



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:38 AM EDT

PDB ID : 1RLO / pdb_00001rlo
Title : Phospho-aspartyl Intermediate Analogue of ybiV from E. coli K12
Authors : Roberts, A.; Lee, S.Y.; McCullagh, E.; Silversmith, R.E.; Wemmer, D.E.
Deposited on : 2003-11-26
Resolution : 2.00 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	:	9.0.015 (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

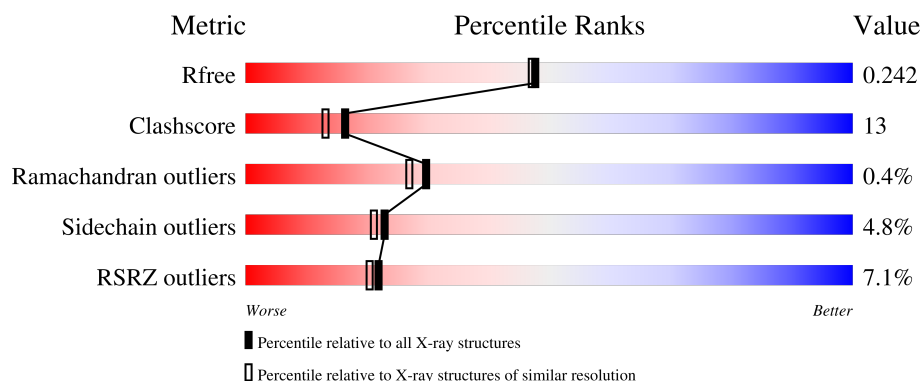
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

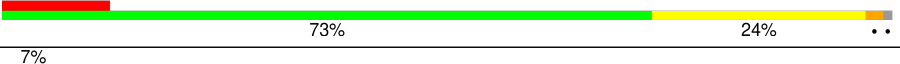
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	271	
1	B	271	
1	C	271	
1	D	271	

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
4	GOL	C	805	-	X	-	-
4	GOL	D	806	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9003 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 Phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2129	1366	361	394	8			
1	B	268	Total	C	N	O	S	0	0	0
			2129	1366	361	394	8			
1	C	268	Total	C	N	O	S	0	0	0
			2129	1366	361	394	8			
1	D	268	Total	C	N	O	S	0	0	0
			2129	1366	361	394	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P75792
A	267	TYR	SER	engineered mutation	UNP P75792
B	2	ALA	SER	engineered mutation	UNP P75792
B	267	TYR	SER	engineered mutation	UNP P75792
C	2	ALA	SER	engineered mutation	UNP P75792
C	267	TYR	SER	engineered mutation	UNP P75792
D	2	ALA	SER	engineered mutation	UNP P75792
D	267	TYR	SER	engineered mutation	UNP P75792

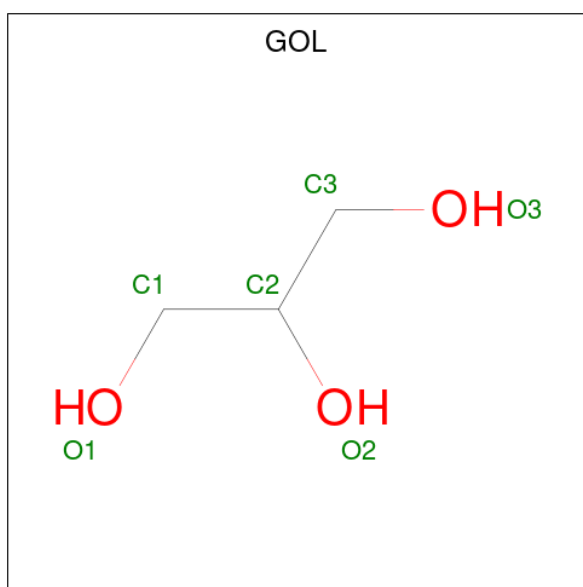
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (CCD ID: HOH) (formula: H_2O).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Be	F	0	0
			4	1	3		
3	B	1	Total	Be	F	0	0
			4	1	3		
3	C	1	Total	Be	F	0	0
			4	1	3		
3	D	1	Total	Be	F	0	0
			4	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	138	Total	O	0	0
			138	138		
5	B	101	Total	O	0	0
			101	101		
5	C	113	Total	O	0	0
			113	113		

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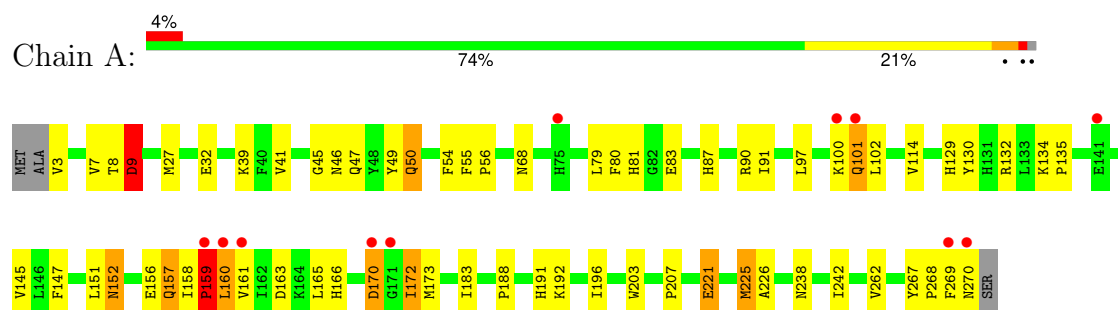
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	103	Total 103	O 103	0	0

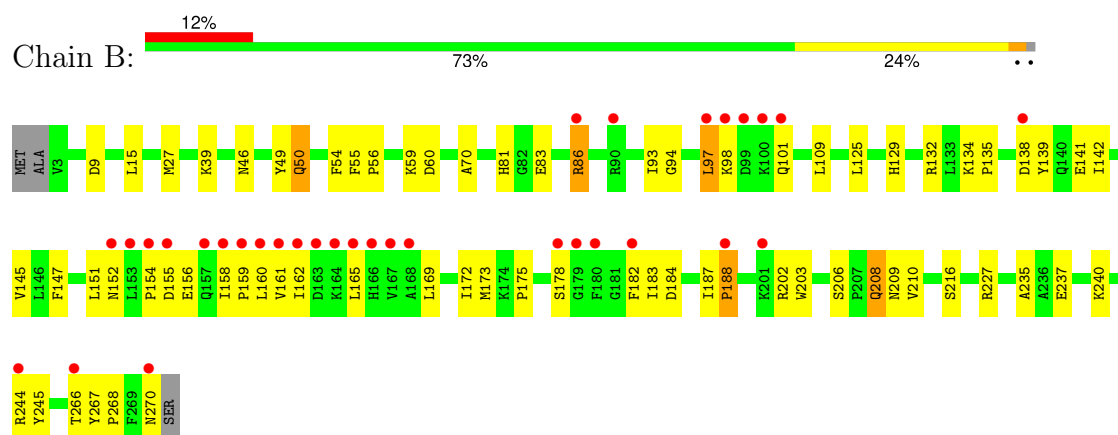
3 Residue-property plots [i](#)

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.

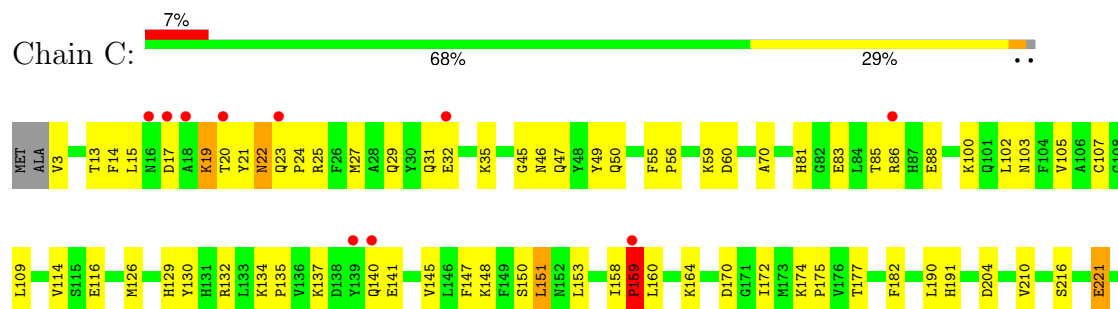
• Molecule 1: Phosphatase

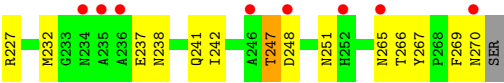


• Molecule 1: Phosphatase

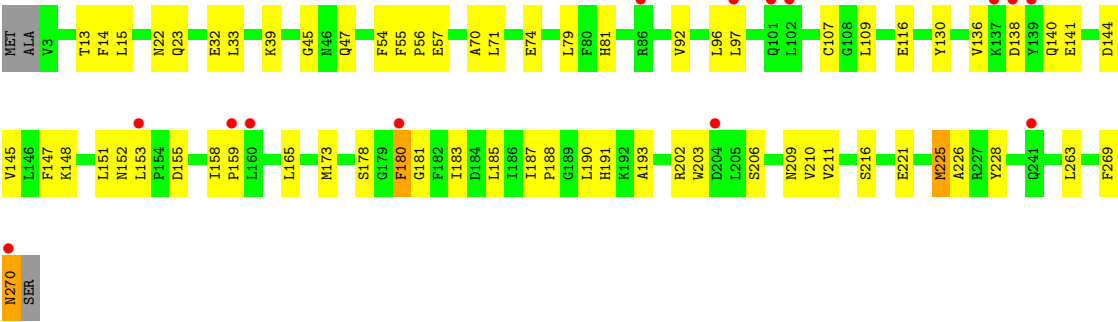
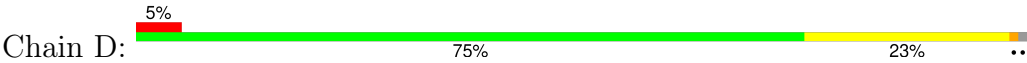


• Molecule 1: Phosphatase





● Molecule 1: Phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.28Å 91.19Å 176.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 2.00 19.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.85-2.00) 98.6 (19.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.29 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.251 0.212 , 0.242	Depositor DCC
R_{free} test set	7906 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.7	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	0.93	EDS
Total number of atoms	9003	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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, MG, BEF

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	0.71	5/2174 (0.2%)	1.08	14/2939 (0.5%)
1	B	0.39	0/2174	0.93	5/2939 (0.2%)
1	C	0.38	0/2174	0.91	4/2939 (0.1%)
1	D	0.37	0/2174	0.87	3/2939 (0.1%)
All	All	0.48	5/8696 (0.1%)	0.95	26/11756 (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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ASP	CA-CB	16.17	1.79	1.53
1	A	9	ASP	CA-C	11.77	1.66	1.52
1	A	9	ASP	N-CA	-11.04	1.32	1.45
1	A	9	ASP	C-O	9.85	1.36	1.23
1	A	8	THR	C-N	8.74	1.45	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASP	CB-CA-C	-13.67	85.10	109.71
1	B	188	PRO	CA-N-CD	-13.11	93.65	112.00
1	A	159	PRO	CA-N-CD	-12.82	94.05	112.00
1	A	9	ASP	CA-C-O	-12.57	106.35	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	PRO	CA-N-CD	-11.78	95.51	112.00
1	A	157	GLN	OE1-CD-NE2	-10.55	112.05	122.60
1	A	8	THR	CA-C-N	-9.18	106.76	122.92
1	A	8	THR	C-N-CA	-9.18	106.76	122.92
1	A	9	ASP	N-CA-CB	-9.17	96.73	110.85
1	C	141	GLU	N-CA-C	-7.39	103.99	113.16
1	A	157	GLN	CG-CD-NE2	7.16	127.14	116.40
1	D	210	VAL	N-CA-C	6.84	118.45	108.53
1	B	210	VAL	N-CA-C	6.75	118.31	108.53
1	A	183	ILE	N-CA-C	6.69	117.92	108.36
1	B	187	ILE	N-CA-C	-6.54	103.00	108.63
1	B	216	SER	N-CA-C	6.19	116.45	108.34
1	C	216	SER	N-CA-C	6.15	117.91	109.18
1	B	9	ASP	N-CA-C	-5.90	102.92	110.53
1	C	210	VAL	N-CA-C	5.80	116.94	108.53
1	A	267	TYR	CA-C-N	5.61	140.46	127.00
1	A	267	TYR	C-N-CA	5.61	140.46	127.00
1	A	9	ASP	O-C-N	-5.59	115.89	123.10
1	A	172	ILE	N-CA-C	-5.42	105.09	110.62
1	D	216	SER	N-CA-C	5.42	116.87	109.18
1	A	170	ASP	N-CA-C	5.38	118.81	111.39
1	D	45	GLY	N-CA-C	-5.30	108.38	115.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	9	ASP	Mainchain

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	2129	0	2119	72	0
1	B	2129	0	2119	51	0
1	C	2129	0	2119	67	0
1	D	2129	0	2119	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	C	6	0	4	2	0
4	D	6	0	4	1	0
5	A	138	0	0	3	0
5	B	101	0	0	3	0
5	C	113	0	0	3	0
5	D	103	0	0	2	0
All	All	9003	0	8484	222	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 13.

All (222) 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:9:ASP:CB	1:A:9:ASP:CA	1.79	1.56
1:A:9:ASP:CB	1:A:9:ASP:C	2.34	0.99
1:A:9:ASP:CB	1:A:9:ASP:N	2.35	0.88
1:D:269:PHE:O	1:D:270:ASN:HB2	1.72	0.86
1:A:81:HIS:H	1:C:86:ARG:HH21	1.22	0.84
1:A:160:LEU:C	1:A:160:LEU:HD23	2.05	0.82
1:C:191:HIS:CG	1:C:221:GLU:HG3	2.16	0.81
1:A:191:HIS:CG	1:A:221:GLU:HG3	2.17	0.80
1:B:83:GLU:HG3	1:B:145:VAL:HG13	1.66	0.78
1:C:13:THR:HG22	1:C:14:PHE:N	1.99	0.77
1:A:207:PRO:HB3	1:A:225:MET:HE3	1.67	0.74
1:C:140:GLN:HA	1:C:140:GLN:NE2	2.04	0.73
1:B:50:GLN:HG2	1:B:129:HIS:O	1.90	0.71
1:B:206:SER:H	1:B:209:ASN:HD22	1.36	0.71
1:A:262:VAL:HG22	1:A:269:PHE:CZ	2.26	0.70
1:B:169:LEU:O	1:B:172:ILE:HG12	1.92	0.70
1:C:160:LEU:O	1:C:164:LYS:HG3	1.91	0.69
1:B:160:LEU:HD13	1:B:160:LEU:O	1.92	0.69
1:C:132:ARG:HD2	1:D:23:GLN:OE1	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:GLU:O	1:C:241:GLN:HG3	1.91	0.69
1:A:207:PRO:CB	1:A:225:MET:HE3	2.23	0.68
1:C:83:GLU:HG3	1:C:145:VAL:HG13	1.75	0.67
1:A:166:HIS:O	1:A:170:ASP:HA	1.94	0.67
1:B:154:PRO:HB2	1:B:156:GLU:HG2	1.78	0.66
1:D:180:PHE:HB3	5:D:907:HOH:O	1.95	0.66
1:B:152:ASN:HD22	1:B:182:PHE:HE1	1.44	0.66
1:A:9:ASP:C	1:A:9:ASP:CG	2.64	0.66
1:A:160:LEU:HG	1:A:160:LEU:O	1.96	0.65
1:B:158:ILE:HA	1:B:161:VAL:HG12	1.79	0.64
1:B:266:THR:OG1	5:B:903:HOH:O	2.15	0.64
1:B:93:ILE:HD13	1:B:139:TYR:HB3	1.79	0.64
1:C:269:PHE:O	1:C:270:ASN:HB2	1.97	0.64
1:A:80:PHE:CD1	1:C:86:ARG:NH2	2.67	0.63
1:A:102:LEU:HD12	1:A:152:ASN:ND2	2.13	0.62
1:C:25:ARG:O	1:C:29:GLN:HG3	1.99	0.62
1:C:105:VAL:HG22	1:C:126:MET:HE3	1.81	0.62
1:C:150:SER:C	1:C:151:LEU:HD12	2.24	0.62
1:A:81:HIS:H	1:C:86:ARG:NH2	1.95	0.62
1:A:100:LYS:HE2	1:A:100:LYS:HA	1.82	0.60
1:C:49:TYR:CG	1:C:132:ARG:HD3	2.36	0.60
1:A:158:ILE:HB	1:A:159:PRO:HD2	1.83	0.60
1:C:172:ILE:N	1:C:172:ILE:HD12	2.17	0.60
1:A:81:HIS:CE1	1:C:86:ARG:HG3	2.37	0.60
1:B:55:PHE:N	1:B:56:PRO:HD3	2.18	0.59
1:D:13:THR:HG22	1:D:14:PHE:N	2.17	0.59
1:A:101:GLN:NE2	1:A:101:GLN:N	2.50	0.58
1:A:269:PHE:O	1:A:270:ASN:HB2	2.02	0.58
1:C:238:ASN:O	1:C:242:ILE:HG12	2.03	0.58
1:D:225:MET:HE2	1:D:226:ALA:N	2.18	0.58
1:C:221:GLU:CD	1:C:221:GLU:H	2.11	0.58
1:B:178:SER:HA	1:B:184:ASP:OD2	2.05	0.57
1:B:206:SER:H	1:B:209:ASN:ND2	2.03	0.57
1:C:227:ARG:HG3	1:C:227:ARG:HH11	1.70	0.57
1:D:158:ILE:HG23	1:D:183:ILE:HD11	1.87	0.57
1:C:45:GLY:HA3	4:C:805:GOL:O3	2.04	0.56
1:D:74:GLU:OE2	1:D:202:ARG:HD3	2.05	0.56
1:C:158:ILE:HB	1:C:159:PRO:HD2	1.88	0.56
1:A:161:VAL:HG12	1:A:165:LEU:CD1	2.36	0.56
1:C:140:GLN:HA	1:C:140:GLN:HE21	1.70	0.56
1:D:79:LEU:HD21	1:D:202:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:O	1:A:161:VAL:N	2.36	0.55
1:A:101:GLN:H	1:A:101:GLN:HE21	1.54	0.54
1:A:221:GLU:CD	1:A:221:GLU:H	2.16	0.54
1:D:79:LEU:HD11	1:D:202:ARG:HD2	1.88	0.54
1:D:22:ASN:C	1:D:22:ASN:HD22	2.15	0.54
1:A:160:LEU:O	1:A:160:LEU:CG	2.55	0.54
1:A:80:PHE:HA	1:C:86:ARG:NH2	2.22	0.54
1:B:138:ASP:OD2	1:B:141:GLU:HG3	2.07	0.54
1:C:46:ASN:OD1	1:C:129:HIS:HD2	1.90	0.54
1:B:208:GLN:NE2	1:B:227:ARG:HG2	2.22	0.53
1:A:160:LEU:HD23	1:A:161:VAL:N	2.24	0.53
1:B:161:VAL:HG22	1:B:165:LEU:HG	1.91	0.53
1:C:31:GLN:HA	1:C:31:GLN:NE2	2.22	0.53
1:D:70:ALA:O	1:D:81:HIS:HA	2.09	0.53
1:A:269:PHE:O	1:A:270:ASN:CB	2.56	0.53
1:D:54:PHE:C	1:D:56:PRO:HD3	2.33	0.53
1:B:151:LEU:O	1:B:182:PHE:HD1	1.92	0.53
1:B:59:LYS:HE3	5:B:880:HOH:O	2.09	0.52
1:A:161:VAL:HG12	1:A:165:LEU:HD12	1.90	0.52
1:D:158:ILE:HB	1:D:159:PRO:HD3	1.92	0.52
1:A:46:ASN:OD1	1:A:129:HIS:HD2	1.93	0.52
1:B:227:ARG:HD2	1:B:244:ARG:NH1	2.25	0.52
1:A:83:GLU:HG2	1:A:145:VAL:HB	1.92	0.52
1:C:19:LYS:N	1:C:19:LYS:HD2	2.24	0.51
1:C:102:LEU:HD11	1:C:151:LEU:HD23	1.92	0.51
1:D:138:ASP:OD2	1:D:140:GLN:HB2	2.11	0.51
1:D:158:ILE:HD11	1:D:181:GLY:HA2	1.91	0.51
1:A:45:GLY:HA2	1:A:68:ASN:N	2.25	0.51
1:A:101:GLN:N	1:A:101:GLN:HE21	2.07	0.51
1:A:87:HIS:O	1:A:91:ILE:HG13	2.11	0.51
1:B:54:PHE:C	1:B:56:PRO:HD3	2.35	0.51
1:C:177:THR:HG22	5:C:878:HOH:O	2.09	0.51
1:A:9:ASP:CA	1:A:9:ASP:CG	2.77	0.51
1:C:105:VAL:CG2	1:C:126:MET:HE3	2.40	0.51
1:B:59:LYS:HE2	1:B:60:ASP:OD1	2.10	0.50
1:C:153:LEU:HD23	1:C:153:LEU:N	2.26	0.50
1:D:187:ILE:HB	1:D:190:LEU:HD12	1.93	0.50
1:B:94:GLY:O	1:B:98:LYS:HG3	2.12	0.50
1:A:81:HIS:HE1	1:C:86:ARG:HG3	1.77	0.50
1:B:39:LYS:HD3	1:B:203:TRP:CE2	2.47	0.50
1:A:49:TYR:CG	1:A:132:ARG:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LEU:HD12	1:C:151:LEU:N	2.26	0.49
1:A:46:ASN:OD1	1:A:129:HIS:CD2	2.65	0.49
1:A:163:ASP:HB2	5:A:893:HOH:O	2.11	0.49
1:D:55:PHE:N	1:D:56:PRO:HD3	2.28	0.49
1:A:192:LYS:O	1:A:196:ILE:HG13	2.11	0.49
1:C:102:LEU:HD21	1:C:151:LEU:HG	1.94	0.49
1:A:45:GLY:HA2	1:A:68:ASN:H	1.78	0.49
1:A:79:LEU:C	1:A:79:LEU:HD23	2.38	0.49
1:C:107:CYS:SG	1:C:148:LYS:HE2	2.53	0.49
1:B:125:LEU:HD21	1:B:182:PHE:CE2	2.48	0.49
1:C:85:THR:OG1	1:C:88:GLU:HG3	2.12	0.48
1:D:191:HIS:CE1	1:D:193:ALA:HB3	2.47	0.48
1:A:191:HIS:ND1	1:A:221:GLU:HG3	2.27	0.48
1:D:152:ASN:HA	1:D:181:GLY:O	2.13	0.48
1:C:22:ASN:OD1	1:C:24:PRO:HD2	2.12	0.48
1:A:79:LEU:HD23	1:A:79:LEU:O	2.13	0.48
1:A:268:PRO:HD2	1:A:269:PHE:CD1	2.49	0.48
1:B:227:ARG:HD2	1:B:244:ARG:HH12	1.78	0.48
1:A:7:VAL:HG22	1:A:41:VAL:HB	1.95	0.48
1:C:49:TYR:CD1	1:C:132:ARG:HD3	2.48	0.48
1:C:221:GLU:HG2	5:C:823:HOH:O	2.13	0.48
1:D:107:CYS:SG	1:D:148:LYS:HE2	2.54	0.48
1:A:225:MET:HE2	1:A:226:ALA:HA	1.95	0.48
1:B:139:TYR:O	1:B:142:ILE:HG13	2.13	0.48
1:A:207:PRO:HA	1:A:225:MET:HE3	1.95	0.48
1:A:87:HIS:CD2	1:A:90:ARG:HH21	2.32	0.48
1:C:269:PHE:C	1:C:270:ASN:HD22	2.22	0.47
1:C:55:PHE:N	1:C:56:PRO:HD3	2.29	0.47
1:B:93:ILE:HG22	1:B:97:LEU:HD22	1.95	0.47
1:B:208:GLN:HE21	1:B:208:GLN:CA	2.27	0.47
1:A:49:TYR:CD1	1:A:132:ARG:HD3	2.49	0.47
1:C:32:GLU:OE1	1:C:35:LYS:HD2	2.14	0.47
1:D:144:ASP:OD2	1:D:145:VAL:N	2.48	0.47
1:A:158:ILE:HG22	1:A:159:PRO:CD	2.45	0.47
1:B:46:ASN:HB3	1:B:50:GLN:CG	2.44	0.47
1:B:158:ILE:N	1:B:159:PRO:CD	2.77	0.47
1:C:20:THR:HG22	1:C:21:TYR:N	2.29	0.47
1:C:116:GLU:OE1	1:C:137:LYS:HG2	2.14	0.47
1:B:267:TYR:CD1	1:B:268:PRO:HA	2.50	0.47
1:D:225:MET:HE2	1:D:226:ALA:CA	2.44	0.47
1:A:3:VAL:N	5:A:815:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PRO:CA	1:A:225:MET:HE3	2.44	0.47
1:A:238:ASN:O	1:A:242:ILE:HG13	2.16	0.46
1:B:158:ILE:O	1:B:162:ILE:HG13	2.15	0.46
1:C:23:GLN:N	1:C:24:PRO:CD	2.79	0.46
1:D:211:VAL:HG22	1:D:228:TYR:HB2	1.97	0.46
1:B:158:ILE:HA	1:B:161:VAL:CG1	2.46	0.46
1:C:182:PHE:HB3	4:C:805:GOL:O2	2.16	0.46
1:A:54:PHE:C	1:A:56:PRO:HD3	2.41	0.46
1:D:39:LYS:HD3	1:D:203:TRP:CE3	2.50	0.46
1:A:221:GLU:HG2	5:A:807:HOH:O	2.15	0.46
1:C:170:ASP:O	1:C:172:ILE:HD12	2.16	0.46
1:D:116:GLU:HA	5:D:906:HOH:O	2.16	0.45
1:C:102:LEU:HD21	1:C:151:LEU:CG	2.46	0.45
1:A:55:PHE:N	1:A:56:PRO:HD3	2.32	0.45
1:C:102:LEU:HD21	1:C:151:LEU:HD23	1.98	0.45
1:B:208:GLN:HE22	1:B:227:ARG:HG2	1.80	0.45
1:C:134:LYS:HA	1:C:135:PRO:HD3	1.87	0.45
1:A:172:ILE:HG22	1:A:173:MET:HG3	1.99	0.45
1:C:102:LEU:HD23	1:C:103:ASN:N	2.32	0.45
1:D:165:LEU:HD13	1:D:185:LEU:HD21	1.97	0.45
1:C:191:HIS:ND1	1:C:221:GLU:HG3	2.33	0.44
1:B:172:ILE:HG22	1:B:173:MET:HG3	2.00	0.44
1:D:138:ASP:OD2	1:D:141:GLU:HG2	2.17	0.44
1:C:47:GLN:HB2	1:C:130:TYR:CD2	2.53	0.44
1:D:206:SER:H	1:D:209:ASN:HD22	1.63	0.44
1:B:152:ASN:ND2	1:B:182:PHE:HE1	2.11	0.44
1:D:92:VAL:O	1:D:96:LEU:HG	2.17	0.44
1:C:247:THR:OG1	1:C:248:ASP:N	2.50	0.44
1:D:116:GLU:HG2	1:D:136:VAL:O	2.18	0.44
1:B:125:LEU:HD21	1:B:182:PHE:HE2	1.83	0.44
1:C:70:ALA:O	1:C:81:HIS:HA	2.17	0.44
1:A:102:LEU:HD11	1:A:151:LEU:HB3	2.00	0.43
1:B:27:MET:HB2	5:B:865:HOH:O	2.18	0.43
1:C:174:LYS:HA	1:C:175:PRO:HD3	1.86	0.43
1:D:178:SER:OG	4:D:806:GOL:O2	2.35	0.43
1:B:158:ILE:HB	1:B:159:PRO:HD3	2.00	0.43
1:A:158:ILE:CB	1:A:159:PRO:HD2	2.47	0.43
1:C:59:LYS:NZ	1:C:60:ASP:OD1	2.51	0.43
1:C:266:THR:O	1:C:267:TYR:C	2.62	0.43
1:A:161:VAL:CG1	1:A:165:LEU:CD1	2.96	0.43
1:D:13:THR:CG2	1:D:14:PHE:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:HB2	1:A:130:TYR:CD2	2.54	0.42
1:B:49:TYR:CD1	1:B:132:ARG:HD3	2.54	0.42
1:D:173:MET:HA	1:D:188:PRO:HD3	2.00	0.42
1:D:47:GLN:HB2	1:D:130:TYR:CD2	2.54	0.42
1:B:154:PRO:CB	1:B:156:GLU:HG2	2.49	0.42
1:B:165:LEU:HD13	1:B:175:PRO:HG3	2.01	0.42
1:B:235:ALA:O	1:B:240:LYS:HE3	2.19	0.42
1:C:3:VAL:N	5:C:821:HOH:O	2.52	0.42
1:D:191:HIS:CD2	1:D:221:GLU:HG2	2.54	0.42
1:B:93:ILE:O	1:B:97:LEU:HB2	2.19	0.42
1:A:9:ASP:CB	1:A:9:ASP:H	2.27	0.42
1:C:17:ASP:CG	1:C:251:ASN:HD21	2.27	0.42
1:A:173:MET:HA	1:A:188:PRO:HD3	2.01	0.42
1:C:102:LEU:HD21	1:C:151:LEU:CD2	2.49	0.41
1:B:155:ASP:HA	1:B:183:ILE:HG12	2.02	0.41
1:C:13:THR:HA	1:C:232:MET:HG3	2.01	0.41
1:C:59:LYS:HE3	1:D:57:GLU:HG2	2.01	0.41
1:D:151:LEU:N	1:D:151:LEU:HD12	2.35	0.41
1:A:156:GLU:H	1:A:156:GLU:CD	2.24	0.41
1:B:70:ALA:O	1:B:81:HIS:HA	2.19	0.41
1:C:31:GLN:HA	1:C:31:GLN:HE21	1.84	0.41
1:A:262:VAL:CG2	1:A:269:PHE:CZ	2.99	0.41
1:B:49:TYR:CG	1:B:132:ARG:HD3	2.56	0.41
1:B:245:TYR:CE2	1:B:268:PRO:HB3	2.56	0.41
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.86	0.41
1:D:33:LEU:HD23	1:D:263:LEU:HD21	2.01	0.41
1:A:39:LYS:HD3	1:A:203:TRP:CE2	2.56	0.41
1:B:134:LYS:HA	1:B:135:PRO:HD3	1.89	0.41
1:A:134:LYS:HA	1:A:135:PRO:HD3	1.82	0.41
1:D:79:LEU:HD13	1:D:202:ARG:NH1	2.36	0.41
1:C:59:LYS:HE3	1:D:57:GLU:CG	2.51	0.41
1:A:114:VAL:O	1:A:135:PRO:HA	2.21	0.40
1:B:86:ARG:NH1	1:B:86:ARG:HG3	2.36	0.40
1:B:266:THR:O	1:B:267:TYR:C	2.64	0.40
1:A:160:LEU:C	1:A:160:LEU:CD2	2.70	0.40
1:D:155:ASP:OD2	1:D:180:PHE:CD2	2.74	0.40
1:A:157:GLN:O	1:A:158:ILE:C	2.64	0.40
1:C:114:VAL:O	1:C:135:PRO:HA	2.21	0.40
1:A:50:GLN:HE21	1:A:50:GLN:C	2.30	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	266/271 (98%)	256 (96%)	10 (4%)	0	100	100
1	B	266/271 (98%)	254 (96%)	11 (4%)	1 (0%)	30	27
1	C	266/271 (98%)	250 (94%)	14 (5%)	2 (1%)	16	11
1	D	266/271 (98%)	253 (95%)	12 (4%)	1 (0%)	30	27
All	All	1064/1084 (98%)	1013 (95%)	47 (4%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	GLN
1	C	22	ASN
1	C	100	LYS
1	D	180	PHE

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	228/230 (99%)	216 (95%)	12 (5%)	20	18
1	B	228/230 (99%)	217 (95%)	11 (5%)	23	21
1	C	228/230 (99%)	216 (95%)	12 (5%)	20	18
1	D	228/230 (99%)	219 (96%)	9 (4%)	28	28
All	All	912/920 (99%)	868 (95%)	44 (5%)	23	21

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	27	MET
1	A	32	GLU
1	A	50	GLN
1	A	97	LEU
1	A	101	GLN
1	A	147	PHE
1	A	152	ASN
1	A	159	PRO
1	A	160	LEU
1	A	221	GLU
1	A	225	MET
1	B	15	LEU
1	B	50	GLN
1	B	86	ARG
1	B	97	LEU
1	B	109	LEU
1	B	147	PHE
1	B	188	PRO
1	B	202	ARG
1	B	208	GLN
1	B	237	GLU
1	B	270	ASN
1	C	15	LEU
1	C	19	LYS
1	C	27	MET
1	C	50	GLN
1	C	109	LEU
1	C	147	PHE
1	C	151	LEU
1	C	159	PRO
1	C	204	ASP
1	C	221	GLU
1	C	247	THR
1	C	265	ASN
1	D	15	LEU
1	D	32	GLU
1	D	71	LEU
1	D	97	LEU
1	D	109	LEU
1	D	147	PHE
1	D	153	LEU

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Mol	Chain	Res	Type
1	D	225	MET
1	D	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	50	GLN
1	A	78	GLN
1	A	101	GLN
1	A	110	GLN
1	A	117	ASN
1	A	129	HIS
1	A	152	ASN
1	A	208	GLN
1	A	265	ASN
1	B	50	GLN
1	B	78	GLN
1	B	103	ASN
1	B	152	ASN
1	B	157	GLN
1	B	194	ASN
1	B	208	GLN
1	B	209	ASN
1	B	238	ASN
1	B	241	GLN
1	C	31	GLN
1	C	50	GLN
1	C	78	GLN
1	C	129	HIS
1	C	140	GLN
1	C	152	ASN
1	C	270	ASN
1	D	22	ASN
1	D	78	GLN
1	D	103	ASN
1	D	140	GLN
1	D	152	ASN
1	D	209	ASN

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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	D	806	-	5,5,5	4.92	5 (100%)	5,5,5	6.03	3 (60%)
4	GOL	C	805	-	5,5,5	4.93	5 (100%)	5,5,5	6.10	3 (60%)
5	BEF	D	807	1	0,3,3	-	-	-		
5	BEF	A	802	1	0,3,3	-	-	-		
5	BEF	B	803	1	0,3,3	-	-	-		
5	BEF	C	806	1	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	806	-	-	2/4/4/4	-
4	GOL	C	805	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	805	GOL	C3-C2	-8.50	1.19	1.51
4	D	806	GOL	C3-C2	-8.27	1.20	1.51
4	D	806	GOL	O1-C1	4.55	1.61	1.42
4	C	805	GOL	O1-C1	4.52	1.61	1.42
4	D	806	GOL	O2-C2	-3.70	1.32	1.43
4	C	805	GOL	O2-C2	-3.23	1.34	1.43
4	C	805	GOL	C1-C2	-3.21	1.39	1.51
4	D	806	GOL	O3-C3	3.02	1.55	1.42
4	D	806	GOL	C1-C2	-3.01	1.40	1.51
4	C	805	GOL	O3-C3	2.87	1.54	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	805	GOL	O3-C3-C2	11.27	161.11	110.38
4	D	806	GOL	O3-C3-C2	11.03	160.03	110.38
4	D	806	GOL	O2-C2-C3	7.01	138.21	109.18
4	C	805	GOL	O2-C2-C3	6.90	137.76	109.18
4	C	805	GOL	O1-C1-C2	3.27	125.09	110.38
4	D	806	GOL	O1-C1-C2	3.23	124.92	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	805	GOL	O1-C1-C2-C3
4	C	805	GOL	C1-C2-C3-O3
4	D	806	GOL	C1-C2-C3-O3
4	D	806	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	806	GOL	1	0
4	C	805	GOL	2	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	268/271 (98%)	-0.00	11 (4%) 41 40	10, 18, 35, 47	0
1	B	268/271 (98%)	0.49	33 (12%) 8 7	11, 23, 60, 75	0
1	C	268/271 (98%)	0.36	18 (6%) 24 22	10, 24, 40, 48	0
1	D	268/271 (98%)	0.23	14 (5%) 33 31	11, 24, 46, 58	0
All	All	1072/1084 (98%)	0.27	76 (7%) 22 20	10, 22, 44, 75	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	LEU	7.1
1	A	270	ASN	5.2
1	B	160	LEU	5.1
1	C	20	THR	4.9
1	B	162	ILE	4.5
1	B	165	LEU	4.2
1	B	180	PHE	4.1
1	B	159	PRO	4.1
1	B	161	VAL	4.1
1	B	167	VAL	4.0
1	B	158	ILE	4.0
1	C	270	ASN	3.9
1	B	153	LEU	3.9
1	D	102	LEU	3.8
1	D	180	PHE	3.8
1	D	270	ASN	3.7
1	B	270	ASN	3.6
1	B	155	ASP	3.6
1	B	179	GLY	3.6
1	A	170	ASP	3.5
1	A	141	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	161	VAL	3.5
1	B	154	PRO	3.4
1	A	159	PRO	3.3
1	C	86	ARG	3.1
1	B	163	ASP	3.1
1	D	86	ARG	3.0
1	C	140	GLN	3.0
1	B	97	LEU	3.0
1	B	100	LYS	2.9
1	A	75	HIS	2.9
1	A	171	GLY	2.9
1	C	23	GLN	2.9
1	C	246	ALA	2.9
1	B	182	PHE	2.8
1	B	98	LYS	2.8
1	B	201	LYS	2.7
1	C	248	ASP	2.7
1	D	138	ASP	2.7
1	B	166	HIS	2.7
1	D	137	LYS	2.6
1	D	101	GLN	2.6
1	C	18	ALA	2.6
1	C	236	ALA	2.6
1	C	17	ASP	2.6
1	D	159	PRO	2.6
1	A	269	PHE	2.5
1	C	139	TYR	2.5
1	D	160	LEU	2.5
1	D	204	ASP	2.5
1	B	188	PRO	2.5
1	B	152	ASN	2.5
1	B	244	ARG	2.4
1	C	235	ALA	2.4
1	A	101	GLN	2.4
1	A	100	LYS	2.4
1	C	252	HIS	2.3
1	D	153	LEU	2.3
1	B	138	ASP	2.3
1	C	265	ASN	2.3
1	B	90	ARG	2.2
1	B	168	ALA	2.2
1	B	178	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	16	ASN	2.2
1	C	234	ASN	2.2
1	D	241	GLN	2.2
1	D	139	TYR	2.2
1	B	266	THR	2.2
1	B	101	GLN	2.1
1	B	157	GLN	2.1
1	B	99	ASP	2.1
1	B	164	LYS	2.1
1	C	159	PRO	2.0
1	C	32	GLU	2.0
1	D	97	LEU	2.0
1	B	86	ARG	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
4	GOL	D	806	6/6	0.76	0.21	32,38,41,41	0
4	GOL	C	805	6/6	0.79	0.16	23,29,32,32	0
2	MG	C	803	1/1	0.91	0.05	22,22,22,22	0
5	BEF	C	806	4/4	0.96	0.07	14,17,18,19	0
5	BEF	D	807	4/4	0.97	0.05	12,13,14,15	0
5	BEF	B	803	4/4	0.97	0.05	13,14,14,14	0
5	BEF	A	802	4/4	0.97	0.06	11,12,12,12	0
2	MG	B	802	1/1	0.98	0.02	11,11,11,11	0
2	MG	A	801	1/1	0.98	0.03	11,11,11,11	0
2	MG	D	804	1/1	0.98	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.