



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:33 PM UTC

PDB ID : 6JMV / pdb_00006jmv
Title : Crystal structure of the GluK3 ligand binding domain complex with SYM and zinc
Authors : Kumari, J.; Kumar, J.
Deposited on : 2019-03-13
Resolution : 1.83 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

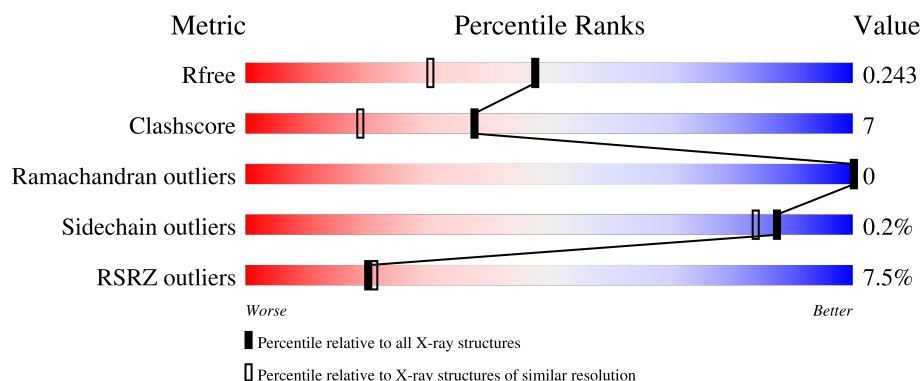
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	257	6% 91% 9%
1	B	257	9% 86% 13% .

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
5	GOL	B	307	-	-	X	-
6	ACT	B	312	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8623 atoms, of which 4160 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.

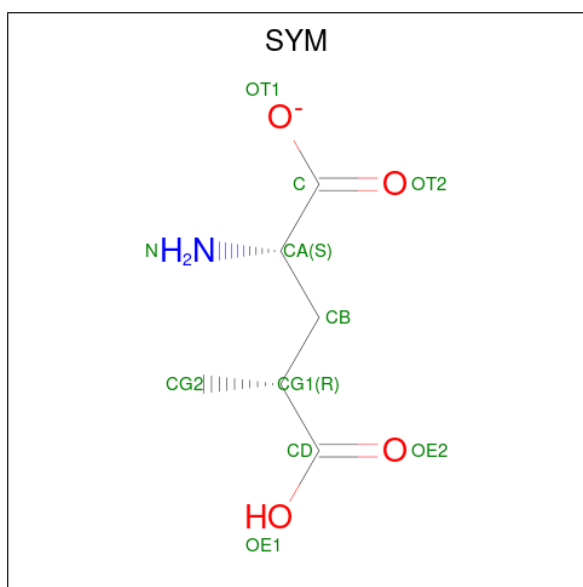
- Molecule 1 is a protein called Glutamate receptor ionotropic, kainate 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	256	Total	C	H	N	O	S	0	1	0
			4094	1298	2058	342	384	12			
1	B	253	Total	C	H	N	O	S	0	0	0
			4038	1283	2027	336	380	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P42264
A	2	SER	-	expression tag	UNP P42264
A	117	GLY	-	linker	UNP P42264
A	118	THR	-	linker	UNP P42264
B	1	GLY	-	expression tag	UNP P42264
B	2	SER	-	expression tag	UNP P42264
B	117	GLY	-	linker	UNP P42264
B	118	THR	-	linker	UNP P42264

- Molecule 2 is 2S,4R-4-METHYLGLUTAMATE (CCD ID: SYM) (formula: C₆H₁₀NO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			20	6	9	1	4		
2	B	1	Total	C	H	N	O	0	0
			20	6	9	1	4		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

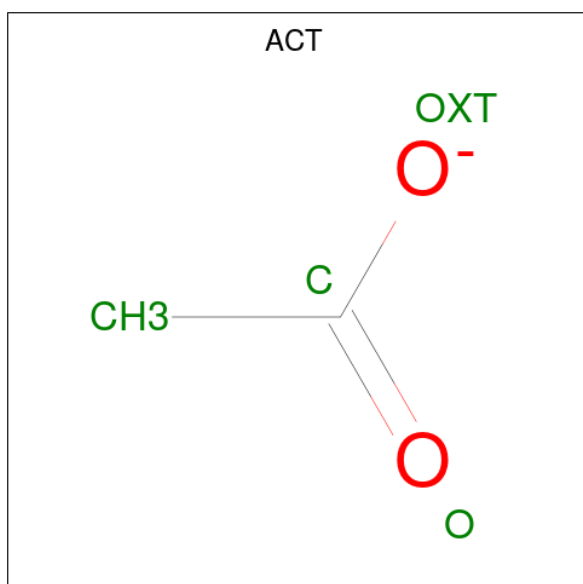
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			13	3	7	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 7 2 3 2	0	0
6	A	1	Total C H O 7 2 3 2	0	0
6	A	1	Total C H O 7 2 3 2	0	0
6	B	1	Total C H O 7 2 3 2	0	0
6	B	1	Total C H O 7 2 3 2	0	0
6	B	1	Total C H O 7 2 3 2	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Na 2 2	0	0

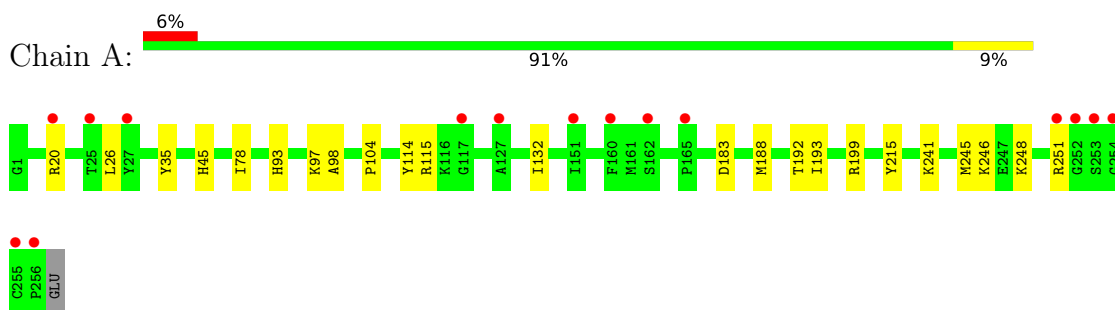
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	198	Total O 198 198	0	0
8	B	132	Total O 132 132	0	0

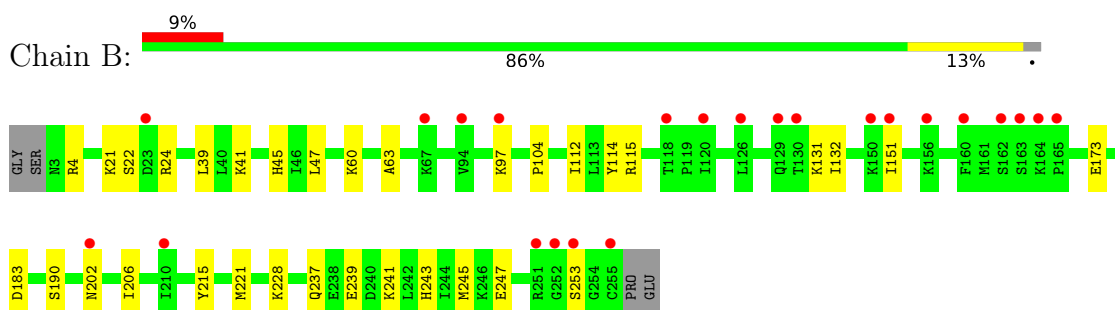
3 Residue-property plots

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: Glutamate receptor ionotropic, kainate 3



- Molecule 1: Glutamate receptor ionotropic, kainate 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 2	Depositor
Cell constants a, b, c, α , β , γ	56.46Å 88.03Å 130.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 1.83 72.97 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.5 (72.97-1.83) 99.5 (72.97-1.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.83Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.203 , 0.242 0.205 , 0.243	Depositor DCC
R_{free} test set	2925 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 56.1	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	0.96	EDS
Total number of atoms	8623	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: CL, NA, ACT, SYM, GOL, ZN

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	0.45	0/2078	0.62	0/2797
1	B	0.38	0/2049	0.55	0/2758
All	All	0.42	0/4127	0.59	0/5555

There are no bond length outliers.

There are no bond angle outliers.

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	2036	2058	2058	26	1
1	B	2011	2027	2027	31	0
2	A	11	9	9	0	0
2	B	11	9	9	0	0
3	A	1	0	0	0	0
3	B	3	0	0	1	0
4	A	2	0	0	0	1
4	B	2	0	0	0	0
5	A	6	8	8	0	0
5	B	24	31	32	10	0
6	A	12	9	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	9	9	4	0
7	B	2	0	0	0	0
8	A	198	0	0	4	3
8	B	132	0	0	7	2
All	All	4463	4160	4161	58	6

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 7.

All (58) 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)
5:B:307:GOL:O1	8:B:401:HOH:O	1.71	1.06
5:B:308:GOL:O3	8:B:402:HOH:O	1.80	0.99
1:B:202:ASN:OD1	8:B:403:HOH:O	1.81	0.96
1:B:45:HIS:ND1	8:B:405:HOH:O	2.15	0.80
1:A:45:HIS:ND1	8:A:402:HOH:O	2.11	0.77
1:A:97:LYS:NZ	8:A:401:HOH:O	1.86	0.76
1:B:60:LYS:NZ	3:B:305:CL:CL	2.56	0.76
1:B:239:GLU:OE1	6:B:312:ACT:H3	1.85	0.76
1:A:188:MET:HE3	1:A:192:THR:HG22	1.73	0.70
1:B:45:HIS:ND1	8:B:407:HOH:O	2.27	0.67
1:A:188:MET:HE3	1:A:192:THR:CG2	2.24	0.67
1:B:243:HIS:HB2	5:B:307:GOL:H32	1.78	0.64
1:A:93:HIS:H	6:A:306:ACT:H1	1.63	0.64
1:B:97:LYS:O	1:B:221:MET:HE1	2.00	0.62
1:B:114:TYR:OH	1:B:183:ASP:OD1	2.19	0.59
1:A:188:MET:HE3	1:A:192:THR:HB	1.85	0.59
1:B:41:LYS:NZ	8:B:404:HOH:O	1.94	0.59
1:A:188:MET:HE3	1:A:192:THR:CB	2.33	0.58
1:A:188:MET:HE2	1:A:193:ILE:N	2.18	0.58
1:B:39:LEU:HB2	1:B:245:MET:HE1	1.86	0.56
1:B:239:GLU:CD	6:B:312:ACT:H3	2.30	0.55
1:B:241:LYS:NZ	6:B:312:ACT:H1	2.24	0.53
1:A:188:MET:HE2	1:A:193:ILE:CG1	2.39	0.53
1:A:188:MET:HE2	1:A:193:ILE:HG13	1.91	0.53
1:B:243:HIS:N	5:B:307:GOL:H32	2.23	0.52
1:B:151:ILE:HD12	1:B:151:ILE:N	2.25	0.52
1:A:188:MET:HE2	1:A:193:ILE:CA	2.40	0.52
1:A:199[A]:ARG:NH2	8:A:403:HOH:O	2.14	0.52
1:B:131:LYS:NZ	1:B:183:ASP:OD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:O	1:A:251:ARG:HG3	2.11	0.51
1:B:115:ARG:NH2	1:B:183:ASP:OD1	2.44	0.50
1:A:241:LYS:NZ	8:A:408:HOH:O	2.44	0.49
1:A:114:TYR:OH	1:A:132:ILE:HD13	2.14	0.47
1:A:78:ILE:HD11	1:A:98:ALA:HB1	1.95	0.47
1:B:190:SER:HB2	6:B:311:ACT:H3	1.96	0.46
1:B:243:HIS:HB2	5:B:307:GOL:C3	2.45	0.46
1:A:20:ARG:HD2	1:A:26:LEU:HD13	1.96	0.46
1:B:112:ILE:HB	1:B:206:ILE:HB	1.98	0.46
1:A:241:LYS:O	1:A:245:MET:HE3	2.17	0.45
1:B:237:GLN:HG3	5:B:307:GOL:O2	2.16	0.45
1:A:188:MET:CE	1:A:192:THR:C	2.90	0.45
1:B:4:ARG:HG3	8:B:489:HOH:O	2.16	0.45
1:B:97:LYS:O	1:B:97:LYS:HG2	2.16	0.45
1:A:115:ARG:NH2	1:A:183:ASP:OD1	2.49	0.44
1:B:114:TYR:OH	1:B:115:ARG:NH2	2.47	0.43
1:A:188:MET:CE	1:A:193:ILE:N	2.82	0.43
1:A:104:PRO:HA	1:A:215:TYR:O	2.19	0.42
1:B:173:GLU:OE1	5:B:309:GOL:O1	2.20	0.42
1:B:114:TYR:OH	1:B:132:ILE:HD13	2.20	0.42
1:A:93:HIS:CE1	5:B:307:GOL:H31	2.55	0.41
1:B:47:LEU:HD22	1:B:228:LYS:HB3	2.00	0.41
1:B:24:ARG:O	5:B:308:GOL:H31	2.19	0.41
1:A:35:TYR:CD2	1:A:35:TYR:C	2.99	0.41
1:B:63:ALA:HB2	5:B:306:GOL:H2	2.03	0.40
1:A:97:LYS:HE3	1:B:247:GLU:OE2	2.22	0.40
1:A:188:MET:CE	1:A:192:THR:HG22	2.48	0.40
1:B:21:LYS:HG3	1:B:22:SER:N	2.36	0.40
1:B:104:PRO:HA	1:B:215:TYR:O	2.21	0.40

All (6) 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)
8:A:451:HOH:O	8:A:552:HOH:O[4_555]	1.79	0.41
8:A:502:HOH:O	8:A:550:HOH:O[4_555]	2.00	0.20
8:B:418:HOH:O	8:B:518:HOH:O[2_556]	2.08	0.12
8:A:538:HOH:O	8:A:574:HOH:O[2_555]	2.13	0.07
1:A:246:LYS:HZ1	4:A:303:ZN:ZN[4_555]	1.55	0.05
8:B:490:HOH:O	8:B:521:HOH:O[2_556]	2.17	0.03

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	255/257 (99%)	245 (96%)	10 (4%)	0	100	100
1	B	251/257 (98%)	243 (97%)	8 (3%)	0	100	100
All	All	506/514 (98%)	488 (96%)	18 (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	221/221 (100%)	221 (100%)	0	100	100
1	B	218/221 (99%)	217 (100%)	1 (0%)	81	75
All	All	439/442 (99%)	438 (100%)	1 (0%)	87	84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	253	SER

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	237	GLN
1	B	64	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 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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	$\# Z > 2$
6	ACT	B	312	-	3,3,3	0.68	0	3,3,3	2.02	2 (66%)
6	ACT	A	308	-	3,3,3	1.26	0	3,3,3	1.33	0
6	ACT	B	310	-	3,3,3	1.22	0	3,3,3	1.71	1 (33%)
2	SYM	A	301	-	8,10,10	1.11	0	8,13,13	1.63	1 (12%)
5	GOL	B	308	-	5,5,5	0.83	0	5,5,5	1.56	1 (20%)
6	ACT	B	311	-	3,3,3	1.21	0	3,3,3	1.81	2 (66%)
6	ACT	A	306	-	3,3,3	1.00	0	3,3,3	1.75	2 (66%)
5	GOL	B	307	-	5,5,5	1.40	0	5,5,5	1.43	1 (20%)
5	GOL	B	309	-	5,5,5	0.74	0	5,5,5	1.24	1 (20%)
5	GOL	A	304	-	5,5,5	0.79	0	5,5,5	1.49	1 (20%)
6	ACT	A	305	-	3,3,3	0.68	0	3,3,3	1.74	2 (66%)
5	GOL	B	306	-	5,5,5	1.20	1 (20%)	5,5,5	1.15	1 (20%)
2	SYM	B	302	-	8,10,10	1.13	0	8,13,13	1.10	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
2	SYM	A	301	-	-	1/12/12/12	-
5	GOL	B	308	-	-	4/4/4/4	-
5	GOL	B	307	-	-	2/4/4/4	-
5	GOL	B	309	-	-	0/4/4/4	-
5	GOL	A	304	-	-	2/4/4/4	-
5	GOL	B	306	-	-	0/4/4/4	-
2	SYM	B	302	-	-	0/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	306	GOL	C1-C2	2.13	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	SYM	OT1-C-OT2	-3.71	115.66	124.08
6	B	312	ACT	O-C-CH3	-2.65	111.66	122.53
5	B	308	GOL	C3-C2-C1	-2.49	102.67	111.80
6	B	310	ACT	OXT-C-O	2.48	131.22	122.03
5	A	304	GOL	C3-C2-C1	-2.43	102.87	111.80
5	B	307	GOL	C3-C2-C1	-2.34	103.20	111.80
6	B	311	ACT	OXT-C-O	2.34	130.70	122.03
6	A	306	ACT	OXT-C-O	2.17	130.08	122.03
6	A	305	ACT	O-C-CH3	-2.14	113.76	122.53
6	B	312	ACT	OXT-C-O	2.13	129.94	122.03
5	B	309	GOL	C3-C2-C1	-2.12	104.01	111.80
6	A	306	ACT	O-C-CH3	-2.11	113.88	122.53
6	B	311	ACT	O-C-CH3	-2.09	113.95	122.53
6	A	305	ACT	OXT-C-O	2.09	129.78	122.03
5	B	306	GOL	C3-C2-C1	-2.06	104.23	111.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	307	GOL	C1-C2-C3-O3
5	B	307	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	308	GOL	O1-C1-C2-C3
5	B	308	GOL	O1-C1-C2-O2
5	A	304	GOL	O2-C2-C3-O3
5	B	308	GOL	O2-C2-C3-O3
5	A	304	GOL	C1-C2-C3-O3
2	A	301	SYM	OT2-C-CA-N
5	B	308	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	312	ACT	3	0
5	B	308	GOL	2	0
6	B	311	ACT	1	0
6	A	306	ACT	1	0
5	B	307	GOL	6	0
5	B	309	GOL	1	0
5	B	306	GOL	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	256/257 (99%)	0.25	15 (5%) 28 30	20, 42, 94, 112	1 (0%)
1	B	253/257 (98%)	0.54	23 (9%) 15 16	26, 53, 102, 118	0
All	All	509/514 (99%)	0.40	38 (7%) 20 21	20, 48, 99, 118	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	GLY	4.0
1	B	255	CYS	3.9
1	B	165	PRO	3.7
1	B	94	VAL	3.6
1	B	97	LYS	3.4
1	B	160	PHE	3.4
1	B	118	THR	3.4
1	B	120	ILE	3.3
1	A	255	CYS	3.3
1	A	251	ARG	3.2
1	A	254	GLY	3.2
1	B	130	THR	2.9
1	A	165	PRO	2.8
1	B	23	ASP	2.7
1	A	256	PRO	2.7
1	B	126	LEU	2.6
1	B	253	SER	2.5
1	A	160	PHE	2.5
1	A	253	SER	2.5
1	B	156	LYS	2.4
1	B	163	SER	2.4
1	B	251	ARG	2.4
1	A	127	ALA	2.4
1	B	164	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	129	GLN	2.3
1	A	25	THR	2.3
1	A	162	SER	2.2
1	B	210	ILE	2.2
1	B	150	LYS	2.2
1	B	252	GLY	2.2
1	A	27	TYR	2.2
1	B	67	LYS	2.2
1	B	162	SER	2.1
1	B	151	ILE	2.1
1	A	117	GLY	2.0
1	A	151	ILE	2.0
1	B	202	ASN	2.0
1	A	20	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(Å ²)	Q<0.9
6	ACT	A	308	4/4	0.76	0.20	47,61,66,68	0
7	NA	B	314	1/1	0.78	0.30	73,73,73,73	0
5	GOL	B	308	6/6	0.81	0.16	43,63,79,95	0
6	ACT	B	311	4/4	0.82	0.18	54,67,72,80	0
6	ACT	A	305	4/4	0.83	0.14	59,72,77,81	0
6	ACT	B	312	4/4	0.85	0.15	64,69,85,85	0
6	ACT	B	310	4/4	0.85	0.18	49,60,71,79	0
3	CL	B	313	1/1	0.86	0.21	91,91,91,91	0
6	ACT	A	306	4/4	0.87	0.16	45,54,72,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	307	6/6	0.89	0.14	37,68,87,87	0
5	GOL	B	309	6/6	0.92	0.10	30,48,60,67	0
5	GOL	A	304	6/6	0.92	0.09	42,53,63,66	0
7	NA	B	315	1/1	0.92	0.23	58,58,58,58	0
3	CL	B	305	1/1	0.93	0.14	72,72,72,72	0
5	GOL	B	306	6/6	0.94	0.08	39,48,68,68	0
4	ZN	A	307	1/1	0.96	0.06	75,75,75,75	0
2	SYM	B	302	11/11	0.97	0.06	29,37,50,60	0
3	CL	A	302	1/1	0.97	0.06	52,52,52,52	0
4	ZN	B	303	1/1	0.97	0.07	60,60,60,60	1
2	SYM	A	301	11/11	0.97	0.05	21,33,40,40	0
3	CL	B	304	1/1	0.99	0.14	44,44,44,44	0
4	ZN	A	303	1/1	1.00	0.04	33,33,33,33	0
4	ZN	B	301	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.