
1	A	211	SER	2.4
1	A	169	GLN	2.4
1	A	87	ILE	2.3
1	A	190	SER	2.3
1	A	133	GLY	2.3
1	A	177	SER	2.3
1	A	234	ASP	2.3
1	A	221	ASN	2.3
1	A	155	LYS	2.2
1	A	88	THR	2.2
1	A	46	GLY	2.2
1	A	161	PRO	2.2
1	A	114	HIS	2.1
1	A	131	PHE	2.1
1	B	136	ARG	2.1
1	A	115	PHE	2.1
2	C	48	SER	2.1
1	A	90	ASP	2.1
1	B	241	GLU	2.0
1	A	119	ARG	2.0
1	A	205	ASP	2.0
1	B	240	ILE	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
3	SO4	B	704	5/5	0.26	0.17	98,103,116,119	0
3	SO4	B	702	5/5	0.60	0.15	59,60,65,69	0
3	SO4	B	705	5/5	0.70	0.16	88,88,93,94	0
3	SO4	A	701	5/5	0.71	0.14	68,69,75,76	0
3	SO4	B	703	5/5	0.76	0.12	43,52,56,62	0
3	SO4	C	101	5/5	0.89	0.10	49,49,55,59	0
3	SO4	B	701	5/5	0.96	0.16	35,39,43,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.