



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:27 PM UTC

PDB ID : 6ROL / pdb_00006rol
Title : Structure of IMP2 KH34 domains
Authors : Bhaskar, V.; Biswas, J.; Singer, R.H.; Chao, J.A.
Deposited on : 2019-05-13
Resolution : 2.10 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

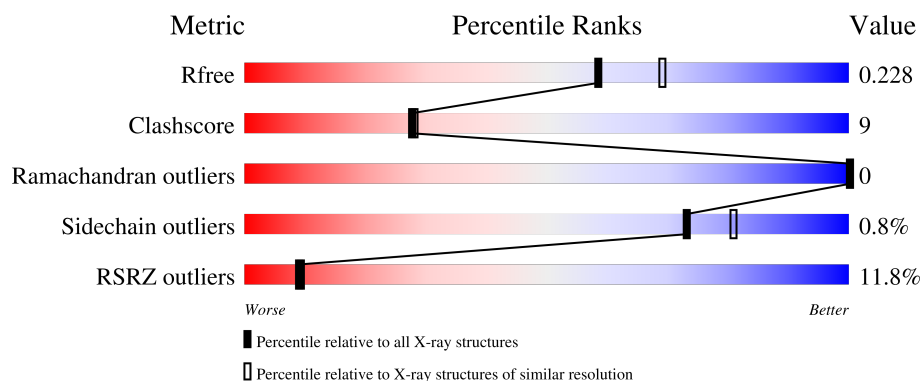
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	166	6% 80% 16% ..
1	B	166	17% 84% 13% .
1	C	166	5% 87% 10% .
1	D	166	18% 84% 12% .

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	606	-	-	X	-
3	PEG	B	603	-	-	X	-
3	PEG	D	606	-	-	X	-
4	SO4	C	613	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10679 atoms, of which 5239 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 Insulin-like growth factor 2 mRNA-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	162	Total	C	H	N	O	S	0	5	0
			2588	807	1315	231	234	1			
1	B	161	Total	C	H	N	O	S	0	0	0
			2415	764	1212	219	219	1			
1	C	161	Total	C	H	N	O	S	0	2	0
			2507	786	1268	223	229	1			
1	D	159	Total	C	H	N	O	S	0	0	0
			2392	757	1200	214	220	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	GLY	-	expression tag	UNP Q9Y6M1
A	424	GLY	-	expression tag	UNP Q9Y6M1
A	425	SER	-	expression tag	UNP Q9Y6M1
B	423	GLY	-	expression tag	UNP Q9Y6M1
B	424	GLY	-	expression tag	UNP Q9Y6M1
B	425	SER	-	expression tag	UNP Q9Y6M1
C	423	GLY	-	expression tag	UNP Q9Y6M1
C	424	GLY	-	expression tag	UNP Q9Y6M1
C	425	SER	-	expression tag	UNP Q9Y6M1
D	423	GLY	-	expression tag	UNP Q9Y6M1
D	424	GLY	-	expression tag	UNP Q9Y6M1
D	425	SER	-	expression tag	UNP Q9Y6M1

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



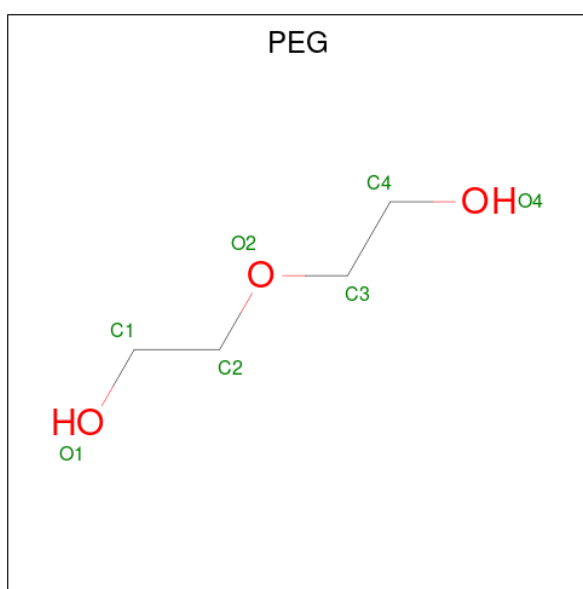
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	116	Total	O	0	0
			116	116		
5	B	44	Total	O	0	0
			44	44		

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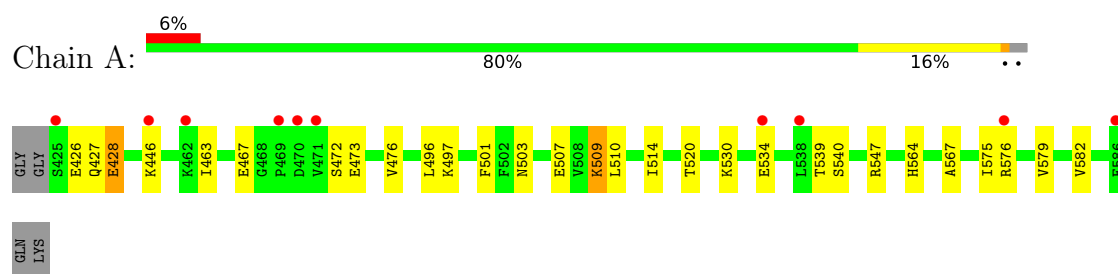
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	129	Total 129	O 129	0	0
5	D	46	Total 46	O 46	0	0

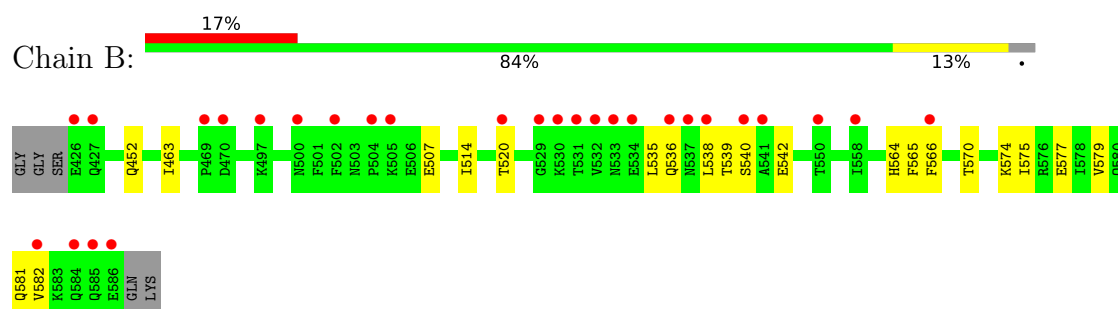
3 Residue-property plots

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.

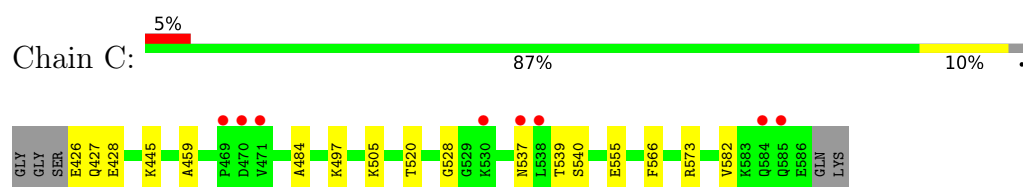
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 2



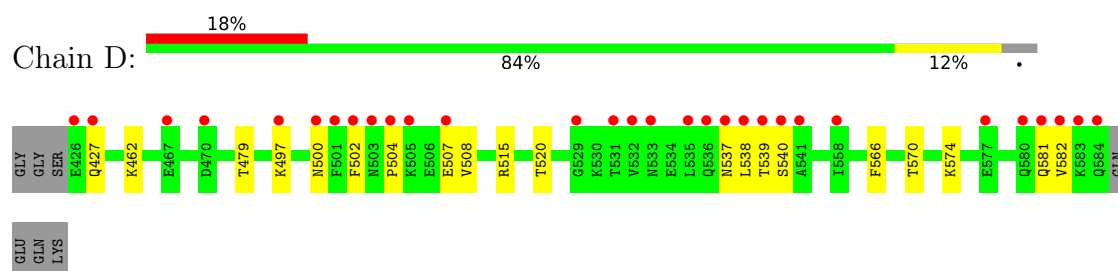
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 2



- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 2



- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.88Å 62.38Å 85.74Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	37.80 – 2.10 37.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (37.80-2.10) 97.0 (37.80-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.198 , 0.224 0.205 , 0.228	Depositor DCC
R_{free} test set	2529 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10679	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4602e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, PEG, SO4

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	0.15	0/1308	0.34	0/1763
1	B	0.15	0/1222	0.35	0/1652
1	C	0.14	0/1264	0.32	0/1705
1	D	0.18	0/1211	0.40	0/1639
All	All	0.15	0/5005	0.35	0/6759

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	1273	1315	1314	23	1
1	B	1203	1212	1211	24	0
1	C	1239	1268	1268	13	1
1	D	1192	1200	1200	26	0
2	A	36	48	48	10	0
2	B	12	16	16	0	0
2	C	42	56	56	2	0
2	D	18	24	24	1	0
3	A	7	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	10	10	11	0
3	C	35	50	50	1	0
3	D	21	30	30	6	0
4	A	10	0	0	0	0
4	C	10	0	0	3	0
5	A	116	0	0	3	1
5	B	44	0	0	3	0
5	C	129	0	0	6	1
5	D	46	0	0	7	0
All	All	5440	5239	5237	93	2

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 9.

All (93) 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)
3:D:605:PEG:O4	5:D:701:HOH:O	1.83	0.96
1:D:538:LEU:HD22	1:D:574:LYS:HE3	1.56	0.88
1:D:566:PHE:N	5:D:701:HOH:O	2.07	0.87
1:A:428:GLU:OE2	1:A:576[B]:ARG:NH1	2.10	0.84
4:C:613:SO4:O2	5:C:701:HOH:O	1.97	0.82
1:A:547:ARG:NH2	5:A:701:HOH:O	2.14	0.80
1:B:538:LEU:HD22	1:B:574:LYS:HE3	1.65	0.79
1:C:573:ARG:NH1	2:D:602:GOL:O2	2.16	0.78
4:C:614:SO4:O4	5:C:702:HOH:O	2.00	0.78
3:D:606:PEG:O1	5:D:702:HOH:O	2.02	0.77
1:D:497:LYS:HA	1:D:502:PHE:CZ	2.22	0.75
1:B:577:GLU:OE2	5:B:701:HOH:O	2.03	0.74
1:C:445:LYS:NZ	5:C:705:HOH:O	2.23	0.69
1:C:537[A]:ASN:ND2	5:C:706:HOH:O	2.24	0.69
1:B:452:GLN:OE1	5:B:702:HOH:O	2.11	0.68
1:B:520:THR:HG21	1:B:579:VAL:HA	1.76	0.67
1:D:581:GLN:NE2	5:D:704:HOH:O	2.27	0.67
3:B:603:PEG:O1	5:B:703:HOH:O	2.12	0.66
1:B:570:THR:HG22	1:B:574:LYS:HE2	1.78	0.66
1:B:520:THR:HG23	1:B:582:VAL:HG21	1.78	0.65
2:C:605:GOL:O3	5:C:703:HOH:O	2.14	0.65
1:D:427:GLN:OE1	1:D:479:THR:HG22	1.97	0.65
2:A:606:GOL:H2	5:A:703:HOH:O	1.97	0.64
1:D:497:LYS:HG2	1:D:502:PHE:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:PHE:CE1	1:D:508:VAL:HG23	2.34	0.62
1:A:501:PHE:O	2:A:601:GOL:O2	2.12	0.61
1:C:520:THR:HG22	1:C:582:VAL:HG11	1.85	0.59
1:A:539:THR:O	1:A:540:SER:OG	2.17	0.58
1:A:427:GLN:NE2	5:A:704:HOH:O	2.27	0.58
1:A:426:GLU:HG3	1:A:427:GLN:H	1.70	0.56
1:D:497:LYS:HG2	1:D:502:PHE:HE1	1.70	0.55
1:D:515:ARG:HE	3:D:606:PEG:H21	1.71	0.55
1:D:538:LEU:HD23	1:D:538:LEU:O	2.06	0.55
1:D:515:ARG:HH21	3:D:606:PEG:H31	1.73	0.54
1:B:566:PHE:HB2	3:B:603:PEG:H11	1.89	0.53
1:A:463:ILE:CD1	1:A:476:VAL:HG22	2.39	0.53
1:A:427:GLN:OE1	1:D:504:PRO:HA	2.08	0.52
1:D:520:THR:HG22	1:D:582:VAL:HG11	1.91	0.52
1:D:462:LYS:NZ	5:D:709:HOH:O	2.42	0.52
1:A:463:ILE:HD12	1:A:476:VAL:HG22	1.92	0.52
1:C:497:LYS:HZ1	2:C:601:GOL:C1	2.23	0.51
2:A:606:GOL:H12	3:B:603:PEG:C4	2.41	0.51
1:D:500:ASN:HA	1:D:502:PHE:CE2	2.46	0.51
1:B:565:PHE:H	3:B:603:PEG:H31	1.76	0.50
1:C:566:PHE:HD2	1:D:497:LYS:HZ2	1.58	0.50
1:D:539:THR:HG22	1:D:570:THR:HG22	1.93	0.50
1:A:472:SER:OG	1:A:473[A]:GLU:OE2	2.25	0.49
1:B:538:LEU:O	1:B:538:LEU:HD23	2.13	0.48
1:A:520[B]:THR:HG22	1:A:582:VAL:HG11	1.96	0.48
1:A:564[B]:HIS:CE1	1:A:567:ALA:HB2	2.48	0.48
1:D:538:LEU:HD23	1:D:538:LEU:C	2.38	0.48
3:D:605:PEG:O4	5:D:703:HOH:O	2.09	0.48
1:B:538:LEU:HD23	1:B:538:LEU:C	2.39	0.48
2:A:606:GOL:H11	1:B:566:PHE:CD2	2.49	0.47
1:C:428:GLU:OE1	5:C:704:HOH:O	2.19	0.47
1:D:497:LYS:HG2	1:D:502:PHE:CZ	2.49	0.47
1:A:497:LYS:HD3	3:B:603:PEG:H12	1.97	0.47
2:A:606:GOL:H12	3:B:603:PEG:O2	2.14	0.47
1:B:570:THR:CG2	1:B:574:LYS:HE2	2.45	0.47
1:D:497:LYS:HE2	1:D:507:GLU:HG3	1.96	0.47
1:B:514:ILE:HD11	1:B:575:ILE:HG21	1.96	0.47
1:A:520[A]:THR:HG21	1:A:579:VAL:HA	1.97	0.46
1:A:509:LYS:O	2:A:601:GOL:H2	2.15	0.46
1:B:507:GLU:OE2	3:B:603:PEG:H42	2.16	0.46
1:D:537:ASN:ND2	5:D:708:HOH:O	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:GLU:HG2	1:C:427:GLN:H	1.82	0.44
1:C:566:PHE:HD2	1:D:497:LYS:NZ	2.15	0.44
1:A:514:ILE:HD11	1:A:575:ILE:HG21	2.00	0.44
1:B:564:HIS:CB	3:B:603:PEG:H22	2.48	0.44
1:B:564:HIS:CB	3:B:603:PEG:C2	2.96	0.44
1:C:505:LYS:NZ	4:C:613:SO4:O4	2.48	0.44
1:B:539:THR:O	1:B:540:SER:OG	2.32	0.43
1:B:564:HIS:HB2	3:B:603:PEG:C2	2.48	0.43
1:A:496:LEU:HD12	1:A:510:LEU:HD11	2.00	0.43
1:B:566:PHE:HB2	3:B:603:PEG:C1	2.49	0.43
1:A:507:GLU:HG2	2:A:606:GOL:H32	2.00	0.43
1:A:473[B]:GLU:OE1	2:A:604:GOL:O3	2.26	0.43
1:A:507:GLU:OE2	2:A:606:GOL:O2	2.37	0.42
1:D:502:PHE:HE1	1:D:508:VAL:HG23	1.83	0.42
1:A:530:LYS:O	1:A:534:GLU:HG2	2.19	0.42
1:B:577:GLU:O	1:B:581:GLN:HG2	2.19	0.42
1:D:515:ARG:NE	3:D:606:PEG:H21	2.34	0.42
2:A:606:GOL:H11	1:B:566:PHE:CE2	2.55	0.42
1:A:426:GLU:CG	1:A:427:GLN:H	2.33	0.42
1:B:536:GLN:OE1	1:B:542:GLU:HG3	2.21	0.41
1:C:459:ALA:HB2	1:C:484:ALA:HB1	2.01	0.41
1:D:570:THR:CG2	1:D:574:LYS:HE2	2.50	0.41
1:B:535:LEU:HD23	1:B:574:LYS:HD3	2.03	0.41
1:C:539:THR:O	1:C:540:SER:HB3	2.21	0.41
1:D:539:THR:O	1:D:540:SER:HB3	2.21	0.41
1:A:446:LYS:HA	1:A:446:LYS:HE2	2.03	0.40
1:B:570:THR:O	1:B:574:LYS:HG3	2.21	0.40
1:C:555:GLU:HB3	3:C:608:PEG:H11	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:714:HOH:O	5:C:746:HOH:O[2_645]	2.02	0.18
1:A:503:ASN:OD1	1:C:528:GLY:H[2_645]	1.53	0.07

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	165/166 (99%)	163 (99%)	2 (1%)	0	100	100
1	B	159/166 (96%)	155 (98%)	4 (2%)	0	100	100
1	C	161/166 (97%)	161 (100%)	0	0	100	100
1	D	157/166 (95%)	154 (98%)	3 (2%)	0	100	100
All	All	642/664 (97%)	633 (99%)	9 (1%)	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	135/136 (99%)	132 (98%)	3 (2%)	45	53
1	B	120/136 (88%)	119 (99%)	1 (1%)	73	81
1	C	129/136 (95%)	129 (100%)	0	100	100
1	D	121/136 (89%)	121 (100%)	0	100	100
All	All	505/544 (93%)	501 (99%)	4 (1%)	73	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	428	GLU
1	A	467	GLU

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Mol	Chain	Res	Type
1	A	509	LYS
1	B	463	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
1	A	489	GLN
1	A	572	GLN
1	B	485	GLN
1	B	489	GLN
1	B	569	GLN
1	B	572	GLN
1	C	485	GLN
1	C	489	GLN
1	C	572	GLN

5.3.3 RNA [i](#)

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](#)

32 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	604	-	5,5,5	0.83	0	5,5,5	1.08	0
4	SO4	C	614	-	4,4,4	0.24	0	6,6,6	0.08	0
2	GOL	B	601	-	5,5,5	0.85	0	5,5,5	1.05	0
2	GOL	C	605	-	5,5,5	0.79	0	5,5,5	0.96	0
4	SO4	C	613	-	4,4,4	0.24	0	6,6,6	0.11	0
2	GOL	A	602	-	5,5,5	0.81	0	5,5,5	0.85	0
4	SO4	A	609	-	4,4,4	0.23	0	6,6,6	0.07	0
3	PEG	C	611	-	6,6,6	0.51	0	5,5,5	0.34	0
2	GOL	A	603	-	5,5,5	0.86	0	5,5,5	1.00	0
2	GOL	D	601	-	5,5,5	0.88	0	5,5,5	1.12	0
3	PEG	B	603	-	6,6,6	0.53	0	5,5,5	0.60	0
3	PEG	D	606	-	6,6,6	0.51	0	5,5,5	0.39	0
3	PEG	D	605	-	6,6,6	0.50	0	5,5,5	0.38	0
2	GOL	C	606	-	5,5,5	0.81	0	5,5,5	0.90	0
3	PEG	A	607	-	6,6,6	0.52	0	5,5,5	0.39	0
2	GOL	C	603	-	5,5,5	0.84	0	5,5,5	1.05	0
3	PEG	C	608	-	6,6,6	0.53	0	5,5,5	0.29	0
2	GOL	C	607	-	5,5,5	0.76	0	5,5,5	0.90	0
3	PEG	C	612	-	6,6,6	0.51	0	5,5,5	0.36	0
2	GOL	D	602	-	5,5,5	0.85	0	5,5,5	0.99	0
2	GOL	B	602	-	5,5,5	0.80	0	5,5,5	0.90	0
2	GOL	A	601	-	5,5,5	0.93	0	5,5,5	0.92	0
3	PEG	D	604	-	6,6,6	0.50	0	5,5,5	0.28	0
4	SO4	A	608	-	4,4,4	0.25	0	6,6,6	0.06	0
2	GOL	A	606	-	5,5,5	0.93	0	5,5,5	1.30	1 (20%)
2	GOL	C	602	-	5,5,5	0.84	0	5,5,5	1.04	0
2	GOL	D	603	-	5,5,5	0.82	0	5,5,5	0.99	0
2	GOL	C	604	-	5,5,5	0.77	0	5,5,5	0.99	0
2	GOL	A	605	-	5,5,5	0.85	0	5,5,5	1.04	0
3	PEG	C	610	-	6,6,6	0.50	0	5,5,5	0.31	0
3	PEG	C	609	-	6,6,6	0.50	0	5,5,5	0.28	0
2	GOL	C	601	-	5,5,5	0.86	0	5,5,5	1.21	1 (20%)

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	604	-	-	2/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-
2	GOL	C	605	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	602	-	-	2/4/4/4	-
3	PEG	C	611	-	-	0/4/4/4	-
2	GOL	A	603	-	-	2/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
3	PEG	B	603	-	-	2/4/4/4	-
3	PEG	D	606	-	-	0/4/4/4	-
3	PEG	D	605	-	-	1/4/4/4	-
2	GOL	C	606	-	-	4/4/4/4	-
3	PEG	A	607	-	-	3/4/4/4	-
2	GOL	C	603	-	-	0/4/4/4	-
3	PEG	C	608	-	-	1/4/4/4	-
2	GOL	C	607	-	-	2/4/4/4	-
3	PEG	C	612	-	-	3/4/4/4	-
2	GOL	D	602	-	-	2/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
3	PEG	D	604	-	-	2/4/4/4	-
2	GOL	A	606	-	-	2/4/4/4	-
2	GOL	C	602	-	-	2/4/4/4	-
2	GOL	D	603	-	-	2/4/4/4	-
2	GOL	C	604	-	-	0/4/4/4	-
2	GOL	A	605	-	-	2/4/4/4	-
3	PEG	C	610	-	-	3/4/4/4	-
3	PEG	C	609	-	-	2/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	606	GOL	C3-C2-C1	-2.41	102.95	111.80
2	C	601	GOL	C3-C2-C1	-2.14	103.95	111.80

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	GOL	O1-C1-C2-C3
2	A	605	GOL	C1-C2-C3-O3
2	C	601	GOL	C1-C2-C3-O3
2	C	602	GOL	O1-C1-C2-C3
2	C	606	GOL	O1-C1-C2-O2
2	C	606	GOL	O1-C1-C2-C3
2	C	607	GOL	C1-C2-C3-O3
2	C	607	GOL	O2-C2-C3-O3
2	A	602	GOL	O2-C2-C3-O3
3	C	608	PEG	O1-C1-C2-O2
3	C	609	PEG	O2-C3-C4-O4
2	A	601	GOL	O1-C1-C2-C3
2	A	602	GOL	C1-C2-C3-O3
2	A	604	GOL	C1-C2-C3-O3
2	A	606	GOL	C1-C2-C3-O3
2	C	605	GOL	O1-C1-C2-C3
2	D	601	GOL	O1-C1-C2-C3
2	D	602	GOL	O1-C1-C2-C3
2	D	603	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	A	603	GOL	O1-C1-C2-O2
2	A	604	GOL	O2-C2-C3-O3
2	A	605	GOL	O2-C2-C3-O3
2	A	606	GOL	O2-C2-C3-O3
2	C	601	GOL	O2-C2-C3-O3
2	C	602	GOL	O1-C1-C2-O2
3	A	607	PEG	O1-C1-C2-O2
3	B	603	PEG	O1-C1-C2-O2
3	B	603	PEG	O2-C3-C4-O4
3	C	612	PEG	O2-C3-C4-O4
3	A	607	PEG	O2-C3-C4-O4
2	D	601	GOL	O1-C1-C2-O2
3	C	609	PEG	C1-C2-O2-C3
2	C	606	GOL	C1-C2-C3-O3
3	C	610	PEG	C1-C2-O2-C3
3	C	610	PEG	O2-C3-C4-O4
3	D	604	PEG	C4-C3-O2-C2
3	A	607	PEG	C4-C3-O2-C2
3	C	610	PEG	O1-C1-C2-O2
2	D	603	GOL	O1-C1-C2-O2
3	D	604	PEG	O1-C1-C2-O2
3	C	612	PEG	C1-C2-O2-C3
2	C	606	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	D	602	GOL	O1-C1-C2-O2
3	C	612	PEG	C4-C3-O2-C2
3	D	605	PEG	O2-C3-C4-O4

There are no ring outliers.

12 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	GOL	1	0
4	C	614	SO4	1	0
2	C	605	GOL	1	0
4	C	613	SO4	2	0
3	B	603	PEG	11	0
3	D	606	PEG	4	0
3	D	605	PEG	2	0
3	C	608	PEG	1	0
2	D	602	GOL	1	0
2	A	601	GOL	2	0
2	A	606	GOL	7	0
2	C	601	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	162/166 (97%)	0.32	10 (6%) 26 28	18, 38, 100, 139	5 (3%)
1	B	161/166 (96%)	1.12	28 (17%) 4 4	28, 60, 118, 145	0
1	C	161/166 (96%)	0.19	8 (4%) 34 36	24, 37, 93, 122	2 (1%)
1	D	159/166 (95%)	1.08	30 (18%) 3 3	31, 59, 125, 170	0
All	All	643/664 (96%)	0.68	76 (11%) 9 9	18, 46, 111, 170	7 (1%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	532	VAL	9.1
1	D	502	PHE	6.1
1	B	537	ASN	5.6
1	D	532	VAL	4.7
1	D	503	ASN	4.6
1	D	504	PRO	4.6
1	A	471	VAL	4.0
1	C	585	GLN	4.0
1	B	582	VAL	3.9
1	A	425	SER	3.9
1	B	497	LYS	3.7
1	B	426	GLU	3.6
1	D	538	LEU	3.5
1	B	585	GLN	3.5
1	D	584	GLN	3.5
1	D	501	PHE	3.4
1	B	533	ASN	3.4
1	D	537	ASN	3.4
1	C	538	LEU	3.4
1	C	530	LYS	3.3
1	D	427	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	469	PRO	3.3
1	D	582	VAL	3.3
1	D	535	LEU	3.2
1	B	584	GLN	3.2
1	C	470	ASP	3.2
1	B	427	GLN	3.2
1	D	558	ILE	3.2
1	A	469	PRO	3.2
1	B	538	LEU	3.1
1	B	534	GLU	3.1
1	D	505	LYS	3.1
1	A	534	GLU	3.0
1	D	536	GLN	3.0
1	A	538	LEU	3.0
1	D	467	GLU	3.0
1	D	529	GLY	2.9
1	D	470	ASP	2.9
1	D	426	GLU	2.9
1	B	558	ILE	2.8
1	B	529	GLY	2.8
1	B	531	THR	2.8
1	A	470	ASP	2.7
1	B	530	LYS	2.7
1	D	497	LYS	2.7
1	D	583	LYS	2.7
1	C	537[A]	ASN	2.7
1	B	540	SER	2.6
1	B	586	GLU	2.5
1	D	500	ASN	2.5
1	D	540	SER	2.5
1	A	576[A]	ARG	2.5
1	A	586	GLU	2.4
1	B	502	PHE	2.4
1	D	580	GLN	2.4
1	B	504	PRO	2.4
1	B	550	THR	2.4
1	D	541	ALA	2.4
1	B	566	PHE	2.4
1	D	539	THR	2.4
1	B	536	GLN	2.3
1	B	470	ASP	2.3
1	C	471	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	520	THR	2.3
1	D	531	THR	2.3
1	D	581	GLN	2.2
1	B	500	ASN	2.2
1	B	541	ALA	2.2
1	B	469	PRO	2.1
1	D	507	GLU	2.1
1	B	505	LYS	2.1
1	D	533	ASN	2.1
1	A	446	LYS	2.1
1	D	577	GLU	2.1
1	A	462	LYS	2.0
1	C	584	GLN	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	C	602	6/6	0.71	0.13	86,106,120,128	0
3	PEG	C	610	7/7	0.71	0.27	93,114,130,130	0
2	GOL	C	605	6/6	0.72	0.26	64,81,111,134	0
2	GOL	A	602	6/6	0.72	0.20	47,73,89,107	14
3	PEG	B	603	7/7	0.73	0.26	71,85,109,122	0
3	PEG	D	606	7/7	0.74	0.20	75,91,111,115	0
2	GOL	D	602	6/6	0.76	0.21	77,92,106,107	14
3	PEG	C	609	7/7	0.77	0.20	79,95,102,107	0
2	GOL	B	601	6/6	0.77	0.17	60,80,90,96	0
2	GOL	C	601	6/6	0.77	0.21	55,76,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	D	605	7/7	0.79	0.27	55,75,97,114	0
2	GOL	C	606	6/6	0.80	0.23	53,81,98,112	0
4	SO4	A	608	5/5	0.80	0.14	66,82,85,94	5
3	PEG	C	612	7/7	0.81	0.20	85,102,108,112	0
2	GOL	D	601	6/6	0.81	0.18	56,78,92,94	0
4	SO4	C	614	5/5	0.81	0.21	90,93,94,95	5
3	PEG	C	611	7/7	0.83	0.27	36,70,104,104	17
4	SO4	A	609	5/5	0.83	0.19	81,82,97,99	5
2	GOL	D	603	6/6	0.83	0.16	77,97,118,126	0
2	GOL	B	602	6/6	0.84	0.18	59,86,100,104	0
2	GOL	A	603	6/6	0.84	0.17	51,71,86,86	14
3	PEG	D	604	7/7	0.84	0.21	65,78,101,106	17
3	PEG	A	607	7/7	0.84	0.16	47,88,123,123	0
2	GOL	A	605	6/6	0.86	0.23	68,82,95,97	0
2	GOL	A	606	6/6	0.86	0.31	49,77,133,153	14
2	GOL	C	607	6/6	0.86	0.11	69,83,90,99	0
2	GOL	A	604	6/6	0.88	0.14	69,83,95,101	0
2	GOL	A	601	6/6	0.89	0.13	33,45,54,54	14
4	SO4	C	613	5/5	0.89	0.23	47,47,57,64	5
2	GOL	C	603	6/6	0.89	0.17	78,96,104,115	0
3	PEG	C	608	7/7	0.90	0.18	25,53,102,102	17
2	GOL	C	604	6/6	0.90	0.15	60,72,80,84	0

6.5 Other polymers

There are no such residues in this entry.