



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:43 AM UTC

PDB ID : 1ZY4 / pdb_00001zy4
Title : Crystal Structure of eIF2alpha Protein Kinase GCN2: R794G Hyperactivating Mutant in Apo Form.
Authors : Padyana, A.K.; Qiu, H.; Roll-Mecak, A.; Hinnebusch, A.G.; Burley, S.K.
Deposited on : 2005-06-09
Resolution : 1.95 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

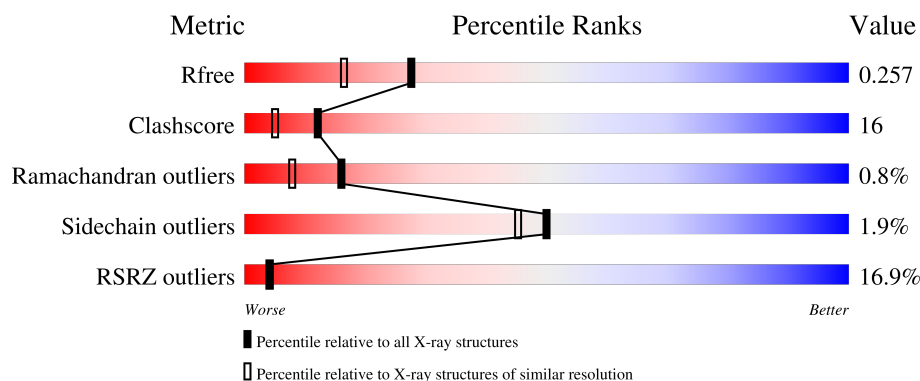
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	303	8% 69% 19% • 11%
1	B	303	21% 53% 27% • 18%

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
2	GOL	A	998	-	X	-	-
2	GOL	B	998	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4539 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.

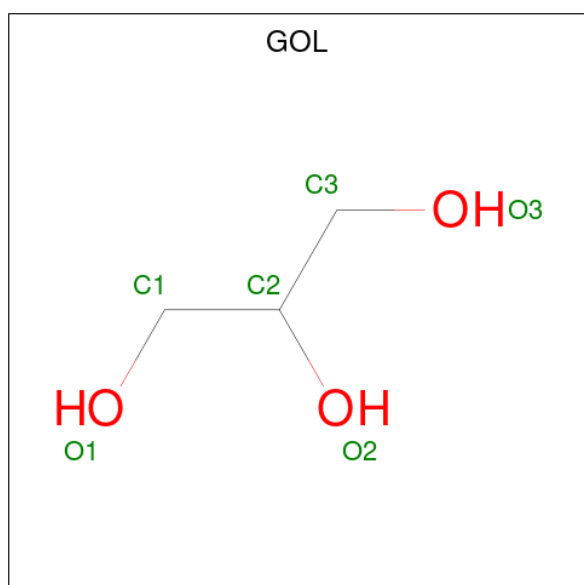
- Molecule 1 is a protein called Serine/threonine-protein kinase GCN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2236	1434	390	403	9			
1	B	249	Total	C	N	O	S	0	0	0
			2057	1326	352	370	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	592	SER	-	cloning artifact	UNP P15442
A	593	LEU	-	cloning artifact	UNP P15442
A	794	GLY	ARG	engineered mutation	UNP P15442
B	592	SER	-	cloning artifact	UNP P15442
B	593	LEU	-	cloning artifact	UNP P15442
B	794	GLY	ARG	engineered mutation	UNP P15442

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

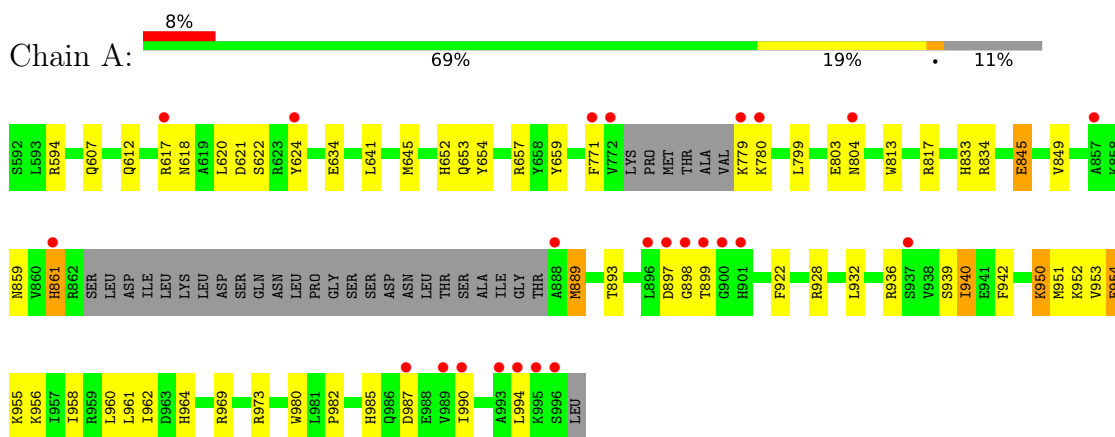
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total	O	0	0
			163	163		
3	B	71	Total	O	0	0
			71	71		

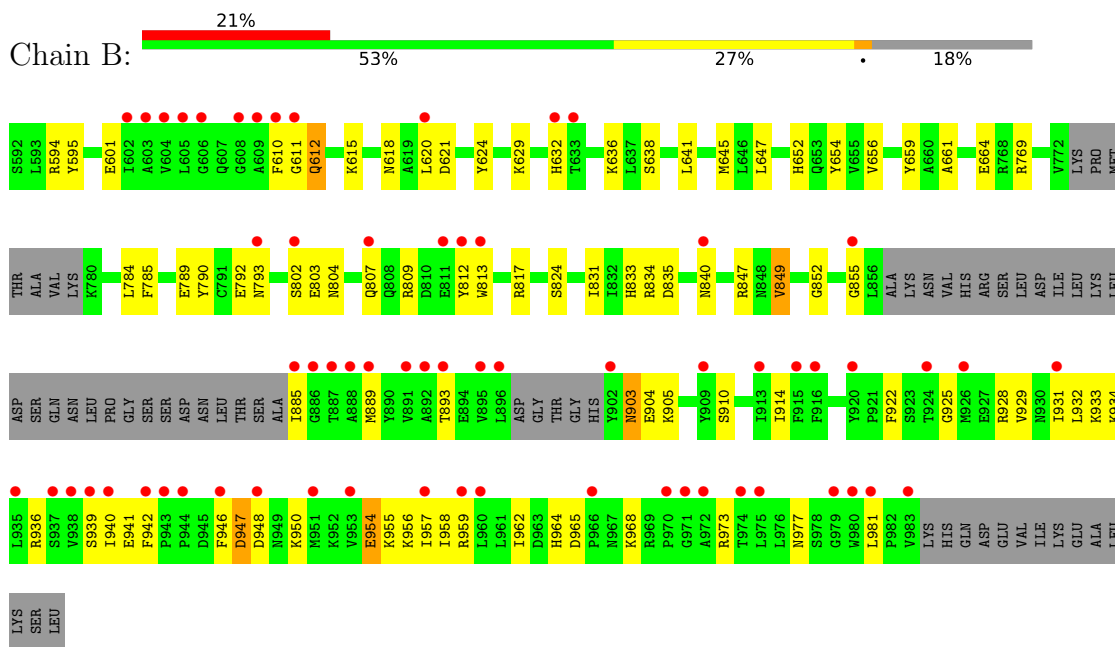
3 Residue-property plots

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: Serine/threonine-protein kinase GCN2



• Molecule 1: Serine/threonine-protein kinase GCN2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.83Å 79.26Å 146.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.72 – 1.95 37.72 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (37.72-1.95) 99.1 (37.72-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.95Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.224 , 0.252 0.222 , 0.257	Depositor DCC
R_{free} test set	1407 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	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	0.95	EDS
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: GOL

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	0.54	0/2281	0.91	3/3068 (0.1%)
1	B	0.43	0/2098	0.86	3/2824 (0.1%)
All	All	0.49	0/4379	0.89	6/5892 (0.1%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	594	ARG	N-CA-C	7.44	120.03	111.11
1	A	594	ARG	N-CA-C	6.99	119.50	111.11
1	B	849	VAL	N-CA-C	6.37	116.99	110.05
1	A	849	VAL	CB-CA-C	-5.72	105.30	111.59
1	B	659	TYR	N-CA-C	5.50	118.45	111.69
1	A	659	TYR	N-CA-C	5.03	117.53	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	TYR	Sidechain

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	2236	0	2253	63	0
1	B	2057	0	2072	77	0
2	A	6	0	4	0	0
2	B	6	0	4	0	0
3	A	163	0	0	8	0
3	B	71	0	0	7	0
All	All	4539	0	4333	135	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 16.

All (135) 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:617:ARG:HH21	1:A:622:SER:HB3	1.17	1.04
1:B:618:ASN:HD21	1:B:620:LEU:HB2	1.35	0.90
1:A:657:ARG:HD3	3:A:95:HOH:O	1.74	0.86
1:A:953:VAL:HG12	3:A:102:HOH:O	1.79	0.81
1:B:958:ILE:O	1:B:962:ILE:HG12	1.81	0.81
1:B:652:HIS:HD2	1:B:654:TYR:H	1.28	0.79
1:B:833:HIS:HD2	1:B:835:ASP:H	1.29	0.79
1:B:790:TYR:CE2	1:B:792:GLU:HB3	2.19	0.78
1:A:617:ARG:NH2	1:A:622:SER:HB3	1.98	0.77
1:B:632:HIS:CE1	1:B:636:LYS:HD2	2.21	0.75
1:A:889:MET:HE2	1:A:936:ARG:HD3	1.68	0.75
1:A:652:HIS:HD2	1:A:654:TYR:H	1.36	0.72
1:A:645:MET:HE3	1:B:784:LEU:HD11	1.70	0.71
1:A:617:ARG:HH21	1:A:622:SER:CB	2.00	0.71
1:B:817:ARG:HH21	1:B:981:LEU:HB2	1.56	0.70
1:B:610:PHE:HB3	3:B:213:HOH:O	1.92	0.69
1:A:641:LEU:HD22	1:B:645:MET:HE3	1.75	0.69
1:A:951:MET:HB3	1:A:954:GLU:HG2	1.75	0.69
1:B:595:TYR:OH	1:B:601:GLU:HB3	1.92	0.68
1:B:903:ASN:HD21	1:B:905:LYS:HB2	1.57	0.68
1:B:618:ASN:ND2	1:B:620:LEU:HB2	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:HIS:CD2	1:A:654:TYR:H	2.14	0.66
1:A:779:LYS:HG3	1:A:780:LYS:H	1.60	0.65
1:A:859:ASN:HD21	1:A:861:HIS:CD2	2.15	0.64
1:B:618:ASN:ND2	1:B:620:LEU:H	1.95	0.64
1:A:618:ASN:HD21	1:A:620:LEU:HB2	1.63	0.64
1:B:652:HIS:CD2	1:B:654:TYR:H	2.12	0.63
1:A:952:LYS:HE2	1:A:956:LYS:NZ	2.13	0.63
1:B:889:MET:HE2	1:B:932:LEU:HB3	1.81	0.62
1:A:950:LYS:NZ	1:A:950:LYS:HB3	2.15	0.61
1:A:942:PHE:CE1	1:A:955:LYS:HG3	2.35	0.61
1:B:889:MET:HE3	1:B:936:ARG:CD	2.31	0.61
1:B:793:ASN:HB3	3:B:136:HOH:O	2.00	0.61
1:A:618:ASN:HD22	1:A:621:ASP:H	1.50	0.60
1:B:618:ASN:HD22	1:B:621:ASP:H	1.50	0.60
1:A:817:ARG:NH2	3:A:116:HOH:O	2.36	0.59
1:A:889:MET:HG2	1:A:932:LEU:CD1	2.32	0.59
1:A:951:MET:HB3	1:A:954:GLU:CG	2.33	0.57
1:B:804:ASN:O	1:B:807:GLN:HG2	2.05	0.56
1:A:845:GLU:HG2	3:A:64:HOH:O	2.04	0.56
1:B:942:PHE:CE1	1:B:955:LYS:HG3	2.41	0.56
1:B:793:ASN:HB2	3:B:87:HOH:O	2.06	0.56
1:B:889:MET:HE3	1:B:936:ARG:HD3	1.86	0.56
1:B:931:ILE:HG23	3:B:195:HOH:O	2.05	0.56
1:A:618:ASN:ND2	1:A:620:LEU:H	2.03	0.56
1:A:960:LEU:O	1:A:969:ARG:HG3	2.05	0.56
1:B:615:LYS:HE2	1:B:624:TYR:CD2	2.41	0.55
1:A:645:MET:HE3	1:B:784:LEU:CD1	2.37	0.55
1:B:833:HIS:HE1	1:B:852:GLY:O	1.91	0.54
1:A:889:MET:HG2	1:A:932:LEU:HD12	1.90	0.54
1:A:950:LYS:HB3	1:A:950:LYS:HZ3	1.73	0.54
1:A:803:GLU:O	1:A:804:ASN:CG	2.51	0.53
1:A:922:PHE:CD2	1:A:928:ARG:HA	2.43	0.53
1:A:942:PHE:CG	1:A:955:LYS:HE3	2.44	0.53
1:A:645:MET:CE	1:B:784:LEU:HD11	2.38	0.52
1:B:893:THR:HG21	1:B:964:HIS:CD2	2.44	0.52
1:B:910:SER:O	1:B:914:ILE:HG13	2.10	0.52
1:A:893:THR:HG21	1:A:964:HIS:CE1	2.45	0.52
1:B:847:ARG:HB3	1:B:847:ARG:NH1	2.24	0.51
1:B:939:SER:HB3	1:B:941:GLU:HG3	1.92	0.51
1:B:954:GLU:O	1:B:958:ILE:HG13	2.10	0.51
1:A:780:LYS:HA	3:A:200:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:ASN:HB3	1:B:621:ASP:OD2	2.10	0.51
1:B:809:ARG:HA	1:B:812:TYR:CE2	2.46	0.51
1:B:904:GLU:N	1:B:904:GLU:OE2	2.39	0.51
1:A:861:HIS:N	1:A:861:HIS:ND1	2.59	0.50
1:B:656:VAL:HG13	1:B:789:GLU:HB3	1.92	0.50
1:A:859:ASN:ND2	1:A:861:HIS:CD2	2.78	0.50
1:B:817:ARG:HH21	1:B:981:LEU:CB	2.21	0.50
1:B:611:GLY:O	1:B:612:GLN:HB3	2.12	0.50
1:B:809:ARG:HG3	1:B:809:ARG:HH11	1.76	0.50
1:B:664:GLU:HB3	1:B:769:ARG:HH12	1.77	0.50
1:B:802:SER:O	1:B:803:GLU:HG3	2.12	0.50
1:A:952:LYS:HE2	1:A:956:LYS:HZ1	1.76	0.49
1:B:824:SER:OG	1:B:973:ARG:HD2	2.12	0.49
1:B:804:ASN:HB3	1:B:807:GLN:HG2	1.94	0.49
1:A:803:GLU:O	1:A:804:ASN:C	2.54	0.49
1:B:929:VAL:O	1:B:933:LYS:HG3	2.13	0.49
1:A:634:GLU:HB3	3:A:217:HOH:O	2.13	0.49
1:A:771:PHE:CD1	1:A:780:LYS:HE2	2.47	0.49
1:A:889:MET:HE3	1:A:889:MET:HA	1.94	0.48
1:B:813:TRP:HH2	1:B:957:ILE:HD12	1.78	0.48
1:A:813:TRP:CE2	1:A:982:PRO:HG2	2.49	0.48
1:B:835:ASP:O	1:B:840:ASN:OD1	2.32	0.47
1:A:990:ILE:O	1:A:994:LEU:HG	2.13	0.47
1:A:645:MET:HE2	1:B:641:LEU:HD22	1.95	0.47
1:B:834:ARG:HD2	1:B:855:GLY:O	2.15	0.47
1:B:973:ARG:HD3	3:B:180:HOH:O	2.14	0.47
1:A:889:MET:HG2	1:A:932:LEU:HD13	1.97	0.46
1:B:946:PHE:O	1:B:948:ASP:N	2.48	0.46
1:A:607:GLN:HG3	1:A:612:GLN:HB3	1.97	0.46
1:B:889:MET:CE	1:B:936:ARG:HD3	2.45	0.46
1:B:889:MET:HE3	1:B:936:ARG:HD2	1.97	0.46
1:A:641:LEU:O	1:A:645:MET:HG2	2.15	0.46
1:B:885:ILE:HG23	1:B:885:ILE:O	2.15	0.46
1:B:638:SER:HA	1:B:641:LEU:HG	1.98	0.45
1:B:940:ILE:O	1:B:940:ILE:HG22	2.16	0.45
1:A:845:GLU:CG	3:A:64:HOH:O	2.65	0.44
1:B:922:PHE:CD2	1:B:928:ARG:HA	2.52	0.44
1:B:903:ASN:H	1:B:903:ASN:HD22	1.65	0.44
1:B:977:ASN:HB3	3:B:156:HOH:O	2.17	0.44
1:A:833:HIS:O	1:A:834:ARG:HB2	2.17	0.44
1:A:961:LEU:O	1:A:969:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:847:ARG:HB3	1:B:847:ARG:HH11	1.82	0.44
1:A:771:PHE:CE1	1:A:780:LYS:HE2	2.53	0.43
1:B:931:ILE:O	1:B:934:LYS:HB2	2.18	0.43
1:A:897:ASP:OD1	1:A:898:GLY:N	2.51	0.43
1:B:661:ALA:HA	1:B:785:PHE:O	2.19	0.43
1:B:947:ASP:HB3	1:B:950:LYS:HB3	2.00	0.43
1:A:952:LYS:HE2	1:A:956:LYS:HZ3	1.80	0.43
1:B:804:ASN:HA	3:B:134:HOH:O	2.17	0.43
1:A:889:MET:HE2	1:A:936:ARG:CD	2.45	0.42
1:A:973:ARG:NH1	3:A:190:HOH:O	2.46	0.42
1:A:653:GLN:HG3	1:A:654:TYR:CD2	2.55	0.42
1:B:903:ASN:ND2	1:B:905:LYS:HB2	2.28	0.42
1:A:922:PHE:CE2	1:A:928:ARG:HA	2.54	0.42
1:B:925:GLY:O	1:B:929:VAL:HG23	2.19	0.42
1:A:939:SER:O	1:A:940:ILE:C	2.61	0.41
1:A:940:ILE:HD11	1:A:964:HIS:HD2	1.84	0.41
1:B:809:ARG:HA	1:B:812:TYR:CZ	2.55	0.41
1:B:817:ARG:NH2	1:B:981:LEU:HB2	2.29	0.41
1:B:959:ARG:HH21	1:B:959:ARG:HG3	1.84	0.41
1:A:956:LYS:HB2	1:A:956:LYS:HE3	1.77	0.41
1:A:958:ILE:O	1:A:962:ILE:HG12	2.19	0.41
1:A:799:LEU:HD12	1:A:799:LEU:HA	1.92	0.41
1:B:981:LEU:N	1:B:981:LEU:HD12	2.36	0.41
1:B:903:ASN:ND2	1:B:903:ASN:C	2.78	0.41
1:B:965:ASP:OD1	1:B:968:LYS:N	2.53	0.41
1:B:847:ARG:HH11	1:B:847:ARG:CB	2.34	0.40
1:A:956:LYS:HD2	1:A:980:TRP:CZ3	2.55	0.40
1:B:965:ASP:OD1	1:B:965:ASP:C	2.64	0.40
1:A:985:HIS:HD2	1:A:987:ASP:H	1.70	0.40
1:B:647:LEU:HD23	1:B:831:ILE:HD13	2.04	0.40
1:B:903:ASN:HD22	1:B:903:ASN:C	2.28	0.40
1:B:611:GLY:HA3	1:B:629:LYS:O	2.21	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	265/303 (88%)	254 (96%)	9 (3%)	2 (1%)	16	8
1	B	241/303 (80%)	222 (92%)	17 (7%)	2 (1%)	16	8
All	All	506/606 (84%)	476 (94%)	26 (5%)	4 (1%)	16	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	947	ASP
1	A	899	THR
1	B	612	GLN
1	A	940	ILE

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	243/271 (90%)	238 (98%)	5 (2%)	47	41
1	B	224/271 (83%)	220 (98%)	4 (2%)	51	47
All	All	467/542 (86%)	458 (98%)	9 (2%)	50	45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	845	GLU
1	A	861	HIS
1	A	889	MET
1	A	950	LYS
1	A	954	GLU
1	B	849	VAL
1	B	903	ASN
1	B	954	GLU

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Mol	Chain	Res	Type
1	B	956	LYS

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	618	ASN
1	A	652	HIS
1	A	787	GLN
1	A	804	ASN
1	A	806	ASN
1	A	807	GLN
1	A	840	ASN
1	A	859	ASN
1	A	930	ASN
1	A	964	HIS
1	A	977	ASN
1	B	618	ASN
1	B	651	ASN
1	B	652	HIS
1	B	787	GLN
1	B	793	ASN
1	B	833	HIS
1	B	840	ASN
1	B	903	ASN
1	B	964	HIS
1	B	977	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

2 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
2	GOL	A	998	-	5,5,5	4.76	5 (100%)	5,5,5	5.96	3 (60%)
2	GOL	B	998	-	5,5,5	4.74	5 (100%)	5,5,5	6.10	3 (60%)

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	GOL	A	998	-	-	2/4/4/4	-
2	GOL	B	998	-	-	3/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	GOL	C3-C2	-8.06	1.21	1.51
2	B	998	GOL	C3-C2	-7.86	1.21	1.51
2	B	998	GOL	O1-C1	4.51	1.61	1.42
2	A	998	GOL	O1-C1	4.08	1.59	1.42
2	B	998	GOL	O3-C3	3.47	1.57	1.42
2	A	998	GOL	O2-C2	-3.41	1.33	1.43
2	A	998	GOL	C1-C2	-3.35	1.39	1.51
2	B	998	GOL	C1-C2	-3.09	1.40	1.51
2	A	998	GOL	O3-C3	3.00	1.55	1.42
2	B	998	GOL	O2-C2	-2.92	1.34	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	GOL	O3-C3-C2	11.01	159.96	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	GOL	O3-C3-C2	10.70	158.56	110.38
2	A	998	GOL	O2-C2-C3	7.33	139.53	109.18
2	B	998	GOL	O2-C2-C3	7.26	139.22	109.18
2	B	998	GOL	O1-C1-C2	3.43	125.81	110.38
2	A	998	GOL	O1-C1-C2	2.93	123.58	110.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	998	GOL	O1-C1-C2-O2
2	A	998	GOL	C1-C2-C3-O3
2	B	998	GOL	C1-C2-C3-O3
2	B	998	GOL	O1-C1-C2-C3
2	B	998	GOL	O1-C1-C2-O2

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

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	271/303 (89%)	0.56	24 (8%) 15 17	19, 37, 73, 91	0
1	B	249/303 (82%)	1.46	64 (25%) 1 1	23, 56, 87, 97	0
All	All	520/606 (85%)	0.99	88 (16%) 4 4	19, 47, 83, 97	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	885	ILE	5.1
1	B	611	GLY	4.6
1	B	886	GLY	4.5
1	B	888	ALA	4.4
1	A	899	THR	4.2
1	B	940	ILE	4.1
1	B	983	VAL	4.1
1	B	620	LEU	4.1
1	B	980	TRP	4.0
1	B	606	GLY	4.0
1	B	608	GLY	4.0
1	B	610	PHE	3.9
1	A	780	LYS	3.9
1	A	996	SER	3.8
1	B	937	SER	3.8
1	B	896	LEU	3.7
1	B	893	THR	3.7
1	B	971	GLY	3.6
1	B	953	VAL	3.6
1	B	605	LEU	3.6
1	A	898	GLY	3.5
1	B	887	THR	3.5
1	B	915	PHE	3.4
1	A	994	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	892	ALA	3.4
1	A	804	ASN	3.4
1	B	604	VAL	3.3
1	B	946	PHE	3.3
1	B	602	ILE	3.3
1	B	942	PHE	3.3
1	B	951	MET	3.2
1	A	900	GLY	3.2
1	A	990	ILE	3.2
1	B	981	LEU	3.2
1	B	840	ASN	3.2
1	A	987	ASP	3.2
1	A	624	TYR	3.1
1	A	989	VAL	3.1
1	A	861	HIS	3.1
1	B	812	TYR	3.1
1	B	902	TYR	3.1
1	B	960	LEU	3.0
1	A	897	ASP	2.9
1	A	993	ALA	2.8
1	B	916	PHE	2.8
1	B	603	ALA	2.7
1	A	995	LYS	2.7
1	B	957	ILE	2.7
1	B	974	THR	2.7
1	B	913	ILE	2.7
1	B	972	ALA	2.6
1	B	944	PRO	2.6
1	B	970	PRO	2.6
1	A	896	LEU	2.6
1	A	901	HIS	2.6
1	B	931	ILE	2.6
1	B	979	GLY	2.6
1	A	772	VAL	2.6
1	B	895	VAL	2.6
1	B	909	TYR	2.5
1	B	920	TYR	2.5
1	B	889	MET	2.5
1	B	924	THR	2.5
1	B	813	TRP	2.5
1	B	926	MET	2.4
1	B	948	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	855	GLY	2.4
1	B	943	PRO	2.3
1	A	937	SER	2.3
1	B	632	HIS	2.3
1	A	771	PHE	2.3
1	B	811	GLU	2.3
1	A	857	ALA	2.2
1	B	802	SER	2.2
1	B	793	ASN	2.2
1	A	617	ARG	2.2
1	B	975	LEU	2.2
1	B	939	SER	2.2
1	B	938	VAL	2.1
1	B	807	GLN	2.1
1	B	633	THR	2.1
1	A	779	LYS	2.1
1	B	935	LEU	2.1
1	B	609	ALA	2.1
1	B	966	PRO	2.0
1	A	888	ALA	2.0
1	B	959	ARG	2.0
1	B	891	VAL	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
2	GOL	A	998	6/6	0.86	0.13	34,42,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	998	6/6	0.88	0.13	62,67,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.