



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2026 – 02:17 PM JST

PDB ID : 21ZX / pdb_000021zx
Title : Crystal structure of Gephyrin E domain with PX-RICS peptide
Authors : Bai, G.; Zhang, M.; Yang, W.
Deposited on : 2026-01-05
Resolution : 2.20 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

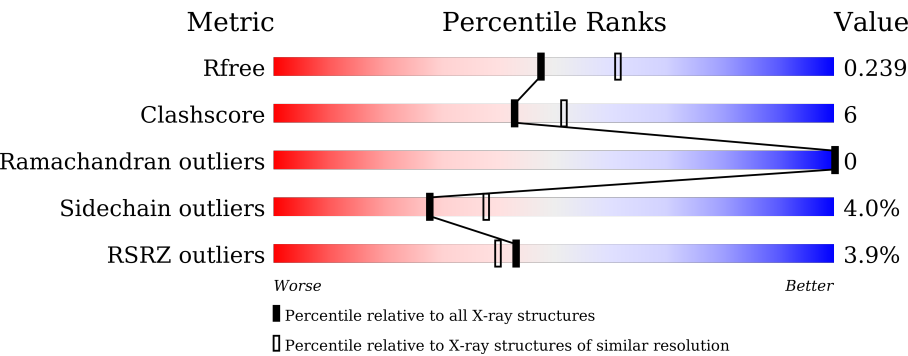
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	425	3% 81%11%7%
1	B	425	3% 78%14%8%
1	C	425	3% 78%14%6%
1	D	425	4% 78%13%7%
2	F	48	8% 21%8%71%
2	G	48	8% 19%6%75%

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
3	GOL	A	802	-	-	X	-
3	GOL	C	801	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12318 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 Isoform 5 of Gephyrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	4	0	0
			2973	1888	516	551	18			
1	B	393	Total	C	N	O	S	1	1	0
			2911	1852	496	545	18			
1	C	399	Total	C	N	O	S	3	0	0
			2972	1887	508	560	17			
1	D	396	Total	C	N	O	S	2	1	0
			2896	1830	506	541	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	GLY	-	expression tag	UNP Q03555
A	313	PRO	-	expression tag	UNP Q03555
A	314	GLY	-	expression tag	UNP Q03555
A	315	SER	-	expression tag	UNP Q03555
A	316	GLU	-	expression tag	UNP Q03555
A	317	PHE	-	expression tag	UNP Q03555
B	312	GLY	-	expression tag	UNP Q03555
B	313	PRO	-	expression tag	UNP Q03555
B	314	GLY	-	expression tag	UNP Q03555
B	315	SER	-	expression tag	UNP Q03555
B	316	GLU	-	expression tag	UNP Q03555
B	317	PHE	-	expression tag	UNP Q03555
C	312	GLY	-	expression tag	UNP Q03555
C	313	PRO	-	expression tag	UNP Q03555
C	314	GLY	-	expression tag	UNP Q03555
C	315	SER	-	expression tag	UNP Q03555
C	316	GLU	-	expression tag	UNP Q03555
C	317	PHE	-	expression tag	UNP Q03555
D	312	GLY	-	expression tag	UNP Q03555
D	313	PRO	-	expression tag	UNP Q03555
D	314	GLY	-	expression tag	UNP Q03555

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Chain	Residue	Modelled	Actual	Comment	Reference
D	315	SER	-	expression tag	UNP Q03555
D	316	GLU	-	expression tag	UNP Q03555
D	317	PHE	-	expression tag	UNP Q03555

- Molecule 2 is a protein called Rho GTPase-activating protein 32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	14	Total	C	N	O	S	1	0	0
			99	62	18	18	1			
2	G	12	Total	C	N	O	S	0	0	0
			82	52	16	13	1			

There are 12 discrepancies between the modelled and reference sequences:

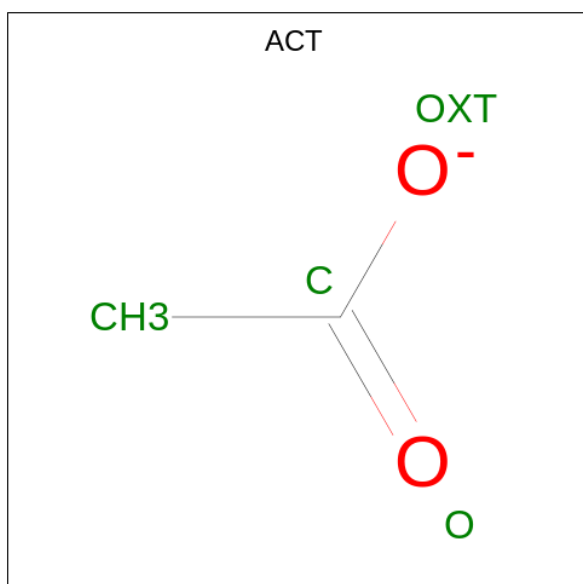
Chain	Residue	Modelled	Actual	Comment	Reference
F	35	GLY	-	expression tag	UNP A7KAX9
F	36	PRO	-	expression tag	UNP A7KAX9
F	37	GLY	-	expression tag	UNP A7KAX9
F	38	SER	-	expression tag	UNP A7KAX9
F	39	GLU	-	expression tag	UNP A7KAX9
F	40	PHE	-	expression tag	UNP A7KAX9
G	35	GLY	-	expression tag	UNP A7KAX9
G	36	PRO	-	expression tag	UNP A7KAX9
G	37	GLY	-	expression tag	UNP A7KAX9
G	38	SER	-	expression tag	UNP A7KAX9
G	39	GLU	-	expression tag	UNP A7KAX9
G	40	PHE	-	expression tag	UNP A7KAX9

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

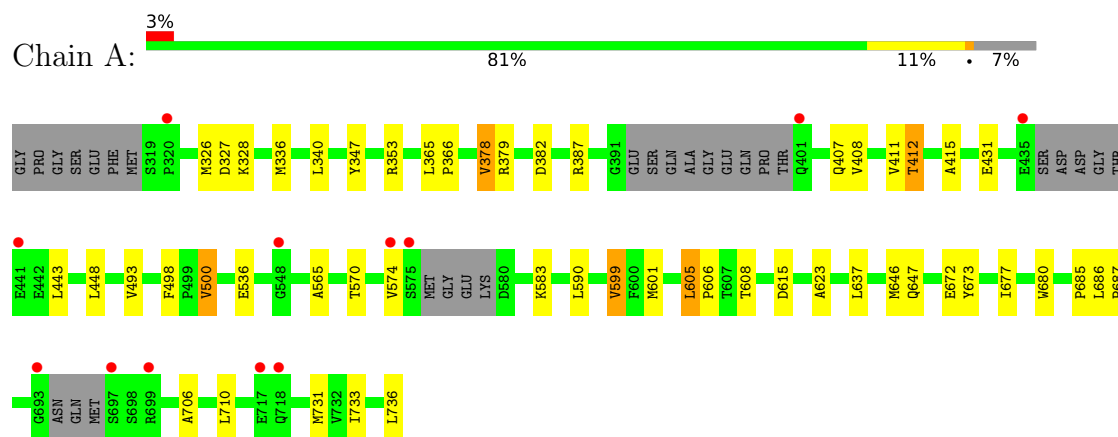
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	B	79	Total	O	0	0
			79	79		
5	C	91	Total	O	0	0
			91	91		
5	D	65	Total	O	0	0
			65	65		

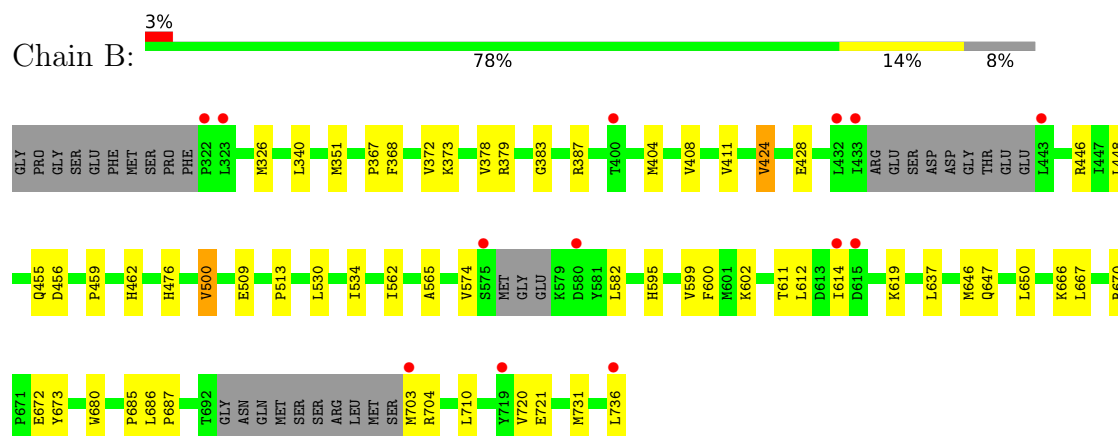
3 Residue-property plots [i](#)

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.

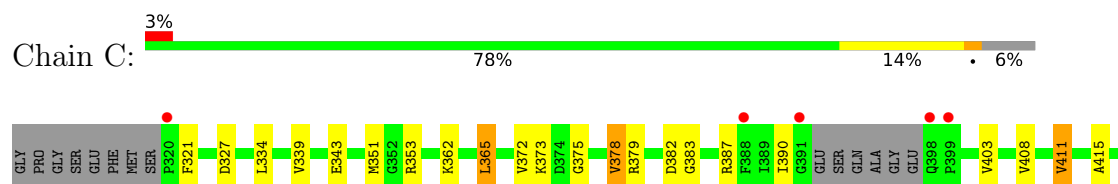
• Molecule 1: Isoform 5 of Gephyrin

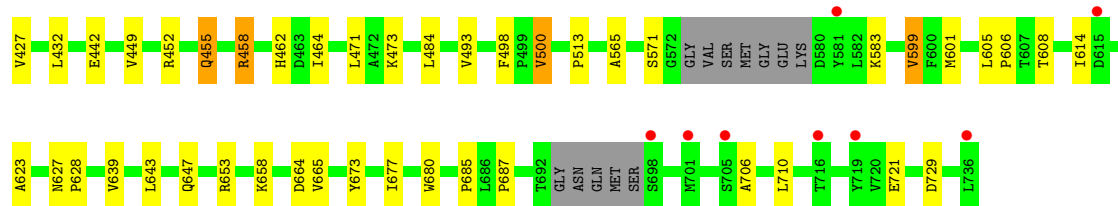


• Molecule 1: Isoform 5 of Gephyrin

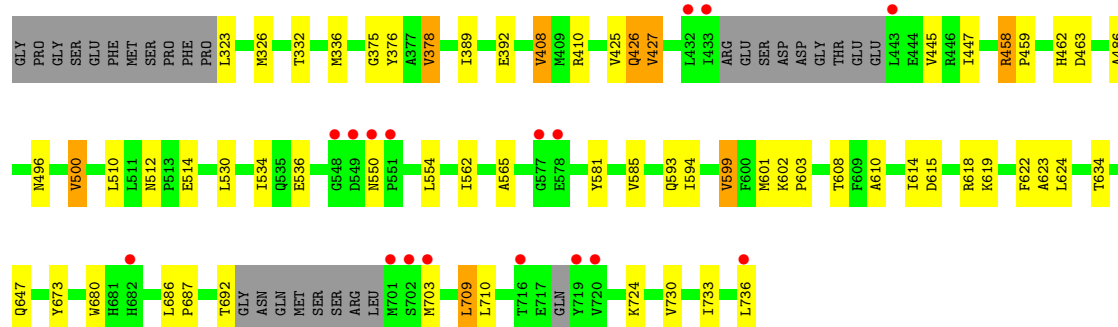
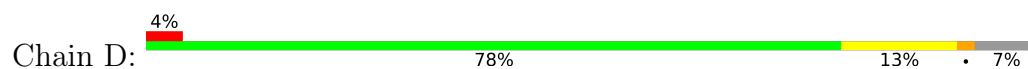


• Molecule 1: Isoform 5 of Gephyrin

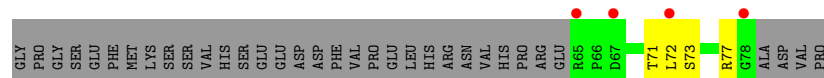




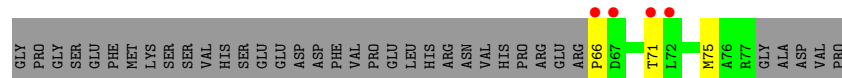
● Molecule 1: Isoform 5 of Gephyrin



● Molecule 2: Rho GTPase-activating protein 32



● Molecule 2: Rho GTPase-activating protein 32



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.51Å 163.04Å 88.05Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	48.01 – 2.20 48.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.01-2.20) 99.2 (48.01-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.190 , 0.238 0.191 , 0.239	Depositor DCC
R_{free} test set	4491 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.6	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	12318	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 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	0.35	0/3027	0.57	0/4118
1	B	0.34	0/2967	0.57	0/4046
1	C	0.34	0/3027	0.56	0/4125
1	D	0.31	0/2950	0.52	0/4025
2	F	0.39	0/101	0.52	0/137
2	G	0.31	0/84	0.44	0/114
All	All	0.34	0/12156	0.56	0/16565

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 [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	2973	0	3002	41	0
1	B	2911	0	2917	36	0
1	C	2972	0	2980	40	0
1	D	2896	0	2862	41	0
2	F	99	0	86	2	0
2	G	82	0	66	6	0
3	A	12	0	15	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	2	0
3	C	6	0	7	8	0
3	D	6	0	8	0	0
4	A	4	0	3	0	0
4	C	4	0	3	0	0
5	A	112	0	0	1	0
5	B	79	0	0	2	0
5	C	91	0	0	0	0
5	D	65	0	0	2	0
All	All	12318	0	11957	149	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 6.

All (149) 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:C:378:VAL:HG22	3:C:801:GOL:H2	1.51	0.91
1:C:382:ASP:HB2	3:C:801:GOL:H32	1.60	0.83
1:D:724:LYS:HZ1	2:G:66:PRO:HD3	1.43	0.82
1:B:650:LEU:HB2	3:B:801:GOL:H32	1.64	0.79
1:A:378:VAL:HG22	3:A:802:GOL:H2	1.66	0.77
1:D:624:LEU:HD22	1:D:634:THR:HG21	1.67	0.76
1:A:431:GLU:HG3	1:A:448:LEU:HD11	1.67	0.76
1:D:392:GLU:HG3	1:D:410:ARG:HB3	1.72	0.71
1:C:375:GLY:HA2	1:C:427:VAL:HG13	1.72	0.71
1:B:612:LEU:HD22	1:B:614:ILE:HG12	1.73	0.70
1:A:686:LEU:HD11	1:B:685:PRO:HB2	1.73	0.70
1:D:599:VAL:HG22	1:D:601:MET:HG2	1.75	0.69
1:B:637:LEU:HD23	1:B:731:MET:HE1	1.73	0.69
1:A:733:ILE:HA	3:A:801:GOL:H2	1.74	0.68
1:C:343:GLU:OE2	1:C:353:ARG:NH2	2.26	0.68
1:B:680:TRP:CH2	1:B:736:LEU:HD13	2.30	0.67
1:D:680:TRP:CH2	1:D:736:LEU:HD13	2.34	0.63
1:A:574:VAL:HG13	1:A:606:PRO:HB2	1.82	0.62
1:C:379:ARG:O	3:C:801:GOL:H31	1.99	0.61
1:D:425:VAL:HG21	1:D:447:ILE:HD12	1.83	0.61
1:C:677:ILE:HD13	1:C:706:ALA:HA	1.83	0.60
1:D:496:ASN:ND2	5:D:901:HOH:O	2.26	0.60
1:A:685:PRO:HB2	1:B:686:LEU:HD21	1.82	0.60
1:C:458:ARG:HD3	1:C:462:HIS:ND1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:GLU:OE2	5:A:901:HOH:O	2.17	0.59
1:C:382:ASP:CB	3:C:801:GOL:H32	2.33	0.58
1:C:680:TRP:CE2	1:C:687:PRO:HB3	2.38	0.58
1:A:608:THR:HB	1:A:623:ALA:HB3	1.84	0.58
1:A:327:ASP:HB3	2:G:71:THR:HG23	1.87	0.57
1:C:353:ARG:HD2	1:C:498:PHE:CE1	2.39	0.56
1:A:387:ARG:HG3	3:A:802:GOL:O2	2.06	0.56
1:D:550:ASN:O	1:D:554:LEU:HB2	2.06	0.55
1:D:594:ILE:HD13	1:D:610:ALA:HB2	1.89	0.55
1:D:709:LEU:HD13	1:D:733:ILE:HD13	1.87	0.55
1:B:500:VAL:HG22	1:B:565:ALA:HA	1.89	0.55
1:A:736:LEU:CD1	1:B:736:LEU:HD11	2.36	0.55
1:D:624:LEU:HD22	1:D:634:THR:CG2	2.35	0.55
1:D:375:GLY:HA2	1:D:427:VAL:HG22	1.89	0.55
1:B:530:LEU:O	1:B:534:ILE:HG12	2.06	0.55
1:D:530:LEU:O	1:D:534:ILE:HG12	2.07	0.54
1:D:500:VAL:HG22	1:D:565:ALA:HA	1.91	0.53
1:A:536:GLU:HB2	1:B:351:MET:HE2	1.88	0.53
1:A:382:ASP:HB2	3:A:802:GOL:H32	1.90	0.53
1:A:673:TYR:HA	1:A:710:LEU:O	2.08	0.53
1:C:608:THR:HB	1:C:623:ALA:HB3	1.91	0.53
1:C:500:VAL:HG22	1:C:565:ALA:HA	1.90	0.53
1:A:340:LEU:HD21	1:A:646:MET:HE2	1.90	0.53
1:C:353:ARG:HD2	1:C:498:PHE:CZ	2.44	0.53
1:C:383:GLY:O	3:C:801:GOL:H11	2.09	0.52
1:B:424:VAL:HG22	1:B:456:ASP:HB3	1.89	0.52
1:C:658:LYS:NZ	1:C:729:ASP:OD1	2.42	0.52
1:A:637:LEU:HD13	1:A:731:MET:HE1	1.90	0.52
2:G:71:THR:O	2:G:75:MET:HG3	2.09	0.52
1:A:407:GLN:O	3:A:802:GOL:O1	2.27	0.52
1:C:665:VAL:O	1:C:721:GLU:HG2	2.08	0.52
1:C:390:ILE:HD11	1:C:403:VAL:HG22	1.92	0.51
1:A:583:LYS:HE2	1:A:608:THR:OG1	2.11	0.51
1:D:608:THR:HB	1:D:623:ALA:HB3	1.92	0.51
1:A:412:THR:HG22	1:A:415:ALA:HB2	1.93	0.51
1:C:387:ARG:HG3	3:C:801:GOL:O2	2.11	0.51
1:A:736:LEU:HD11	1:B:736:LEU:HD11	1.93	0.50
1:D:622:PHE:HB3	1:D:624:LEU:HD21	1.92	0.50
1:B:383:GLY:O	1:B:387:ARG:NH2	2.39	0.50
1:A:365:LEU:HA	1:A:366:PRO:C	2.37	0.49
1:C:372:VAL:HG12	1:C:373:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ASP:HB2	3:C:801:GOL:C3	2.38	0.49
1:C:627:ASN:HD22	1:C:628:PRO:HD2	1.77	0.49
1:C:471:LEU:HD21	1:C:484:LEU:HD23	1.94	0.49
1:A:379:ARG:H	3:A:802:GOL:H12	1.77	0.48
1:C:664:ASP:HB3	1:C:721:GLU:OE2	2.13	0.48
1:A:680:TRP:CE2	1:A:687:PRO:HB3	2.48	0.48
1:B:372:VAL:HG12	1:B:373:LYS:HG2	1.95	0.48
1:C:351:MET:HE2	1:D:536:GLU:HB2	1.95	0.48
1:D:332:THR:O	1:D:336:MET:HG2	2.13	0.48
1:C:327:ASP:HB3	2:F:71:THR:HG23	1.96	0.48
1:B:340:LEU:HD21	1:B:646:MET:HE2	1.96	0.47
1:D:389:ILE:HD11	1:D:445:VAL:HB	1.97	0.47
1:A:340:LEU:HG	1:A:646:MET:HB3	1.97	0.47
1:A:570:THR:OG1	1:A:623:ALA:HA	2.15	0.47
1:A:605:LEU:HB3	1:A:606:PRO:HD3	1.96	0.47
1:C:452:ARG:O	1:C:455:GLN:HB3	2.13	0.47
1:B:670:ARG:HD2	5:B:971:HOH:O	2.14	0.47
1:B:562:ILE:HG23	1:B:619:LYS:HD2	1.96	0.47
1:B:574:VAL:HG13	1:B:582:LEU:HD23	1.96	0.47
1:C:432:LEU:HD11	1:C:442:GLU:HB3	1.97	0.47
1:C:599:VAL:HG22	1:C:601:MET:HG2	1.97	0.47
1:B:476:HIS:HB2	3:B:801:GOL:H12	1.96	0.47
1:D:710:LEU:HD23	1:D:730:VAL:HG22	1.96	0.46
1:C:321:PHE:CE1	1:C:583:LYS:HD3	2.50	0.46
1:A:382:ASP:HB2	3:A:802:GOL:H11	1.97	0.46
1:B:424:VAL:HG22	1:B:456:ASP:CB	2.45	0.46
1:C:685:PRO:HB2	1:D:686:LEU:HD21	1.96	0.46
1:D:336:MET:HE3	1:D:618:ARG:HH12	1.79	0.46
1:A:500:VAL:HG22	1:A:565:ALA:HA	1.97	0.46
1:A:382:ASP:OD2	3:A:802:GOL:H11	2.16	0.46
1:B:602:LYS:HD3	1:B:672:GLU:HG3	1.98	0.46
1:C:605:LEU:HB3	1:C:606:PRO:HD3	1.99	0.45
1:D:614:ILE:HG22	1:D:615:ASP:OD1	2.17	0.45
1:A:336:MET:HE1	1:C:339:VAL:HG21	1.99	0.45
1:B:326:MET:HG3	1:B:673:TYR:OH	2.16	0.45
1:D:512:ASN:HB3	1:D:514:GLU:OE1	2.17	0.44
1:C:411:VAL:HG22	1:C:415:ALA:HB3	2.00	0.44
1:A:599:VAL:HG22	1:A:601:MET:HG2	2.00	0.44
1:B:673:TYR:HA	1:B:710:LEU:O	2.17	0.44
1:B:446:ARG:HG2	1:B:448:LEU:HD23	1.98	0.44
1:D:680:TRP:CE2	1:D:687:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:TRP:CE2	1:B:687:PRO:HB3	2.52	0.44
1:B:404:MET:HE3	1:B:404:MET:HA	1.99	0.44
1:D:376:TYR:HB3	1:D:408:VAL:HG13	1.99	0.44
1:C:513:PRO:HG3	1:D:486:ALA:HB1	2.00	0.44
1:D:458:ARG:NH1	1:D:463:ASP:OD2	2.50	0.43
1:D:459:PRO:HD2	1:D:462:HIS:HB2	2.00	0.43
2:G:75:MET:HE3	2:G:75:MET:HB3	1.75	0.43
1:A:677:ILE:HD13	1:A:706:ALA:HA	2.00	0.43
1:D:724:LYS:NZ	2:G:66:PRO:HD3	2.24	0.43
1:A:680:TRP:CH2	1:A:736:LEU:HD13	2.54	0.43
1:C:673:TYR:HA	1:C:710:LEU:O	2.17	0.43
1:B:600:PHE:CZ	1:B:670:ARG:HG3	2.53	0.43
1:C:365:LEU:HB2	1:C:464:ILE:HB	2.01	0.42
1:B:602:LYS:O	1:B:672:GLU:HA	2.20	0.42
1:A:326:MET:HE1	2:G:75:MET:HE1	2.01	0.42
1:A:353:ARG:HD3	1:A:498:PHE:CE1	2.54	0.42
1:B:367:PRO:HG2	1:B:368:PHE:CD2	2.55	0.42
1:D:562:ILE:O	1:D:619:LYS:HE3	2.19	0.42
1:D:581:TYR:O	1:D:585:VAL:HG23	2.19	0.42
1:C:653:ARG:HB2	2:F:77:ARG:HA	2.02	0.41
1:D:323:LEU:HA	1:D:323:LEU:HD23	1.84	0.41
1:A:590:LEU:HD23	1:A:590:LEU:HA	1.69	0.41
1:D:326:MET:HE2	1:D:673:TYR:OH	2.20	0.41
1:B:379:ARG:HD3	5:B:920:HOH:O	2.20	0.41
1:D:392:GLU:HG3	1:D:410:ARG:CB	2.47	0.41
1:A:378:VAL:CG2	3:A:802:GOL:H2	2.44	0.41
1:A:599:VAL:O	1:A:605:LEU:HA	2.20	0.41
1:B:509:GLU:H	1:B:509:GLU:CD	2.26	0.41
1:D:602:LYS:HA	1:D:603:PRO:HA	1.88	0.41
1:A:379:ARG:N	3:A:802:GOL:H12	2.35	0.41
1:B:459:PRO:HD2	1:B:462:HIS:HB2	2.02	0.41
1:D:378:VAL:HG22	5:D:955:HOH:O	2.20	0.41
1:D:426:GLN:H	1:D:426:GLN:HG3	1.58	0.41
1:C:639:VAL:O	1:C:643:LEU:HG	2.21	0.41
1:A:328:LYS:HB2	1:D:703:MET:HE2	2.02	0.41
1:B:595:HIS:NE2	1:B:611:THR:OG1	2.31	0.41
1:B:703:MET:HB3	1:B:704:ARG:H	1.69	0.41
1:C:334:LEU:HD23	1:C:334:LEU:HA	1.93	0.41
1:A:347:TYR:OH	1:B:513:PRO:HG2	2.21	0.41
1:D:326:MET:HG3	1:D:673:TYR:OH	2.21	0.40
1:D:703:MET:H	1:D:703:MET:HG3	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:LYS:HA	1:B:721:GLU:HG2	2.04	0.40
1:C:379:ARG:O	3:C:801:GOL:O1	2.38	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	387/425 (91%)	379 (98%)	8 (2%)	0	100	100
1	B	386/425 (91%)	377 (98%)	9 (2%)	0	100	100
1	C	391/425 (92%)	386 (99%)	5 (1%)	0	100	100
1	D	389/425 (92%)	381 (98%)	8 (2%)	0	100	100
2	F	12/48 (25%)	12 (100%)	0	0	100	100
2	G	10/48 (21%)	10 (100%)	0	0	100	100
All	All	1575/1796 (88%)	1545 (98%)	30 (2%)	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	321/360 (89%)	310 (97%)	11 (3%)	32	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	310/360 (86%)	299 (96%)	11 (4%)	32	43
1	C	321/360 (89%)	306 (95%)	15 (5%)	23	31
1	D	303/360 (84%)	291 (96%)	12 (4%)	28	38
2	F	8/42 (19%)	6 (75%)	2 (25%)	0	0
2	G	5/42 (12%)	5 (100%)	0	100	100
All	All	1268/1524 (83%)	1217 (96%)	51 (4%)	28	38

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	VAL
1	A	408	VAL
1	A	411	VAL
1	A	412	THR
1	A	443	LEU
1	A	493	VAL
1	A	500	VAL
1	A	599	VAL
1	A	605	LEU
1	A	615	ASP
1	A	647	GLN
1	B	378	VAL
1	B	408	VAL
1	B	411	VAL
1	B	424	VAL
1	B	428	GLU
1	B	455	GLN
1	B	500	VAL
1	B	599	VAL
1	B	647	GLN
1	B	667	LEU
1	B	720	VAL
1	C	362	LYS
1	C	365	LEU
1	C	378	VAL
1	C	408	VAL
1	C	411	VAL
1	C	449	VAL
1	C	455	GLN
1	C	458	ARG

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Mol	Chain	Res	Type
1	C	473	LYS
1	C	493	VAL
1	C	500	VAL
1	C	571	SER
1	C	599	VAL
1	C	614	ILE
1	C	647	GLN
1	D	378	VAL
1	D	408	VAL
1	D	426	GLN
1	D	427	VAL
1	D	458	ARG
1	D	500	VAL
1	D	510	LEU
1	D	593	GLN
1	D	599	VAL
1	D	647	GLN
1	D	692	THR
1	D	709	LEU
2	F	72	LEU
2	F	73	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	462	HIS
1	A	535	GLN
1	A	591	HIS
1	C	593	GLN
1	C	627	ASN
1	C	647	GLN
1	D	401	GLN
1	D	426	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	801	-	5,5,5	1.15	0	5,5,5	0.82	0
3	GOL	A	802	-	5,5,5	1.53	1 (20%)	5,5,5	0.60	0
4	ACT	A	803	-	3,3,3	1.34	0	3,3,3	1.34	0
3	GOL	B	801	-	5,5,5	0.95	0	5,5,5	0.79	0
3	GOL	C	801	-	5,5,5	1.86	1 (20%)	5,5,5	0.53	0
3	GOL	D	801	-	5,5,5	1.21	0	5,5,5	1.11	0
4	ACT	C	802	-	3,3,3	1.30	0	3,3,3	1.40	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	A	801	-	-	4/4/4/4	-
3	GOL	A	802	-	-	2/4/4/4	-
3	GOL	B	801	-	-	4/4/4/4	-
3	GOL	C	801	-	-	2/4/4/4	-
3	GOL	D	801	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	GOL	O2-C2	-3.72	1.32	1.43
3	A	802	GOL	O2-C2	-3.07	1.34	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	GOL	O1-C1-C2-C3
3	D	801	GOL	O1-C1-C2-C3
3	A	801	GOL	C1-C2-C3-O3
3	A	802	GOL	C1-C2-C3-O3
3	B	801	GOL	O1-C1-C2-C3
3	B	801	GOL	C1-C2-C3-O3
3	C	801	GOL	O1-C1-C2-C3
3	D	801	GOL	O1-C1-C2-O2
3	A	801	GOL	O2-C2-C3-O3
3	B	801	GOL	O2-C2-C3-O3
3	D	801	GOL	O2-C2-C3-O3
3	A	802	GOL	O2-C2-C3-O3
3	C	801	GOL	O1-C1-C2-O2
3	A	801	GOL	O1-C1-C2-O2
3	B	801	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GOL	1	0
3	A	802	GOL	9	0
3	B	801	GOL	2	0
3	C	801	GOL	8	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	397/425 (93%)	0.02	12 (3%)	52	49	22, 36, 57, 78	15 (3%)
1	B	393/425 (92%)	0.08	13 (3%)	49	46	22, 38, 59, 78	10 (2%)
1	C	399/425 (93%)	0.07	13 (3%)	49	46	24, 37, 64, 94	12 (3%)
1	D	396/425 (93%)	0.34	17 (4%)	40	36	25, 43, 68, 83	12 (3%)
2	F	14/48 (29%)	1.59	4 (28%)	1	1	50, 63, 68, 69	2 (14%)
2	G	12/48 (25%)	1.74	4 (33%)	1	0	50, 67, 72, 72	0
All	All	1611/1796 (89%)	0.15	63 (3%)	43	40	22, 39, 65, 94	51 (3%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	67	ASP	4.3
1	D	577	GLY	4.1
1	D	702	SER	4.1
2	F	72	LEU	3.9
1	C	716	THR	3.9
1	C	399	PRO	3.7
1	C	719	TYR	3.5
1	D	719	TYR	3.4
2	F	67	ASP	3.4
1	C	398	GLN	3.4
1	B	615	ASP	3.4
1	A	693	GLY	3.2
1	B	443	LEU	3.2
1	C	701	MET	3.2
1	B	433	ILE	3.2
1	A	575	SER	3.2
1	D	433	ILE	3.2
1	D	443	LEU	3.2
1	B	322	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	720	VAL	3.1
1	A	441	GLU	3.0
1	C	736	LEU	3.0
1	B	703	MET	2.9
1	B	432	LEU	2.8
2	F	65	ARG	2.8
2	G	71	THR	2.8
1	B	323	LEU	2.8
1	D	550	ASN	2.7
2	G	66	PRO	2.7
1	D	703	MET	2.6
1	A	574	VAL	2.6
1	B	614	ILE	2.6
1	C	705	SER	2.5
1	C	320	PRO	2.5
1	C	391	GLY	2.4
1	D	551	PRO	2.4
1	A	548	GLY	2.4
2	F	78	GLY	2.4
1	B	575	SER	2.4
1	D	432	LEU	2.4
1	B	719	TYR	2.3
1	C	615	ASP	2.3
1	D	716	THR	2.3
1	D	701	MET	2.3
1	A	435	GLU	2.3
1	C	698	SER	2.3
1	D	736	LEU	2.3
1	A	320	PRO	2.3
1	C	581	TYR	2.3
1	D	682	HIS	2.2
1	C	388	PHE	2.1
1	D	578	GLU	2.1
1	A	697	SER	2.1
1	D	548	GLY	2.1
1	A	699	ARG	2.1
1	A	718	GLN	2.1
1	B	736	LEU	2.0
1	A	717	GLU	2.0
1	B	400	THR	2.0
1	A	401	GLN	2.0
1	B	580	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	549	ASP	2.0
2	G	72	LEU	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
3	GOL	D	801	6/6	0.79	0.18	41,54,57,58	0
4	ACT	C	802	4/4	0.83	0.15	42,49,51,55	0
3	GOL	A	802	6/6	0.88	0.15	30,37,38,40	6
3	GOL	A	801	6/6	0.89	0.14	27,31,33,35	6
3	GOL	C	801	6/6	0.89	0.16	29,40,42,43	6
4	ACT	A	803	4/4	0.90	0.09	36,43,45,48	0
3	GOL	B	801	6/6	0.93	0.15	34,36,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.