



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:29 AM UTC

PDB ID : 3L4Q / pdb_00003l4q
Title : Structural insights into phosphoinositide 3-kinase activation by the influenza A virus NS1 protein
Authors : Hale, B.G.; Kerry, P.S.; Jackson, D.; Precious, B.L.; Gray, A.; Killip, M.J.; Randall, R.E.; Russell, R.J.
Deposited on : 2009-12-21
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

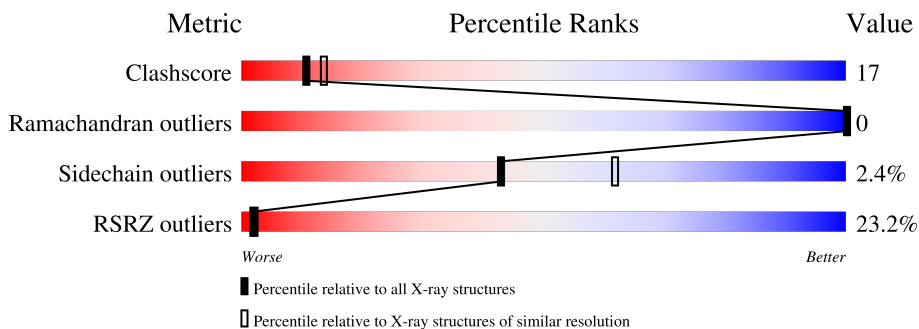
1 Overall quality at a glance

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))
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	164	
1	B	164	
2	C	170	
2	D	170	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4923 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			933	593	158	176	6			
1	B	119	Total	C	N	O	S	0	0	0
			927	590	157	174	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	HIS	-	expression tag	UNP P03496
A	68	HIS	-	expression tag	UNP P03496
A	69	HIS	-	expression tag	UNP P03496
A	70	HIS	-	expression tag	UNP P03496
A	71	HIS	-	expression tag	UNP P03496
A	72	HIS	-	expression tag	UNP P03496
B	67	HIS	-	expression tag	UNP P03496
B	68	HIS	-	expression tag	UNP P03496
B	69	HIS	-	expression tag	UNP P03496
B	70	HIS	-	expression tag	UNP P03496
B	71	HIS	-	expression tag	UNP P03496
B	72	HIS	-	expression tag	UNP P03496

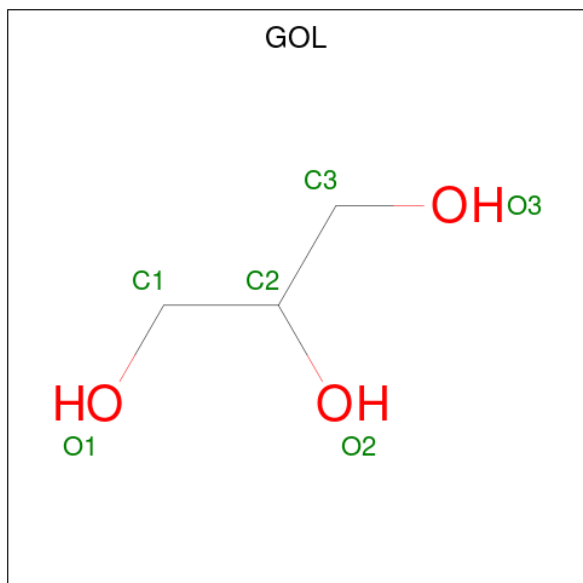
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	163	Total	C	N	O	S	0	0	0
			1385	855	256	270	4			
2	D	163	Total	C	N	O	S	0	0	0
			1385	855	256	270	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	495	SER	CYS	engineered mutation	UNP P23726
D	495	SER	CYS	engineered mutation	UNP P23726

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

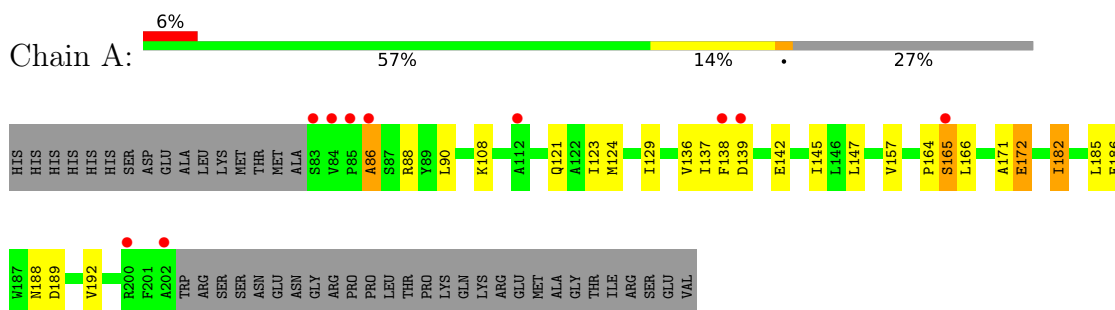
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	72	Total O 72 72	0	0
4	C	76	Total O 76 76	0	0
4	B	68	Total O 68 68	0	0
4	D	65	Total O 65 65	0	0

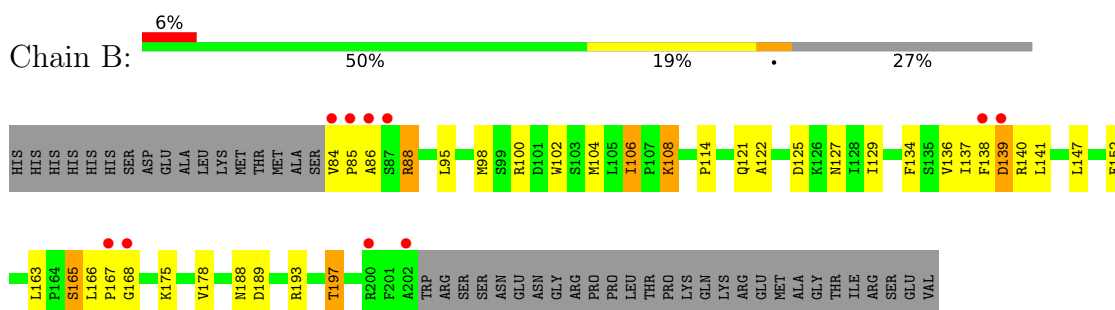
3 Residue-property plots

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.

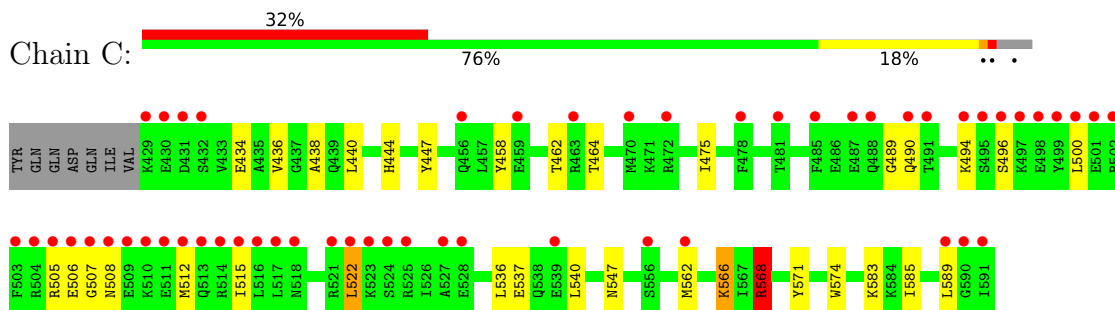
- Molecule 1: Non-structural protein 1



- Molecule 1: Non-structural protein 1

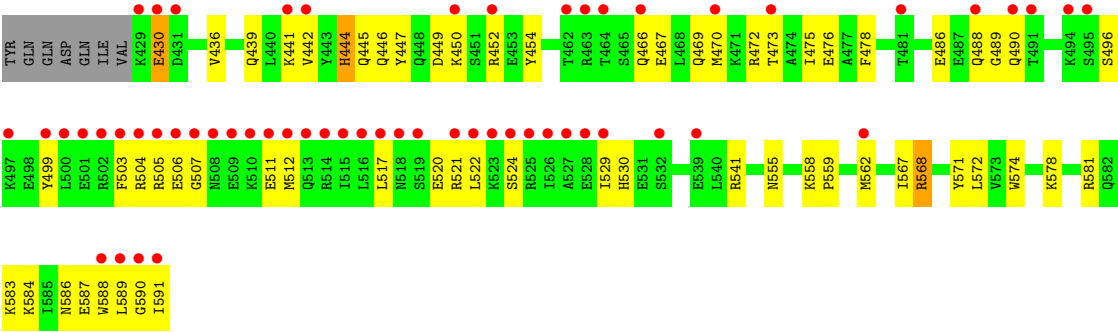


- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit beta



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.95Å 98.67Å 149.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 2.30 49.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.97-2.30) 95.2 (49.97-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.232 , 0.292 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.7	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	0.93	EDS
Total number of atoms	4923	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% 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	1.41	2/948 (0.2%)	1.28	4/1285 (0.3%)
1	B	1.44	6/942 (0.6%)	1.27	2/1277 (0.2%)
2	C	1.14	5/1401 (0.4%)	1.12	4/1868 (0.2%)
2	D	1.05	3/1401 (0.2%)	1.14	5/1868 (0.3%)
All	All	1.24	16/4692 (0.3%)	1.19	15/6298 (0.2%)

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	2
2	C	0	1
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	ILE	CA-CB	7.94	1.61	1.54
1	A	185	LEU	CA-C	7.45	1.62	1.52
2	C	568	ARG	CA-C	6.22	1.60	1.52
1	B	178	VAL	CA-C	5.92	1.60	1.52
2	C	438	ALA	CA-CB	5.68	1.62	1.53
2	C	566	LYS	C-O	5.51	1.30	1.24
2	C	434	GLU	C-O	-5.49	1.17	1.24
2	D	488	GLN	CD-OE1	5.47	1.33	1.23
1	B	100	ARG	C-O	-5.46	1.17	1.23
1	A	171	ALA	CA-CB	-5.45	1.44	1.53
2	D	568	ARG	CA-C	5.42	1.59	1.52
1	B	129	ILE	CA-CB	5.39	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	586	ASN	C-O	-5.30	1.17	1.24
2	C	444	HIS	ND1-CE1	5.27	1.37	1.32
1	B	175	LYS	C-O	-5.22	1.18	1.24
1	B	108	LYS	CA-C	5.08	1.58	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ASP	N-CA-C	-7.70	101.83	112.30
2	D	447	TYR	N-CA-C	7.23	119.24	111.36
2	D	517	LEU	N-CA-C	-6.32	105.59	113.55
2	D	444	HIS	N-CA-C	-6.31	104.33	111.14
2	C	444	HIS	CB-CG-CD2	-6.29	123.02	131.20
2	C	574	TRP	N-CA-C	-6.29	104.50	111.36
1	A	182	ILE	CA-C-N	5.71	126.17	119.94
1	A	182	ILE	C-N-CA	5.71	126.17	119.94
2	C	438	ALA	N-CA-C	-5.57	104.84	111.69
2	D	489	GLY	N-CA-C	-5.45	107.57	114.16
1	A	172	GLU	N-CA-C	5.44	117.29	111.36
1	A	192	VAL	N-CA-C	5.41	115.64	107.80
1	B	88	ARG	N-CA-C	5.40	116.49	108.60
2	D	430	GLU	N-CA-C	-5.38	106.30	112.92
2	C	444	HIS	CB-CG-ND1	5.08	130.32	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	SER	Peptide
1	A	86	ALA	Peptide
2	C	568	ARG	Sidechain

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	933	0	955	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	927	0	950	46	0
2	C	1385	0	1385	31	0
2	D	1385	0	1385	60	0
3	C	6	0	8	0	0
3	D	6	0	8	3	0
4	A	72	0	0	5	0
4	B	68	0	0	8	0
4	C	76	0	0	3	0
4	D	65	0	0	15	0
All	All	4923	0	4691	156	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 17.

All (156) 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:165:SER:HB3	1:A:166:LEU:CD2	1.68	1.22
2:C:506:GLU:CB	2:C:507:GLY:HA2	1.65	1.20
1:A:165:SER:CB	1:A:166:LEU:HD22	1.74	1.18
1:A:165:SER:HB3	1:A:166:LEU:HD22	1.20	1.15
1:B:84:VAL:HB	1:B:85:PRO:HD3	1.14	1.11
2:C:506:GLU:HB3	2:C:507:GLY:HA2	1.31	1.08
2:D:449:ASP:OD1	2:D:452:ARG:NH1	1.97	0.97
2:C:506:GLU:HB2	2:C:507:GLY:HA2	1.44	0.97
1:B:134:PHE:CZ	1:B:197:THR:CG2	2.52	0.92
1:B:84:VAL:CB	1:B:85:PRO:HD3	2.00	0.90
1:B:134:PHE:CZ	1:B:197:THR:HG22	2.08	0.88
2:C:506:GLU:HB3	2:C:507:GLY:CA	2.03	0.88
2:C:506:GLU:CB	2:C:507:GLY:CA	2.51	0.88
1:B:84:VAL:HB	1:B:85:PRO:CD	2.00	0.88
2:C:585:ILE:O	2:C:589:LEU:HD13	1.78	0.83
1:B:134:PHE:CD1	1:B:141:LEU:HD13	2.14	0.83
2:D:590:GLY:O	2:D:591:ILE:HG22	1.79	0.81
1:B:134:PHE:HZ	1:B:197:THR:CG2	1.94	0.78
1:B:163:LEU:HD12	1:B:166:LEU:CD1	2.13	0.78
2:C:489:GLY:HA2	2:C:522:LEU:HD21	1.65	0.78
1:A:165:SER:OG	1:A:166:LEU:HD22	1.85	0.77
1:A:165:SER:HB3	1:A:166:LEU:HD23	1.63	0.77
1:B:134:PHE:CE2	1:B:197:THR:HG22	2.20	0.76
2:C:571:TYR:CE2	1:B:167:PRO:HB2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PRO:HA	1:B:166:LEU:HD13	1.68	0.75
2:C:489:GLY:CA	2:C:522:LEU:HD21	2.16	0.75
2:D:469:GLN:OE1	4:D:233:HOH:O	2.05	0.73
1:B:134:PHE:CD1	1:B:141:LEU:CD1	2.72	0.73
2:D:467:GLU:HA	2:D:470:MET:HE3	1.72	0.71
2:D:590:GLY:O	2:D:591:ILE:CG2	2.39	0.70
2:C:505:ARG:O	4:C:45:HOH:O	2.10	0.69
1:A:189:ASP:OD2	4:A:265:HOH:O	2.09	0.69
2:D:524:SER:HB2	4:D:67:HOH:O	1.91	0.69
2:D:590:GLY:O	2:D:591:ILE:CB	2.40	0.69
1:B:163:LEU:HD12	1:B:166:LEU:HD12	1.73	0.69
1:B:125:ASP:HB3	4:B:251:HOH:O	1.94	0.68
2:D:441:LYS:HG3	2:D:588:TRP:O	1.92	0.68
2:D:503:PHE:CZ	2:D:512:MET:SD	2.87	0.68
1:B:163:LEU:HB2	1:B:166:LEU:HD12	1.75	0.67
2:C:475:ILE:HG13	2:C:536:LEU:HD23	1.76	0.66
1:B:134:PHE:CE2	1:B:197:THR:CG2	2.79	0.66
1:A:165:SER:CB	1:A:166:LEU:CD2	2.49	0.65
1:B:163:LEU:CD1	1:B:166:LEU:HD12	2.27	0.65
2:C:583:LYS:NZ	4:C:78:HOH:O	2.25	0.64
2:D:524:SER:CB	4:D:67:HOH:O	2.45	0.64
1:B:134:PHE:HZ	1:B:197:THR:HG22	1.57	0.63
2:D:590:GLY:O	2:D:591:ILE:HB	1.99	0.62
1:A:138:PHE:CE2	2:D:559:PRO:HB3	2.36	0.61
1:B:163:LEU:CD1	1:B:166:LEU:CD1	2.79	0.60
1:B:85:PRO:O	1:B:86:ALA:C	2.44	0.59
2:D:439:GLN:NE2	4:D:188:HOH:O	2.34	0.59
1:A:166:LEU:HD12	2:D:436:VAL:CG2	2.32	0.59
2:C:508:ASN:O	2:C:512:MET:HB3	2.02	0.59
1:B:165:SER:O	1:B:165:SER:OG	2.20	0.59
1:B:134:PHE:HZ	1:B:197:THR:HG23	1.67	0.58
1:B:95:LEU:HG	3:D:1:GOL:H2	1.86	0.58
1:A:147:LEU:C	1:A:147:LEU:HD23	2.29	0.58
2:D:496:SER:HA	2:D:499:TYR:HD2	1.67	0.58
1:B:134:PHE:CZ	1:B:197:THR:HG23	2.38	0.57
2:D:530:HIS:CE1	4:D:129:HOH:O	2.58	0.57
2:D:442:VAL:HB	4:D:188:HOH:O	2.04	0.57
2:D:444:HIS:HD2	2:D:589:LEU:O	1.88	0.56
2:D:590:GLY:C	2:D:591:ILE:HG22	2.31	0.56
1:A:124:MET:HE3	4:A:265:HOH:O	2.05	0.56
1:B:188:ASN:O	1:B:189:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:CD1	2:D:436:VAL:CG2	2.83	0.55
2:D:444:HIS:CD2	2:D:589:LEU:O	2.59	0.55
1:B:125:ASP:CB	4:B:251:HOH:O	2.52	0.55
2:D:472:ARG:O	2:D:476:GLU:HG2	2.06	0.55
2:C:440:LEU:HD21	2:C:589:LEU:CD1	2.36	0.54
2:C:458:TYR:O	2:C:462:THR:HG23	2.07	0.54
2:D:503:PHE:CE1	2:D:512:MET:SD	3.01	0.54
2:D:541:ARG:CD	4:D:160:HOH:O	2.56	0.53
2:C:489:GLY:HA3	2:C:522:LEU:HD21	1.89	0.53
1:B:166:LEU:C	1:B:167:PRO:O	2.46	0.53
2:D:530:HIS:HE1	4:D:129:HOH:O	1.89	0.53
1:A:164:PRO:O	1:A:165:SER:C	2.50	0.53
1:A:166:LEU:CD1	2:D:436:VAL:HG21	2.39	0.53
1:A:86:ALA:HA	4:A:240:HOH:O	2.08	0.52
1:A:88:ARG:HA	2:C:562:MET:CE	2.39	0.52
2:C:537:GLU:OE2	2:C:540:LEU:HD23	2.10	0.52
1:A:108:LYS:HD2	1:A:121:GLN:CD	2.35	0.52
2:C:496:SER:O	2:C:500:LEU:HG	2.11	0.51
1:B:84:VAL:CB	1:B:85:PRO:CD	2.71	0.51
1:B:108:LYS:HD3	1:B:121:GLN:CD	2.35	0.51
2:D:499:TYR:O	2:D:503:PHE:HB2	2.11	0.50
2:D:520:GLU:OE1	2:D:521:ARG:HG3	2.12	0.50
2:D:449:ASP:HA	2:D:452:ARG:NH1	2.27	0.49
1:B:134:PHE:HD1	1:B:141:LEU:CD1	2.23	0.49
4:B:270:HOH:O	3:D:1:GOL:H31	2.12	0.49
2:D:496:SER:HA	2:D:499:TYR:CD2	2.47	0.49
1:B:139:ASP:HA	4:B:250:HOH:O	2.13	0.49
1:A:166:LEU:HD12	2:D:436:VAL:HG22	1.95	0.48
2:C:436:VAL:HG13	2:C:571:TYR:CD1	2.48	0.48
1:A:137:ILE:HG12	1:A:142:GLU:HB2	1.96	0.48
2:C:440:LEU:HD21	2:C:589:LEU:HD12	1.94	0.48
2:C:505:ARG:HA	4:C:30:HOH:O	2.14	0.48
2:D:470:MET:O	2:D:473:THR:HG22	2.13	0.47
1:A:138:PHE:O	4:A:240:HOH:O	2.20	0.47
2:D:541:ARG:HD3	4:D:160:HOH:O	2.13	0.47
1:A:188:ASN:O	1:A:189:ASP:HB2	2.14	0.47
1:B:114:PRO:CA	1:B:166:LEU:HD13	2.42	0.47
1:B:147:LEU:HD23	1:B:147:LEU:C	2.40	0.47
2:D:473:THR:HA	2:D:476:GLU:CG	2.45	0.47
2:D:505:ARG:HG3	2:D:506:GLU:HG2	1.97	0.47
2:D:473:THR:HA	2:D:476:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD12	1:A:136:VAL:HG13	1.97	0.46
2:C:464:THR:OG1	2:C:547:ASN:OD1	2.32	0.46
1:B:85:PRO:HG2	1:B:88:ARG:HD3	1.98	0.46
2:D:466:GLN:HB2	4:D:261:HOH:O	2.16	0.46
1:B:137:ILE:O	1:B:138:PHE:HB2	2.14	0.46
2:D:504:ARG:HG3	4:D:81:HOH:O	2.15	0.46
2:D:568:ARG:HH22	3:D:1:GOL:H11	1.81	0.46
2:D:486:GLU:O	2:D:490:GLN:HG2	2.16	0.46
2:D:555:ASN:HA	2:D:558:LYS:HD2	1.98	0.46
2:C:490:GLN:O	2:C:494:LYS:HB2	2.15	0.45
2:D:574:TRP:CH2	2:D:578:LYS:HG3	2.51	0.45
2:C:506:GLU:HB3	2:C:508:ASN:H	1.81	0.45
2:C:571:TYR:CD2	1:B:167:PRO:HB2	2.51	0.45
1:A:88:ARG:HA	2:C:562:MET:SD	2.56	0.45
1:A:165:SER:HA	4:A:2:HOH:O	2.16	0.45
1:B:168:GLY:HA2	4:B:236:HOH:O	2.17	0.45
2:D:445:GLN:O	2:D:446:GLN:C	2.60	0.45
2:D:583:LYS:O	2:D:587:GLU:HG3	2.17	0.44
1:A:166:LEU:HD12	2:D:436:VAL:HG21	1.99	0.44
2:C:475:ILE:HG13	2:C:536:LEU:CD2	2.45	0.44
2:D:442:VAL:CB	4:D:188:HOH:O	2.65	0.44
2:D:572:LEU:C	2:D:572:LEU:HD23	2.42	0.44
2:D:439:GLN:HG2	2:D:571:TYR:CE1	2.53	0.44
2:D:581:ARG:NH2	4:D:52:HOH:O	2.50	0.44
2:D:507:GLY:O	2:D:511:GLU:HB2	2.18	0.43
1:A:182:ILE:O	1:A:186:GLU:HG3	2.19	0.43
2:D:503:PHE:HZ	2:D:512:MET:SD	2.39	0.43
2:C:447:TYR:CD1	2:C:568:ARG:NH1	2.87	0.43
1:B:193:ARG:HG2	4:B:249:HOH:O	2.19	0.43
2:D:574:TRP:CZ3	2:D:578:LYS:HG3	2.54	0.43
2:D:584:LYS:HA	2:D:584:LYS:HD2	1.84	0.42
1:B:165:SER:HB3	4:B:33:HOH:O	2.19	0.42
2:D:454:TYR:CD2	2:D:454:TYR:C	2.98	0.42
2:D:478:PHE:CD1	2:D:529:ILE:HD11	2.54	0.42
1:A:138:PHE:HZ	2:D:562:MET:HE1	1.84	0.42
2:C:489:GLY:HA2	2:C:522:LEU:CD2	2.43	0.42
1:B:137:ILE:HD12	1:B:137:ILE:HA	1.94	0.42
1:B:127:ASN:ND2	1:B:152:GLU:OE2	2.51	0.42
2:D:541:ARG:HD2	4:D:160:HOH:O	2.17	0.41
1:B:106:ILE:HD12	1:B:122:ALA:HB2	2.02	0.41
1:B:140:ARG:HB3	4:B:275:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HD11	2:C:566:LYS:HD2	2.02	0.41
2:D:503:PHE:HB3	4:D:81:HOH:O	2.21	0.41
1:B:102:TRP:CZ3	1:B:104:MET:HG3	2.56	0.41
2:D:430:GLU:O	2:D:430:GLU:CD	2.64	0.40
2:D:467:GLU:CA	2:D:470:MET:HE3	2.47	0.40
1:B:134:PHE:HB2	1:B:141:LEU:HD11	2.03	0.40
1:B:95:LEU:HD23	1:B:98:MET:HE3	2.03	0.40
1:A:108:LYS:HD2	1:A:121:GLN:NE2	2.37	0.40
1:A:123:ILE:HG13	1:A:157:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	118/164 (72%)	116 (98%)	2 (2%)	0	100	100
1	B	117/164 (71%)	114 (97%)	3 (3%)	0	100	100
2	C	161/170 (95%)	158 (98%)	3 (2%)	0	100	100
2	D	161/170 (95%)	155 (96%)	6 (4%)	0	100	100
All	All	557/668 (83%)	543 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	104/143 (73%)	101 (97%)	3 (3%)	37	55
1	B	103/143 (72%)	100 (97%)	3 (3%)	37	55
2	C	150/157 (96%)	148 (99%)	2 (1%)	61	77
2	D	150/157 (96%)	146 (97%)	4 (3%)	39	58
All	All	507/600 (84%)	495 (98%)	12 (2%)	43	62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ILE
1	A	139	ASP
1	A	172	GLU
2	C	515	ILE
2	C	522	LEU
1	B	136	VAL
1	B	165	SER
1	B	197	THR
2	D	450	LYS
2	D	475	ILE
2	D	522	LEU
2	D	567	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	444	HIS
2	C	513	GLN
1	B	121	GLN
2	D	448	GLN
2	D	508	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	$\# Z > 2$
3	GOL	C	1	-	5,5,5	0.49	0	5,5,5	0.76	0
3	GOL	D	1	-	5,5,5	0.38	0	5,5,5	0.31	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
3	GOL	C	1	-	-	4/4/4/4	-
3	GOL	D	1	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	GOL	O1-C1-C2-C3
3	C	1	GOL	C1-C2-C3-O3
3	C	1	GOL	O1-C1-C2-O2
3	C	1	GOL	O2-C2-C3-O3
3	D	1	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	GOL	3	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	120/164 (73%)	0.38	10 (8%) 17 19	17, 30, 57, 75	0
1	B	119/164 (72%)	0.28	10 (8%) 17 18	13, 28, 57, 68	0
2	C	163/170 (95%)	1.51	54 (33%) 1 1	19, 48, 137, 142	0
2	D	163/170 (95%)	1.76	57 (34%) 1 1	17, 53, 137, 141	0
All	All	565/668 (84%)	1.08	131 (23%) 2 2	13, 41, 131, 142	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	591	ILE	7.6
2	C	516	LEU	6.9
2	D	515	ILE	6.4
2	D	517	LEU	6.2
2	C	503	PHE	6.2
2	C	500	LEU	6.0
2	C	515	ILE	5.9
2	C	512	MET	5.8
2	D	500	LEU	5.7
2	C	470	MET	5.6
2	C	495	SER	5.4
2	D	495	SER	5.2
1	B	84	VAL	5.0
2	D	508	ASN	4.9
2	D	429	LYS	4.8
2	D	430	GLU	4.8
1	B	202	ALA	4.6
2	D	499	TYR	4.6
2	D	589	LEU	4.6
1	A	84	VAL	4.6
2	D	491	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	138	PHE	4.5
2	D	590	GLY	4.5
2	D	503	PHE	4.5
2	D	516	LEU	4.4
2	D	497	LYS	4.3
2	D	494	LYS	4.3
2	C	510	LYS	4.2
2	D	512	MET	4.2
2	C	591	ILE	4.2
2	C	429	LYS	4.1
2	D	509	GLU	4.1
2	C	499	TYR	4.1
2	D	490	GLN	4.0
2	D	507	GLY	3.9
1	A	86	ALA	3.9
2	C	517	LEU	3.8
2	C	459	GLU	3.8
2	D	518	ASN	3.8
2	C	506	GLU	3.8
2	C	511	GLU	3.7
2	C	513	GLN	3.7
2	D	521	ARG	3.6
1	B	85	PRO	3.6
2	C	523	LYS	3.6
2	C	514	ARG	3.6
2	D	504	ARG	3.6
2	D	532	SER	3.5
2	C	521	ARG	3.5
2	D	523	LYS	3.5
2	D	514	ARG	3.5
1	A	85	PRO	3.4
2	C	488	GLN	3.4
2	C	507	GLY	3.4
2	C	491	THR	3.4
2	C	502	ARG	3.4
2	C	498	GLU	3.3
1	B	86	ALA	3.3
1	A	165	SER	3.3
2	C	508	ASN	3.2
2	D	522	LEU	3.2
2	D	466	GLN	3.2
2	C	522	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	589	LEU	3.2
2	D	525	ARG	3.1
2	D	562	MET	3.2
1	A	83	SER	3.1
2	D	526	ILE	3.1
2	D	470	MET	3.1
2	C	497	LYS	3.1
2	D	442	VAL	3.0
2	D	505	ARG	2.9
2	C	430	GLU	2.9
2	C	494	LYS	2.9
2	D	524	SER	2.9
2	D	502	ARG	2.9
2	D	527	ALA	2.8
2	D	510	LYS	2.8
2	D	488	GLN	2.8
2	C	539	GLU	2.8
2	C	562	MET	2.8
2	D	528	GLU	2.8
1	B	168	GLY	2.7
2	C	505	ARG	2.7
2	C	431	ASP	2.7
2	C	518	ASN	2.7
2	C	504	ARG	2.7
2	D	506	GLU	2.7
2	D	513	GLN	2.6
2	C	525	ARG	2.6
2	C	496	SER	2.6
2	C	490	GLN	2.6
2	D	519	SER	2.6
2	D	441	LYS	2.6
2	D	511	GLU	2.6
2	D	588	TRP	2.6
2	D	463	ARG	2.6
1	A	138	PHE	2.6
1	A	139	ASP	2.6
2	D	529	ILE	2.5
2	C	478	PHE	2.5
1	A	200	ARG	2.5
2	C	487	GLU	2.5
1	A	202	ALA	2.4
2	C	556	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	2.4
2	C	472	ARG	2.4
2	C	501	GLU	2.4
1	B	167	PRO	2.4
2	C	590	GLY	2.4
2	C	481	THR	2.3
1	B	200	ARG	2.3
2	C	432	SER	2.3
2	D	431	ASP	2.2
2	C	528	GLU	2.2
2	D	501	GLU	2.2
2	C	509	GLU	2.2
2	C	527	ALA	2.1
2	D	452	ARG	2.1
2	D	539	GLU	2.1
2	C	485	PHE	2.1
2	D	464	THR	2.1
2	C	524	SER	2.1
1	A	112	ALA	2.1
1	B	87	SER	2.0
2	D	462	THR	2.0
2	D	473	THR	2.0
2	D	481	THR	2.0
2	C	456	GLN	2.0
2	C	463	ARG	2.0
2	D	450	LYS	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	GOL	C	1	6/6	0.59	0.24	20,20,20,20	0
3	GOL	D	1	6/6	0.86	0.17	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.