



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:22 AM UTC

PDB ID : 5XUJ / pdb_00005xuj
Title : Crystal structure of PDE10A in complex with 7-(4-chlorophenyl)-2-methylpyrazolo[1,5-a]pyrimidine
Authors : Amano, Y.; Honbou, K.
Deposited on : 2017-06-23
Resolution : 2.44 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

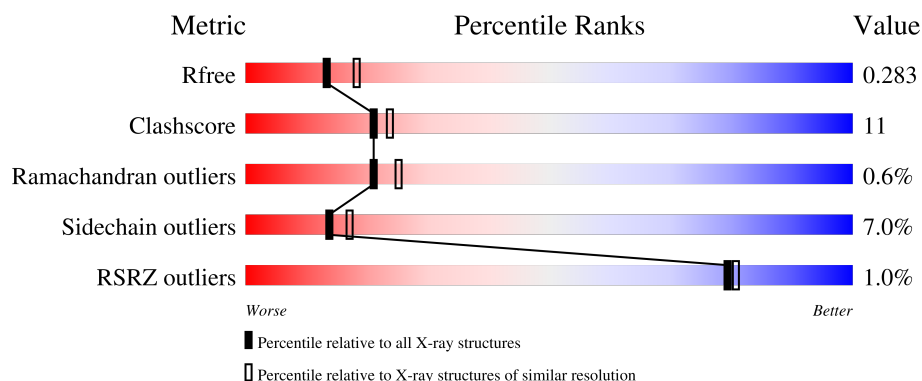
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	345	% 63% 23% • 11%
1	B	345	65% 26% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5218 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 cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2492	1587	425	455	25			
1	B	322	Total	C	N	O	S	0	0	0
			2610	1667	443	475	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	-	expression tag	UNP Q9Y233
A	446	SER	-	expression tag	UNP Q9Y233
A	447	HIS	-	expression tag	UNP Q9Y233
A	448	MET	-	expression tag	UNP Q9Y233
B	445	GLY	-	expression tag	UNP Q9Y233
B	446	SER	-	expression tag	UNP Q9Y233
B	447	HIS	-	expression tag	UNP Q9Y233
B	448	MET	-	expression tag	UNP Q9Y233

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

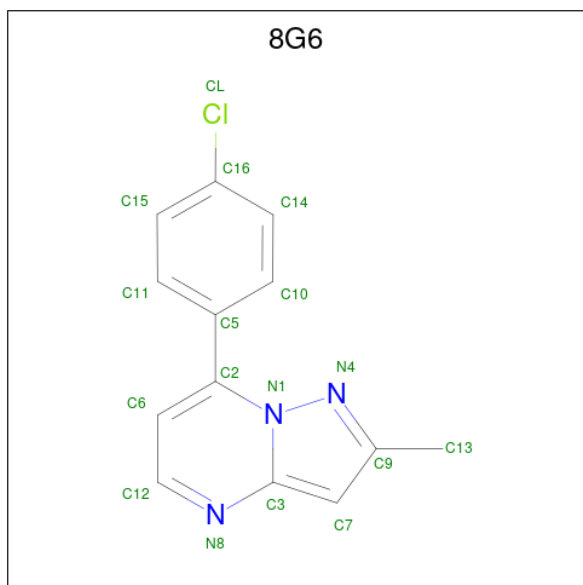
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 7-(4-chlorophenyl)-2-methyl-pyrazolo[1,5-a]pyrimidine (CCD ID: 8G6) (formula: C₁₃H₁₀ClN₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			17	13	1	3		

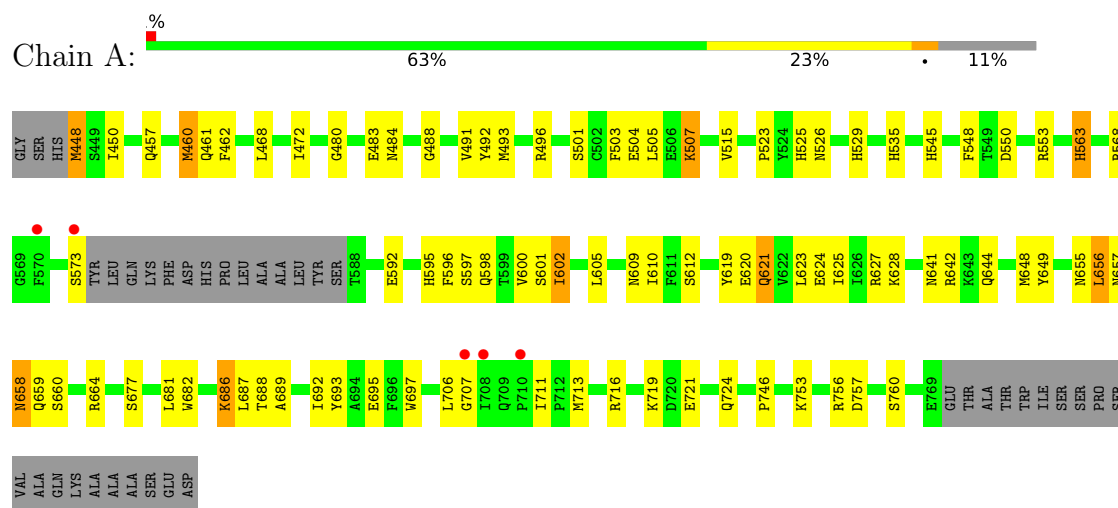
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	57	Total	O	0	0
			57	57		

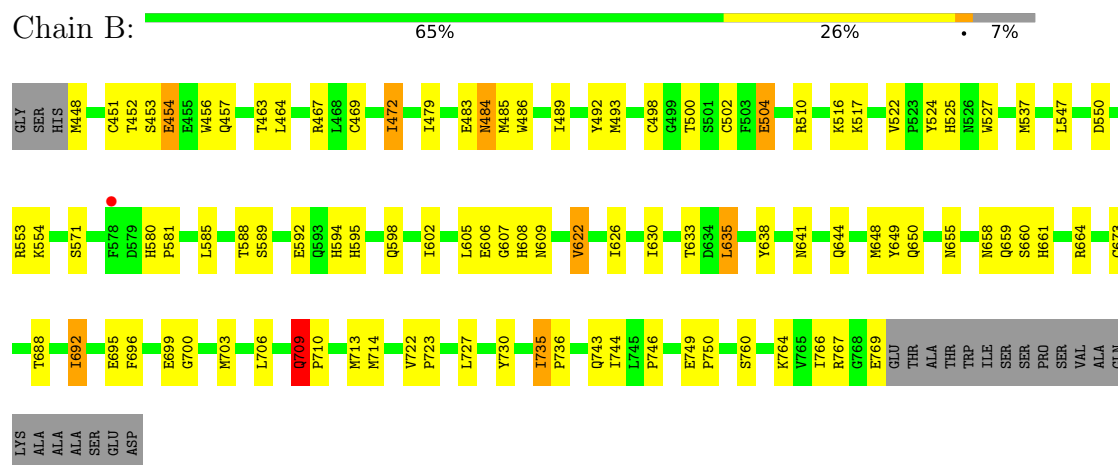
3 Residue-property plots

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: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.34Å 81.30Å 157.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.80 – 2.44 78.80 – 2.44	Depositor EDS
% Data completeness (in resolution range)	92.1 (78.80-2.44) 92.1 (78.80-2.44)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.71 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.198 , 0.280 0.199 , 0.283	Depositor DCC
R_{free} test set	1156 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5218	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: MG, ZN, 8G6

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	0.78	0/2550	1.07	6/3449 (0.2%)
1	B	0.77	0/2674	1.09	9/3620 (0.2%)
All	All	0.78	0/5224	1.08	15/7069 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	ILE	CB-CA-C	-8.28	105.83	113.70
1	A	480	GLY	CA-C-N	7.56	127.23	119.82
1	A	480	GLY	C-N-CA	7.56	127.23	119.82
1	B	485	MET	N-CA-C	6.40	120.69	113.01
1	A	746	PRO	N-CA-C	6.31	118.40	110.70
1	B	522	VAL	CA-C-N	-6.30	112.35	119.28
1	B	522	VAL	C-N-CA	-6.30	112.35	119.28
1	B	746	PRO	N-CA-C	6.25	118.33	110.70
1	B	709	GLN	CA-C-N	5.82	125.79	120.03
1	B	709	GLN	C-N-CA	5.82	125.79	120.03
1	B	735	ILE	N-CA-CB	5.57	114.25	110.52
1	A	460	MET	N-CA-C	5.57	118.07	111.33
1	A	483	GLU	N-CA-C	5.30	117.06	111.28
1	B	744	ILE	CB-CA-C	-5.29	105.15	112.24
1	A	515	VAL	N-CA-C	-5.23	105.28	110.62

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	2492	0	2460	56	0
1	B	2610	0	2575	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	17	0	0	1	0
5	A	38	0	0	5	0
5	B	57	0	0	0	0
All	All	5218	0	5035	112	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 11.

All (112) 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:612:SER:HB2	5:A:909:HOH:O	1.28	1.32
1:A:641:ASN:ND2	1:A:664:ARG:HH11	1.54	1.03
1:A:641:ASN:HD22	1:A:664:ARG:NH1	1.57	1.01
1:B:655:ASN:H	1:B:661:HIS:HD2	1.17	0.91
1:A:658:ASN:HD22	1:A:658:ASN:C	1.84	0.85
1:A:724:GLN:HG3	5:A:932:HOH:O	1.78	0.83
1:B:655:ASN:H	1:B:661:HIS:CD2	2.02	0.77
1:A:548:PHE:O	1:A:553:ARG:NH1	2.18	0.77
1:A:641:ASN:HD22	1:A:664:ARG:HH11	0.83	0.76
1:B:735:ILE:HB	1:B:736:PRO:HD3	1.70	0.73
1:A:655:ASN:HD22	1:A:657:ASN:H	1.37	0.73
1:B:448:MET:HE1	1:B:598:GLN:OE1	1.88	0.73
1:A:525:HIS:NE2	5:A:902:HOH:O	2.22	0.72
1:A:448:MET:HE1	1:A:598:GLN:OE1	1.89	0.72
1:A:756:ARG:HH22	1:B:484:ASN:HD21	1.41	0.68
1:A:655:ASN:ND2	1:A:657:ASN:H	1.92	0.67
1:B:722:VAL:HB	1:B:723:PRO:HD3	1.78	0.65
1:A:658:ASN:HD22	1:A:659:GLN:N	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:ILE:O	1:B:633:THR:OG1	2.13	0.65
1:A:658:ASN:C	1:A:658:ASN:ND2	2.55	0.63
1:A:550:ASP:OD1	1:A:553:ARG:NH2	2.32	0.63
1:A:529:HIS:NE2	1:A:563:HIS:HE1	1.97	0.63
1:A:612:SER:CB	5:A:909:HOH:O	2.08	0.63
1:A:644:GLN:O	1:A:648:MET:HG3	2.01	0.61
1:B:464:LEU:HD23	1:B:469:CYS:SG	2.41	0.60
1:B:472:ILE:HD11	1:B:489:ILE:HG23	1.82	0.60
1:A:507:LYS:NZ	1:A:609:ASN:O	2.35	0.59
1:B:700:GLY:HA3	1:B:714:MET:O	2.04	0.57
1:A:573:SER:OG	5:A:901:HOH:O	2.17	0.57
1:B:709:GLN:HE21	1:B:709:GLN:HA	1.71	0.56
1:A:697:TRP:CH2	1:A:719:LYS:HG2	2.41	0.56
1:A:624:GLU:HG3	1:A:628:LYS:HE3	1.88	0.56
1:B:498:CYS:HB3	1:B:502:CYS:SG	2.47	0.55
1:B:658:ASN:C	1:B:658:ASN:HD22	2.13	0.55
4:A:803:8G6:C11	4:A:803:8G6:N4	2.68	0.55
1:B:605:LEU:O	1:B:608:HIS:HB2	2.07	0.54
1:A:529:HIS:CD2	1:A:563:HIS:HE1	2.26	0.54
1:A:677:SER:OG	1:A:688:THR:HG21	2.08	0.53
1:A:448:MET:HG3	1:A:602:ILE:HG12	1.90	0.53
1:A:468:LEU:O	1:A:472:ILE:HG22	2.09	0.52
1:B:594:HIS:CE1	1:B:598:GLN:NE2	2.78	0.52
1:A:689:ALA:O	1:A:692:ILE:HG22	2.11	0.51
1:A:448:MET:HG2	1:A:601:SER:HB3	1.91	0.51
1:B:524:TYR:HB3	1:B:695:GLU:OE1	2.09	0.51
1:B:658:ASN:C	1:B:658:ASN:ND2	2.65	0.51
1:B:580:HIS:CG	1:B:581:PRO:HD2	2.46	0.50
1:B:598:GLN:O	1:B:602:ILE:HG13	2.11	0.50
1:B:592:GLU:HA	1:B:595:HIS:HD2	1.77	0.49
1:A:493:MET:SD	1:A:535:HIS:HA	2.52	0.49
1:B:483:GLU:HA	1:B:486:TRP:CE2	2.48	0.49
1:B:502:CYS:SG	1:B:554:LYS:HE2	2.52	0.49
1:B:537:MET:HE2	1:B:673:CYS:SG	2.53	0.49
1:A:462:PHE:CD2	1:A:488:GLY:HA3	2.48	0.48
1:A:596:PHE:O	1:A:600:VAL:HG23	2.12	0.48
1:B:696:PHE:HB3	1:B:714:MET:HG2	1.94	0.48
1:A:619:TYR:O	1:A:621:GLN:N	2.47	0.48
1:B:525:HIS:ND1	1:B:695:GLU:OE2	2.44	0.47
1:B:655:ASN:N	1:B:661:HIS:HD2	1.99	0.47
1:B:730:TYR:O	1:B:735:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ILE:HG22	1:A:605:LEU:HD13	1.96	0.47
1:A:460:MET:HE3	1:A:505:LEU:HD23	1.96	0.47
1:B:588:THR:O	1:B:589:SER:C	2.56	0.47
1:A:492:TYR:CE1	1:A:496:ARG:HG3	2.50	0.47
1:B:658:ASN:HD22	1:B:659:GLN:N	2.13	0.47
1:B:502:CYS:SG	1:B:554:LYS:CE	3.03	0.47
1:A:504:GLU:O	1:A:505:LEU:C	2.58	0.46
1:A:523:PRO:HD2	1:A:695:GLU:HG3	1.97	0.46
1:A:655:ASN:HD22	1:A:655:ASN:C	2.23	0.46
1:A:716:ARG:O	1:A:719:LYS:HG3	2.16	0.46
1:B:452:THR:OG1	1:B:454:GLU:HG2	2.15	0.46
1:B:727:LEU:HD22	1:B:766:ILE:HD12	1.98	0.46
1:B:472:ILE:HG21	1:B:492:TYR:HE2	1.81	0.45
1:B:592:GLU:HA	1:B:595:HIS:CD2	2.51	0.45
1:A:457:GLN:O	1:A:461:GLN:OE1	2.35	0.45
1:B:692:ILE:HD11	1:B:696:PHE:CZ	2.51	0.45
1:B:510:ARG:NH1	1:B:607:GLY:HA3	2.31	0.45
1:B:504:GLU:H	1:B:504:GLU:HG2	1.53	0.45
1:B:594:HIS:CE1	1:B:598:GLN:HE21	2.34	0.45
1:A:649:TYR:CD1	1:A:649:TYR:C	2.95	0.45
1:B:688:THR:O	1:B:692:ILE:HG22	2.16	0.44
1:B:571:SER:OG	1:B:699:GLU:OE2	2.22	0.44
1:B:453:SER:HA	1:B:456:TRP:NE1	2.33	0.44
1:A:713:MET:HE2	1:A:713:MET:HB3	1.89	0.44
1:B:622:VAL:O	1:B:626:ILE:HG13	2.18	0.44
1:B:463:THR:HG22	1:B:464:LEU:N	2.33	0.44
1:A:592:GLU:HA	1:A:595:HIS:CD2	2.53	0.43
1:A:503:PHE:CD1	1:A:610:ILE:HB	2.54	0.43
1:B:644:GLN:HG3	1:B:664:ARG:CZ	2.48	0.43
1:B:451:CYS:HA	1:B:517:LYS:HD2	1.99	0.43
1:B:489:ILE:HG22	1:B:493:MET:HE2	1.99	0.43
1:A:529:HIS:CD2	1:A:563:HIS:CE1	3.05	0.43
1:A:760:SER:HB2	1:B:467:ARG:HH22	1.83	0.43
1:A:682:TRP:CZ2	1:A:686:LYS:HG3	2.54	0.42
1:B:635:LEU:HD22	1:B:638:TYR:HB3	2.01	0.42
1:B:703:MET:HB2	1:B:710:PRO:HG3	2.02	0.42
1:A:596:PHE:CD2	1:A:627:ARG:HG3	2.55	0.42
1:B:550:ASP:OD1	1:B:553:ARG:NH2	2.51	0.42
1:A:491:VAL:O	1:A:492:TYR:C	2.63	0.42
1:A:523:PRO:O	1:A:526:ASN:ND2	2.53	0.41
1:A:448:MET:HG2	1:A:601:SER:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ASN:HD22	1:B:664:ARG:HH11	1.68	0.41
1:B:749:GLU:N	1:B:750:PRO:CD	2.83	0.41
1:A:592:GLU:HA	1:A:595:HIS:HD2	1.85	0.41
1:B:479:ILE:O	1:B:486:TRP:NE1	2.42	0.41
1:A:656:LEU:HD12	1:A:656:LEU:HA	1.79	0.41
1:A:692:ILE:HG23	1:A:693:TYR:N	2.36	0.41
1:B:764:LYS:HG2	1:B:767:ARG:NH2	2.36	0.41
1:B:644:GLN:O	1:B:648:MET:HG3	2.21	0.41
1:A:689:ALA:O	1:A:692:ILE:CG2	2.69	0.40
1:A:753:LYS:NZ	1:A:757:ASP:OD2	2.54	0.40
1:B:516:LYS:HA	1:B:527:TRP:CE3	2.56	0.40
1:B:649:TYR:CZ	1:B:743:GLN:HB3	2.57	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	304/345 (88%)	285 (94%)	16 (5%)	3 (1%)	12	13
1	B	320/345 (93%)	301 (94%)	18 (6%)	1 (0%)	36	44
All	All	624/690 (90%)	586 (94%)	34 (5%)	4 (1%)	21	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	620	GLU
1	A	621	GLN
1	A	707	GLY
1	B	609	ASN

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	279/308 (91%)	258 (92%)	21 (8%)	12	15
1	B	291/308 (94%)	272 (94%)	19 (6%)	15	20
All	All	570/616 (92%)	530 (93%)	40 (7%)	14	17

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	448	MET
1	A	484	ASN
1	A	501	SER
1	A	507	LYS
1	A	545	HIS
1	A	563	HIS
1	A	568	ARG
1	A	597	SER
1	A	602	ILE
1	A	623	LEU
1	A	625	ILE
1	A	642	ARG
1	A	656	LEU
1	A	658	ASN
1	A	660	SER
1	A	681	LEU
1	A	686	LYS
1	A	687	LEU
1	A	706	LEU
1	A	711	ILE
1	A	721	GLU
1	B	454	GLU
1	B	457	GLN
1	B	472	ILE
1	B	484	ASN
1	B	500	THR
1	B	504	GLU

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Mol	Chain	Res	Type
1	B	547	LEU
1	B	585	LEU
1	B	606	GLU
1	B	622	VAL
1	B	635	LEU
1	B	650	GLN
1	B	660	SER
1	B	692	ILE
1	B	706	LEU
1	B	709	GLN
1	B	713	MET
1	B	760	SER
1	B	769	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	HIS
1	A	641	ASN
1	A	655	ASN
1	A	658	ASN
1	A	690	ASN
1	A	726	GLN
1	B	476	HIS
1	B	484	ASN
1	B	544	ASN
1	B	545	HIS
1	B	593	GLN
1	B	594	HIS
1	B	598	GLN
1	B	641	ASN
1	B	655	ASN
1	B	658	ASN
1	B	661	HIS
1	B	690	ASN
1	B	709	GLN
1	B	726	GLN
1	B	731	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 ⓘ

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
4	8G6	A	803	-	19,19,19	1.21	1 (5%)	27,27,27	2.85	7 (25%)

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	8G6	A	803	-	-	4/4/4/4	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	8G6	C6-C12	3.29	1.47	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	8G6	C12-C6-C2	-11.37	113.23	120.69
4	A	803	8G6	C6-C2-N1	5.05	121.22	115.22
4	A	803	8G6	C12-N8-C3	4.35	117.79	115.82
4	A	803	8G6	C7-C3-N1	3.04	107.46	105.65
4	A	803	8G6	N1-C3-N8	-2.87	119.64	121.61
4	A	803	8G6	C9-N4-N1	2.61	106.66	104.40
4	A	803	8G6	C5-C2-C6	-2.52	117.51	123.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	8G6	C6-C2-C5-C10
4	A	803	8G6	C6-C2-C5-C11
4	A	803	8G6	N1-C2-C5-C10
4	A	803	8G6	N1-C2-C5-C11

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	8G6	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 [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	308/345 (89%)	-0.18	5 (1%) 70 72	28, 50, 86, 122	0
1	B	322/345 (93%)	-0.27	1 (0%) 90 91	26, 49, 79, 99	0
All	All	630/690 (91%)	-0.22	6 (0%) 79 81	26, 50, 82, 122	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	GLY	3.5
1	A	708	ILE	2.6
1	A	710	PRO	2.4
1	A	570	PHE	2.4
1	A	573	SER	2.3
1	B	578	PHE	2.3

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
4	8G6	A	803	17/17	0.81	0.15	49,68,82,99	0
3	MG	B	802	1/1	0.99	0.02	34,34,34,34	0
3	MG	A	802	1/1	0.99	0.03	27,27,27,27	0
2	ZN	B	801	1/1	1.00	0.02	38,38,38,38	0
2	ZN	A	801	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.