



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:38 PM UTC

PDB ID : 1WPR / pdb_00001wpr
Title : Crystal structure of RsbQ inhibited by PMSF
Authors : Kaneko, T.; Tanaka, N.; Kumasaka, T.
Deposited on : 2004-09-11
Resolution : 2.60 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

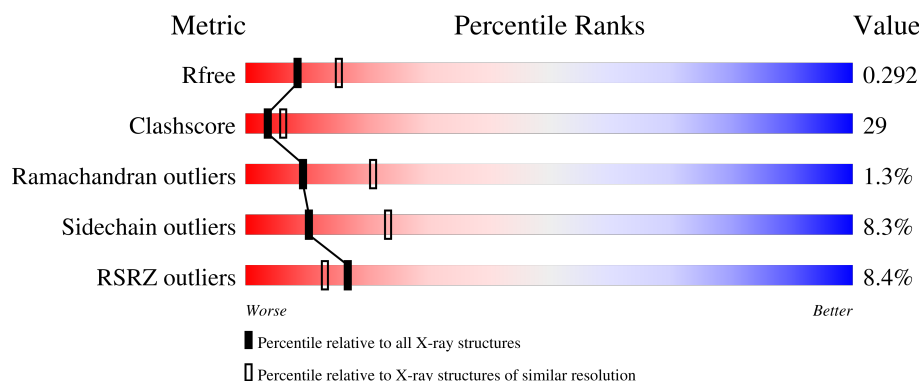
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	5% 57% 32% 8% ..
1	B	271	12% 46% 46% 6% .

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	PMS	A	1001	-	-	X	-
3	GOL	A	2002	-	-	X	-
3	GOL	A	2004	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4284 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.

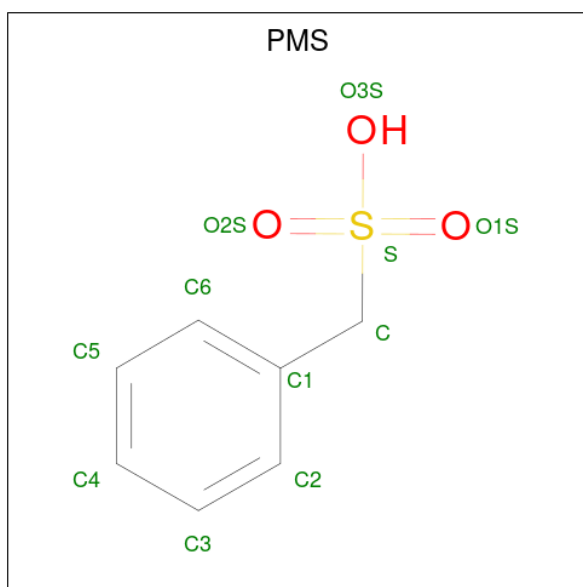
- Molecule 1 is a protein called Sigma factor sigB regulation protein rsbQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	1	0
			2062	1313	347	388	14			
1	B	265	Total	C	N	O	S	0	0	0
			2008	1278	340	376	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	cloning artifact	UNP O07015
A	0	GLY	-	cloning artifact	UNP O07015
A	1	HIS	-	cloning artifact	UNP O07015
A	2	MET	-	cloning artifact	UNP O07015
A	3	THR	-	cloning artifact	UNP O07015
A	4	SER	-	cloning artifact	UNP O07015
B	-1	ALA	-	cloning artifact	UNP O07015
B	0	GLY	-	cloning artifact	UNP O07015
B	1	HIS	-	cloning artifact	UNP O07015
B	2	MET	-	cloning artifact	UNP O07015
B	3	THR	-	cloning artifact	UNP O07015
B	4	SER	-	cloning artifact	UNP O07015

- Molecule 2 is phenylmethanesulfonic acid (CCD ID: PMS) (formula: C₇H₈O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			10	7	2	1		
2	B	1	Total	C	O	S	0	0
			10	7	2	1		

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



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		

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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		

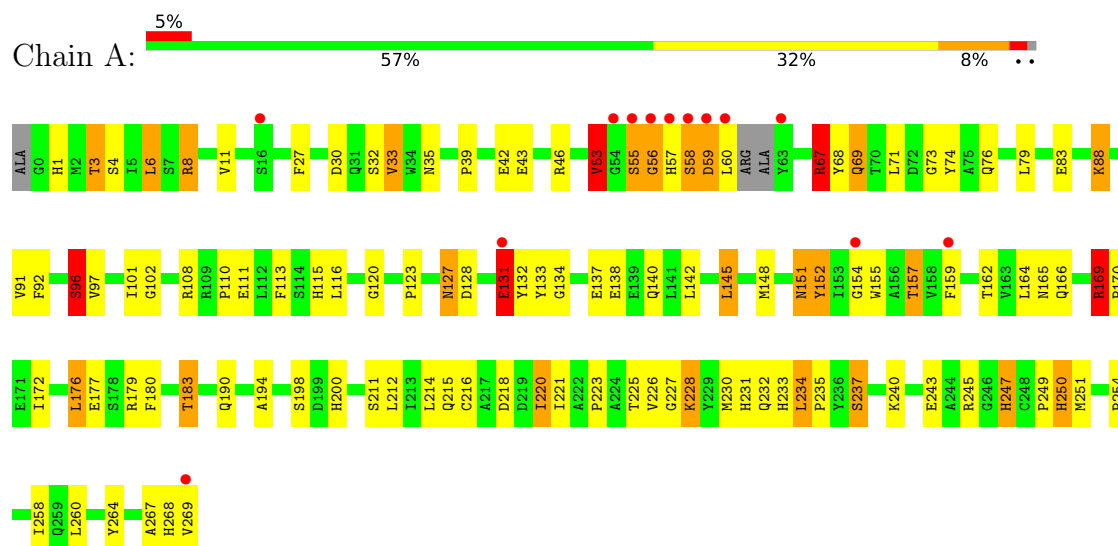
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	45	Total	O	0	0
			45	45		

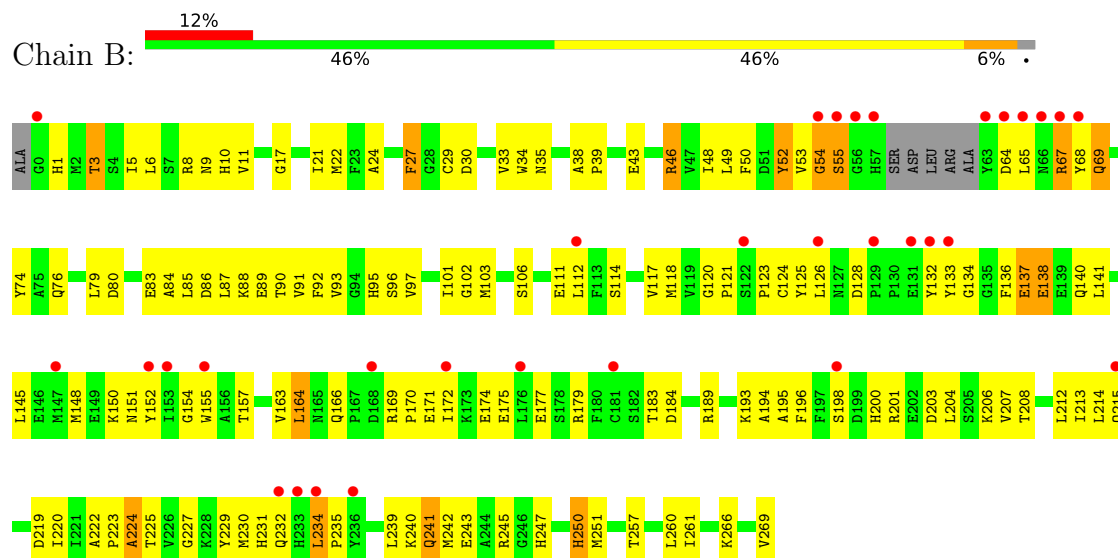
3 Residue-property plots

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: Sigma factor sigB regulation protein rsbQ



- Molecule 1: Sigma factor sigB regulation protein rsbQ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.20Å 81.00Å 136.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.86 – 2.60 35.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.86-2.60) 99.5 (35.86-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.292 0.232 , 0.292	Depositor DCC
R_{free} test set	1339 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4284	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: PMS, 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	0.70	0/2119	1.19	22/2880 (0.8%)
1	B	0.53	0/2058	1.07	14/2798 (0.5%)
All	All	0.62	0/4177	1.14	36/5678 (0.6%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	N-CA-C	-9.10	102.19	113.38
1	A	46	ARG	N-CA-C	-7.68	98.45	109.96
1	B	35	ASN	N-CA-C	7.61	120.54	111.33
1	A	169	ARG	CA-C-N	7.51	128.18	119.47
1	A	169	ARG	C-N-CA	7.51	128.18	119.47
1	B	46	ARG	N-CA-C	-7.10	98.39	109.25
1	A	131	GLU	N-CA-C	7.07	122.00	113.23
1	A	152	TYR	N-CA-C	7.02	118.63	110.97
1	A	59	ASP	N-CA-C	6.62	120.12	109.79
1	B	152	TYR	N-CA-C	6.39	118.13	111.03
1	B	55	SER	N-CA-C	6.33	118.49	110.33
1	A	220	ILE	CB-CA-C	-6.29	101.90	112.16
1	A	88	LYS	N-CA-C	-6.20	105.85	113.41
1	B	96	SER	CB-CA-C	-6.06	109.57	116.54
1	A	8	ARG	N-CA-C	6.06	118.68	111.71
1	B	88	LYS	N-CA-C	-6.01	104.07	111.40
1	A	53	VAL	N-CA-C	-5.82	103.78	111.05
1	B	52	TYR	N-CA-C	-5.81	101.89	110.48
1	B	11	VAL	N-CA-C	5.74	116.47	109.30
1	A	58	SER	N-CA-C	5.68	116.58	108.74
1	A	35	ASN	N-CA-C	5.56	118.86	111.75
1	B	234	LEU	CA-C-N	5.42	126.62	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	LEU	C-N-CA	5.42	126.62	119.84
1	A	237	SER	N-CA-C	5.37	117.14	109.14
1	B	68	TYR	N-CA-C	-5.37	107.28	112.97
1	A	96	SER	CB-CA-C	-5.33	110.41	116.54
1	B	243	GLU	N-CA-C	-5.32	106.30	112.89
1	A	56	GLY	N-CA-C	-5.31	100.60	113.18
1	A	166	GLN	CA-C-N	5.25	124.92	119.56
1	A	166	GLN	C-N-CA	5.25	124.92	119.56
1	A	127	ASN	N-CA-C	-5.21	101.47	109.76
1	B	69	GLN	N-CA-C	-5.19	105.24	112.45
1	A	67	ARG	N-CA-C	5.17	118.69	112.38
1	A	91	VAL	N-CA-C	-5.17	102.41	109.55
1	A	243	GLU	N-CA-C	-5.01	105.92	112.23
1	A	247	HIS	N-CA-C	5.01	119.39	113.28

There are no chirality outliers.

There are no planarity outliers.

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	2062	0	1955	116	0
1	B	2008	0	1896	117	0
2	A	10	0	7	4	0
2	B	10	0	7	0	0
3	A	24	0	32	18	0
4	A	125	0	0	7	0
4	B	45	0	0	1	0
All	All	4284	0	3897	233	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 29.

All (233) 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:215:GLN:HE21	1:A:227:GLY:HA3	1.30	0.95
1:B:8:ARG:HH21	1:B:9:ASN:HD21	1.16	0.93
1:A:108:ARG:HD2	3:A:2002:GOL:H11	1.55	0.87
1:A:212:LEU:HD11	1:A:240:LYS:HD3	1.54	0.87
1:A:108:ARG:HH21	3:A:2002:GOL:H11	1.40	0.87
1:A:32:SER:HB3	1:A:179:ARG:HH22	1.40	0.87
1:A:111:GLU:HA	3:A:2004:GOL:C3	2.09	0.81
1:A:97:VAL:HG23	2:A:1001:PMS:O2S	1.79	0.80
1:A:113:PHE:O	3:A:2004:GOL:C1	2.29	0.80
1:B:124:CYS:HB3	1:B:132:TYR:CE2	2.17	0.79
1:B:203:ASP:HA	1:B:206:LYS:HE2	1.65	0.78
1:B:93:VAL:HG22	1:B:117:VAL:HB	1.66	0.78
1:B:103:MET:HE2	1:B:207:VAL:HG21	1.68	0.76
1:B:240:LYS:HE2	1:B:260:LEU:HD21	1.67	0.76
1:A:56:GLY:HA3	4:A:2008:HOH:O	1.87	0.74
1:A:113:PHE:O	3:A:2004:GOL:H11	1.86	0.74
1:A:223:PRO:O	1:A:226:VAL:HG22	1.89	0.71
1:A:111:GLU:HA	3:A:2004:GOL:H31	1.70	0.71
1:B:215:GLN:CG	1:B:227:GLY:HA3	2.21	0.71
1:B:8:ARG:NH2	1:B:9:ASN:HD21	1.87	0.70
1:A:67:ARG:O	1:A:73:GLY:HA3	1.91	0.70
1:B:200:HIS:O	1:B:204:LEU:HD13	1.92	0.70
1:A:113:PHE:O	3:A:2004:GOL:H12	1.92	0.69
1:B:133:TYR:CB	1:B:225:THR:HG21	2.22	0.69
1:A:53:VAL:O	1:A:55:SER:N	2.21	0.69
1:A:108:ARG:NH2	3:A:2002:GOL:H11	2.07	0.68
1:A:30:ASP:OD1	1:A:32:SER:HB3	1.94	0.68
1:A:53:VAL:C	1:A:55:SER:H	2.02	0.68
1:A:215:GLN:NE2	1:A:227:GLY:HA3	2.04	0.67
1:B:124:CYS:HB3	1:B:132:TYR:HE2	1.55	0.67
1:A:111:GLU:HA	3:A:2004:GOL:H32	1.76	0.66
1:A:111:GLU:CA	3:A:2004:GOL:H31	2.26	0.66
1:A:231:HIS:HD2	1:A:237:SER:OG	1.79	0.66
1:A:245:ARG:NH1	1:A:245:ARG:HB3	2.11	0.65
1:A:180:PHE:O	1:A:183:THR:HG22	1.96	0.65
1:B:215:GLN:OE1	1:B:224:ALA:HA	1.97	0.65
1:B:33:VAL:HA	1:B:179:ARG:HH21	1.61	0.64
1:A:32:SER:CB	1:A:179:ARG:HH22	2.08	0.64
1:B:118:MET:HE3	1:B:121:PRO:HG3	1.80	0.64
1:B:8:ARG:HH21	1:B:9:ASN:ND2	1.94	0.64
1:A:39:PRO:HA	1:A:42:GLU:HG3	1.79	0.63
1:A:159:PHE:HE1	2:A:1001:PMS:C3	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASP:N	1:B:132:TYR:O	2.30	0.63
1:B:257:THR:O	1:B:261:ILE:HG13	1.99	0.63
1:B:166:GLN:HB3	1:B:169:ARG:HG3	1.81	0.62
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.81	0.62
1:A:88:LYS:HD3	4:A:2101:HOH:O	1.99	0.61
1:B:194:ALA:O	1:B:198:SER:HB3	2.00	0.61
1:A:228:LYS:NZ	1:A:232:GLN:NE2	2.48	0.61
1:A:110:PRO:O	3:A:2004:GOL:H31	2.00	0.61
1:B:21:ILE:HG12	1:B:91:VAL:HB	1.83	0.60
1:A:164:LEU:CD1	1:A:176:LEU:HD12	2.31	0.60
1:B:33:VAL:CA	1:B:179:ARG:HH21	2.13	0.60
1:A:164:LEU:HD21	1:A:172:ILE:HG22	1.83	0.60
1:B:231:HIS:HB2	1:B:239:LEU:HD22	1.84	0.60
1:B:240:LYS:HE2	1:B:260:LEU:CD2	2.32	0.60
1:B:5:ILE:HD13	1:B:80:ASP:HB3	1.84	0.59
1:B:164:LEU:HD12	1:B:166:GLN:HB2	1.84	0.59
1:A:169:ARG:HG3	1:A:169:ARG:HH11	1.68	0.59
1:B:231:HIS:CB	1:B:239:LEU:HD22	2.33	0.59
1:A:53:VAL:C	1:A:55:SER:N	2.60	0.58
1:B:55:SER:CB	1:B:184:ASP:H	2.15	0.58
1:B:171:GLU:HG2	1:B:172:ILE:N	2.18	0.58
1:A:92:PHE:CE2	1:A:102:GLY:HA3	2.39	0.57
1:A:180:PHE:O	1:A:183:THR:CG2	2.52	0.57
1:A:8:ARG:HD3	4:A:2079:HOH:O	2.05	0.57
1:A:221:ILE:HG21	2:A:1001:PMS:H2A	1.87	0.57
1:B:215:GLN:HG3	1:B:227:GLY:HA3	1.85	0.57
1:A:53:VAL:HG22	1:A:68:TYR:OH	2.05	0.56
1:A:1:HIS:CD2	1:A:3:THR:HG23	2.40	0.56
1:A:231:HIS:O	4:A:2129:HOH:O	2.18	0.56
1:B:97:VAL:HG11	1:B:195:ALA:CB	2.35	0.56
1:A:131:GLU:CD	1:A:131:GLU:H	2.14	0.56
1:B:27:PHE:CD1	1:B:27:PHE:C	2.82	0.56
1:B:223:PRO:C	1:B:225:THR:H	2.13	0.56
1:B:214:LEU:HD11	1:B:260:LEU:HD13	1.87	0.56
1:A:108:ARG:HH21	3:A:2002:GOL:C1	2.16	0.56
1:A:267:ALA:C	1:A:269:VAL:H	2.14	0.56
1:B:48:ILE:HD13	1:B:85:LEU:HD12	1.86	0.56
1:A:111:GLU:C	3:A:2004:GOL:H31	2.30	0.56
1:B:97:VAL:HG11	1:B:195:ALA:HB2	1.88	0.56
1:A:6:LEU:HD12	1:A:11:VAL:HB	1.87	0.55
1:A:43:GLU:OE2	1:A:43:GLU:HA	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG22	1:A:68:TYR:CZ	2.41	0.55
1:B:103:MET:HE2	1:B:234:LEU:HD21	1.88	0.55
1:A:133:TYR:HB2	1:A:225:THR:HG21	1.88	0.55
1:A:58:SER:CB	4:A:2070:HOH:O	2.53	0.55
1:A:228:LYS:O	1:A:232:GLN:HG3	2.07	0.55
1:B:29:CYS:HB3	1:B:33:VAL:HG11	1.88	0.55
1:A:4:SER:O	1:A:8:ARG:HG2	2.07	0.55
1:B:145:LEU:O	1:B:148:MET:HB2	2.06	0.55
1:B:33:VAL:HA	1:B:179:ARG:NH2	2.22	0.54
1:B:151:ASN:HD21	1:B:154:GLY:HA3	1.72	0.54
1:B:214:LEU:HG	1:B:242:MET:SD	2.48	0.54
1:A:220:ILE:HG22	1:A:220:ILE:O	2.07	0.53
1:A:251:MET:HE3	3:A:2001:GOL:H12	1.90	0.53
1:A:27:PHE:CD1	1:A:27:PHE:C	2.87	0.53
1:A:30:ASP:O	1:A:33:VAL:HG22	2.07	0.53
1:A:159:PHE:CE1	2:A:1001:PMS:C3	2.90	0.53
1:B:266:LYS:O	1:B:269:VAL:HG12	2.08	0.53
1:A:264:TYR:O	1:A:268:HIS:HD2	1.91	0.53
1:A:169:ARG:N	1:A:170:PRO:CD	2.71	0.53
1:B:103:MET:CE	1:B:234:LEU:HD21	2.38	0.53
1:A:30:ASP:OD1	1:A:32:SER:CB	2.56	0.53
1:A:1:HIS:HD2	1:A:3:THR:HG23	1.74	0.53
1:A:198:SER:HB2	1:A:200:HIS:CE1	2.43	0.53
1:A:57:HIS:HA	1:A:183:THR:HB	1.91	0.52
1:B:67:ARG:HH11	1:B:76:GLN:HB3	1.75	0.52
1:B:125:TYR:HD1	1:B:196:PHE:HA	1.75	0.52
1:B:223:PRO:C	1:B:225:THR:N	2.67	0.52
1:B:215:GLN:CD	1:B:227:GLY:HA3	2.35	0.52
1:A:254:PRO:O	1:A:258:ILE:HG13	2.11	0.51
1:A:194:ALA:O	1:A:198:SER:HB3	2.11	0.51
1:B:8:ARG:HE	1:B:9:ASN:ND2	2.07	0.51
1:A:111:GLU:CA	3:A:2004:GOL:C3	2.86	0.51
1:B:250:HIS:CD2	1:B:250:HIS:H	2.28	0.50
1:B:125:TYR:O	1:B:136:PHE:HB2	2.11	0.50
1:A:145:LEU:HA	1:A:148:MET:HE3	1.93	0.50
1:A:164:LEU:HD13	1:A:176:LEU:HD12	1.93	0.50
1:A:245:ARG:HB3	1:A:245:ARG:HH11	1.76	0.50
1:B:17:GLY:O	1:B:46:ARG:NH1	2.45	0.50
1:B:33:VAL:N	1:B:179:ARG:HH21	2.09	0.50
1:B:240:LYS:HD3	1:B:241:GLN:N	2.27	0.50
1:B:8:ARG:HG2	1:B:53:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:SER:CB	1:B:183:THR:HG23	2.42	0.49
1:B:123:PRO:HD3	1:B:230:MET:SD	2.53	0.49
1:B:83:GLU:O	1:B:86:ASP:N	2.44	0.49
1:A:245:ARG:HH11	1:A:245:ARG:CB	2.26	0.49
1:B:1:HIS:CD2	1:B:3:THR:HG23	2.48	0.49
1:B:29:CYS:HB3	1:B:33:VAL:CG1	2.42	0.49
1:B:164:LEU:CD1	1:B:166:GLN:HB2	2.42	0.49
1:A:215:GLN:NE2	1:A:227:GLY:CA	2.75	0.48
1:B:53:VAL:HG12	1:B:53:VAL:O	2.13	0.48
1:B:145:LEU:HD21	1:B:196:PHE:HD2	1.79	0.48
1:A:162:THR:HG22	1:A:221:ILE:HD11	1.94	0.48
1:B:126:LEU:O	1:B:134:GLY:HA3	2.14	0.48
1:B:169:ARG:N	1:B:170:PRO:CD	2.76	0.48
1:B:171:GLU:HG2	1:B:172:ILE:H	1.77	0.48
1:A:6:LEU:HD12	1:A:11:VAL:CB	2.44	0.48
1:A:212:LEU:HD22	1:A:264:TYR:CG	2.48	0.48
1:B:137:GLU:O	1:B:138:GLU:C	2.55	0.48
1:B:175:GLU:OE1	1:B:179:ARG:NH1	2.47	0.48
1:A:59:ASP:O	1:A:60:LEU:CB	2.61	0.47
1:A:115:HIS:HD2	1:A:264:TYR:OH	1.97	0.47
1:B:83:GLU:O	1:B:84:ALA:C	2.57	0.47
1:B:48:ILE:CD1	1:B:87:LEU:HD11	2.45	0.47
1:B:163:VAL:HG13	1:B:247:HIS:HB3	1.97	0.47
1:A:212:LEU:HD22	1:A:264:TYR:CB	2.44	0.47
1:B:214:LEU:HD11	1:B:260:LEU:CD1	2.45	0.47
1:B:220:ILE:HG22	1:B:220:ILE:O	2.14	0.47
1:A:269:VAL:HG12	1:A:269:VAL:O	2.14	0.47
1:A:4:SER:O	1:A:8:ARG:CG	2.63	0.47
1:B:95:HIS:HE1	1:B:247:HIS:O	1.98	0.47
1:B:103:MET:HG3	1:B:207:VAL:HG22	1.96	0.47
1:A:108:ARG:HD2	3:A:2002:GOL:O3	2.14	0.46
1:B:223:PRO:O	1:B:225:THR:N	2.48	0.46
1:B:92:PHE:C	1:B:92:PHE:CD2	2.93	0.46
1:A:230:MET:O	1:A:234:LEU:HB2	2.16	0.46
1:A:137:GLU:O	1:A:138:GLU:C	2.58	0.46
1:B:24:ALA:C	1:B:34:TRP:HE1	2.24	0.46
1:B:241:GLN:NE2	1:B:242:MET:O	2.49	0.46
1:A:128:ASP:N	1:A:132:TYR:O	2.37	0.46
1:A:218:ASP:OD1	1:A:245:ARG:NH2	2.48	0.45
1:A:233:HIS:O	1:A:235:PRO:HD3	2.17	0.45
1:B:27:PHE:CE1	1:B:155:TRP:HH2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HB	1:A:177:GLU:CD	2.41	0.45
1:A:214:LEU:HD22	1:A:260:LEU:HD13	1.98	0.45
1:A:164:LEU:HD21	1:A:172:ILE:CG2	2.46	0.45
1:B:174:GLU:O	1:B:177:GLU:HB3	2.16	0.45
1:A:151:ASN:OD1	1:A:151:ASN:C	2.60	0.45
1:B:120:GLY:N	1:B:121:PRO:CD	2.79	0.45
1:A:137:GLU:O	1:A:140:GLN:N	2.49	0.45
1:A:228:LYS:HZ3	1:A:232:GLN:NE2	2.15	0.45
1:B:189:ARG:NH2	1:B:193:LYS:NZ	2.64	0.45
1:B:166:GLN:OE1	1:B:169:ARG:HD3	2.16	0.44
1:B:250:HIS:CD2	1:B:250:HIS:N	2.85	0.44
1:A:250:HIS:H	1:A:250:HIS:CD2	2.36	0.44
1:B:97:VAL:O	1:B:101:ILE:HG13	2.17	0.44
1:B:10:HIS:HD2	4:B:1008:HOH:O	2.00	0.43
1:B:111:GLU:HG2	1:B:112:LEU:N	2.33	0.43
1:A:74:TYR:HB3	1:A:101:ILE:HD13	2.00	0.43
1:B:33:VAL:HG13	1:B:179:ARG:HE	1.83	0.43
1:A:212:LEU:HD22	1:A:264:TYR:HB2	2.00	0.43
1:B:189:ARG:CZ	1:B:193:LYS:HZ3	2.31	0.43
1:B:242:MET:HG2	1:B:260:LEU:CD1	2.48	0.43
1:B:22:MET:HA	1:B:48:ILE:HB	1.99	0.43
1:A:179:ARG:NH1	1:A:179:ARG:HG2	2.34	0.43
1:A:96:SER:HB3	1:A:97:VAL:H	1.64	0.43
1:A:216:CYS:SG	1:A:249:PRO:HD3	2.59	0.43
1:B:137:GLU:HB2	1:B:140:GLN:HG3	2.01	0.43
1:B:49:LEU:O	1:B:50:PHE:HB3	2.19	0.42
1:A:120:GLY:O	1:A:247:HIS:HE1	2.03	0.42
1:B:87:LEU:HD13	1:B:90:THR:HB	2.00	0.42
1:B:92:PHE:CE2	1:B:102:GLY:HA3	2.55	0.42
1:A:152:TYR:O	1:A:155:TRP:HB3	2.18	0.42
1:A:108:ARG:HB3	3:A:2002:GOL:H12	2.01	0.42
1:A:164:LEU:O	1:A:165:ASN:C	2.62	0.42
1:B:29:CYS:SG	1:B:33:VAL:HG11	2.60	0.42
1:B:125:TYR:CD1	1:B:196:PHE:HA	2.54	0.42
1:B:30:ASP:C	1:B:30:ASP:OD1	2.62	0.42
1:A:250:HIS:CD2	1:A:250:HIS:N	2.88	0.42
1:B:67:ARG:C	1:B:69:GLN:H	2.27	0.42
1:B:80:ASP:O	1:B:83:GLU:HB3	2.20	0.42
1:B:214:LEU:HD12	1:B:214:LEU:HA	1.97	0.42
1:A:76:GLN:OE1	1:A:108:ARG:NH1	2.31	0.42
1:A:123:PRO:HD2	1:A:132:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HA	1:A:177:GLU:HG3	2.01	0.41
1:B:126:LEU:N	1:B:126:LEU:HD12	2.36	0.41
1:A:154:GLY:O	1:A:157:THR:HG23	2.20	0.41
1:B:52:TYR:C	1:B:54:GLY:H	2.29	0.41
1:B:123:PRO:HB3	1:B:204:LEU:HD11	2.02	0.41
1:B:229:TYR:O	1:B:232:GLN:HB2	2.21	0.41
1:A:56:GLY:CA	4:A:2008:HOH:O	2.54	0.41
1:B:30:ASP:O	1:B:33:VAL:HG22	2.20	0.41
1:A:108:ARG:NH2	3:A:2002:GOL:C1	2.79	0.41
1:A:116:LEU:HB2	1:A:211:SER:OG	2.20	0.41
1:B:8:ARG:HE	1:B:9:ASN:HD21	1.68	0.41
1:B:201:ARG:O	1:B:204:LEU:HB2	2.21	0.41
1:B:212:LEU:HD12	1:B:213:ILE:N	2.36	0.41
1:A:69:GLN:HE21	1:A:69:GLN:HB3	1.68	0.41
1:B:245:ARG:HD3	1:B:245:ARG:N	2.36	0.41
1:A:67:ARG:HG2	1:A:68:TYR:CE1	2.56	0.41
1:A:67:ARG:HD2	1:A:68:TYR:CZ	2.55	0.40
1:B:48:ILE:HD13	1:B:85:LEU:CD1	2.50	0.40
1:B:219:ASP:OD1	1:B:222:ALA:N	2.37	0.40
1:A:190:GLN:NE2	4:A:2005:HOH:O	2.50	0.40
1:B:55:SER:CB	1:B:183:THR:HA	2.52	0.40
1:B:89:GLU:CD	1:B:114:SER:HB3	2.45	0.40
1:B:239:LEU:O	1:B:239:LEU:HG	2.19	0.40
1:A:39:PRO:O	1:A:42:GLU:HG3	2.20	0.40
1:A:127:ASN:HA	1:A:134:GLY:H	1.86	0.40
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.85	0.40
1:B:74:TYR:HB3	1:B:101:ILE:HD13	2.03	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	265/271 (98%)	250 (94%)	14 (5%)	1 (0%)	30	51
1	B	261/271 (96%)	233 (89%)	22 (8%)	6 (2%)	5	9
All	All	526/542 (97%)	483 (92%)	36 (7%)	7 (1%)	9	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	ASP
1	B	65	LEU
1	A	55	SER
1	B	150	LYS
1	B	224	ALA
1	B	235	PRO
1	B	54	GLY

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	216/229 (94%)	196 (91%)	20 (9%)	8	18
1	B	207/229 (90%)	192 (93%)	15 (7%)	13	30
All	All	423/458 (92%)	388 (92%)	35 (8%)	10	23

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	6	LEU
1	A	33	VAL
1	A	53	VAL
1	A	67	ARG
1	A	69	GLN
1	A	79	LEU
1	A	83	GLU
1	A	96	SER

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Mol	Chain	Res	Type
1	A	131	GLU
1	A	142	LEU
1	A	145	LEU
1	A	151	ASN
1	A	157	THR
1	A	169	ARG
1	A	176	LEU
1	A	183	THR
1	A	228	LYS
1	A	234	LEU
1	A	250	HIS
1	B	3	THR
1	B	6	LEU
1	B	27	PHE
1	B	43	GLU
1	B	79	LEU
1	B	106	SER
1	B	137	GLU
1	B	138	GLU
1	B	141	LEU
1	B	157	THR
1	B	164	LEU
1	B	208	THR
1	B	241	GLN
1	B	250	HIS
1	B	251	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	66	ASN
1	A	69	GLN
1	A	166	GLN
1	A	200	HIS
1	A	215	GLN
1	A	231	HIS
1	A	232	GLN
1	A	250	HIS
1	A	268	HIS
1	B	1	HIS
1	B	9	ASN

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Mol	Chain	Res	Type
1	B	31	GLN
1	B	95	HIS
1	B	151	ASN
1	B	231	HIS
1	B	241	GLN
1	B	250	HIS
1	B	259	GLN

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 ⓘ

6 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	2001	-	5,5,5	0.27	0	5,5,5	0.38	0
3	GOL	A	2002	-	5,5,5	0.23	0	5,5,5	0.30	0
3	GOL	A	2004	-	5,5,5	0.27	0	5,5,5	0.45	0
2	PMS	A	1001	1	7,10,11	0.71	0	11,12,15	1.27	2 (18%)
2	PMS	B	1002	1	7,10,11	0.83	0	11,12,15	1.01	1 (9%)
3	GOL	A	2003	-	5,5,5	0.40	0	5,5,5	0.33	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	2001	-	-	0/4/4/4	-
3	GOL	A	2002	-	-	0/4/4/4	-
3	GOL	A	2004	-	-	0/4/4/4	-
2	PMS	A	1001	1	-	0/4/4/5	0/1/1/1
2	PMS	B	1002	1	-	2/4/4/5	0/1/1/1
3	GOL	A	2003	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	PMS	O2S-S-C	3.13	110.96	105.55
2	B	1002	PMS	O2S-S-C	2.83	110.45	105.55
2	A	1001	PMS	O1S-S-C	2.60	110.04	105.55

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1002	PMS	C1-C-S-O2S
2	B	1002	PMS	C1-C-S-O1S

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	GOL	1	0
3	A	2002	GOL	7	0
3	A	2004	GOL	10	0
2	A	1001	PMS	4	0

5.7 Other polymers [i](#)

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	268/271 (98%)	0.17	13 (4%) 35 29	23, 43, 67, 97	1 (0%)
1	B	265/271 (97%)	0.84	32 (12%) 8 6	37, 66, 90, 105	0
All	All	533/542 (98%)	0.51	45 (8%) 17 13	23, 54, 86, 105	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	LEU	6.5
1	A	57	HIS	6.4
1	A	58	SER	4.7
1	B	66	ASN	4.7
1	B	152	TYR	4.6
1	A	56	GLY	4.3
1	A	63	TYR	4.3
1	A	59	ASP	3.8
1	B	67	ARG	3.8
1	B	63	TYR	3.6
1	B	155	TRP	3.4
1	B	153	ILE	3.3
1	B	54	GLY	3.1
1	B	129	PRO	3.0
1	A	55	SER	3.0
1	B	236	TYR	2.9
1	B	133	TYR	2.8
1	B	234	LEU	2.6
1	A	131	GLU	2.6
1	A	16	SER	2.6
1	B	232	GLN	2.6
1	B	198	SER	2.5
1	A	54	GLY	2.5
1	A	154	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	65	LEU	2.4
1	B	57	HIS	2.4
1	B	172	ILE	2.4
1	B	131	GLU	2.4
1	B	233	HIS	2.3
1	B	147	MET	2.3
1	B	56	GLY	2.3
1	B	68	TYR	2.3
1	B	168	ASP	2.3
1	B	55	SER	2.3
1	A	159	PHE	2.3
1	B	64	ASP	2.2
1	B	122	SER	2.2
1	B	112	LEU	2.1
1	B	176	LEU	2.1
1	B	126	LEU	2.1
1	B	132	TYR	2.1
1	B	0	GLY	2.1
1	B	215	GLN	2.0
1	B	181	CYS	2.0
1	A	269	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	A	2003	6/6	0.82	0.11	91,92,92,93	0
3	GOL	A	2002	6/6	0.83	0.23	82,83,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PMS	B	1002	10/11	0.89	0.19	79,81,83,83	0
3	GOL	A	2004	6/6	0.90	0.16	53,56,57,58	0
2	PMS	A	1001	10/11	0.91	0.15	59,60,61,61	0
3	GOL	A	2001	6/6	0.92	0.13	72,73,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.