Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 09:02 AM EST

PDB ID	:	3C66
Title	:	Yeast poly(A) polymerase in complex with Fip1 residues 80-105
Authors	:	Bohm, A.; Meinke, G.
Deposited on	:	2008-02-02
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 (i) 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 (i)) were used in the production of this report:

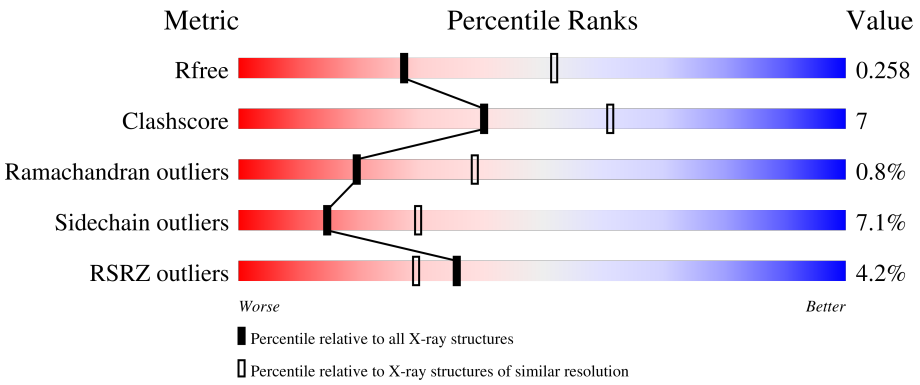
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	537	5% 75% 20% • •
1	B	537	3% 79% 16% • •
2	C	26	4% 77% 15% 8%
2	D	26	4% 58% 31% 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
4	GOL	A	540	-	-	-	X
4	GOL	A	541	-	-	-	X
4	GOL	B	544	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9172 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 Poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	529	4259	2737	728	778	16	0	7	0
1	B	529	4247	2726	716	788	17	0	4	0

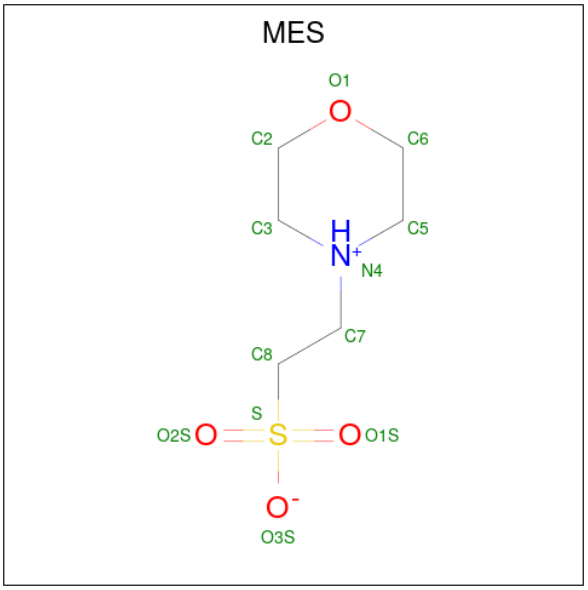
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	527	LYS	-	expression tag	UNP P29468
A	528	ARG	-	expression tag	UNP P29468
A	529	PRO	-	expression tag	UNP P29468
A	530	SER	-	expression tag	UNP P29468
A	531	LYS	-	expression tag	UNP P29468
A	532	LYS	-	expression tag	UNP P29468
A	533	SER	-	expression tag	UNP P29468
A	534	LYS	-	expression tag	UNP P29468
A	535	ARG	-	expression tag	UNP P29468
A	536	LYS	-	expression tag	UNP P29468
A	537	ASN	-	expression tag	UNP P29468
B	527	LYS	-	expression tag	UNP P29468
B	528	ARG	-	expression tag	UNP P29468
B	529	PRO	-	expression tag	UNP P29468
B	530	SER	-	expression tag	UNP P29468
B	531	LYS	-	expression tag	UNP P29468
B	532	LYS	-	expression tag	UNP P29468
B	533	SER	-	expression tag	UNP P29468
B	534	LYS	-	expression tag	UNP P29468
B	535	ARG	-	insertion	UNP P29468
B	536	LYS	-	expression tag	UNP P29468
B	537	ASN	-	expression tag	UNP P29468

- Molecule 2 is a protein called Pre-mRNA polyadenylation factor FIP1.

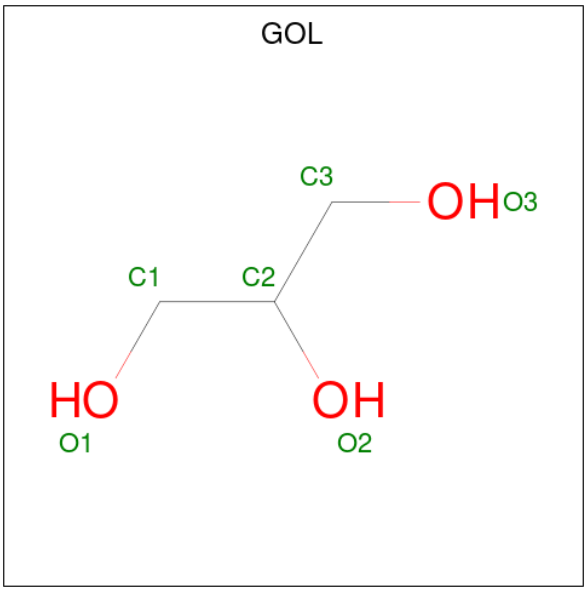
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	24	176	114	28	34	0	0	0
			Total	C	N	O			
2	D	23	178	114	27	37	0	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	B	1	12	6	1	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	110	110	110	0	0

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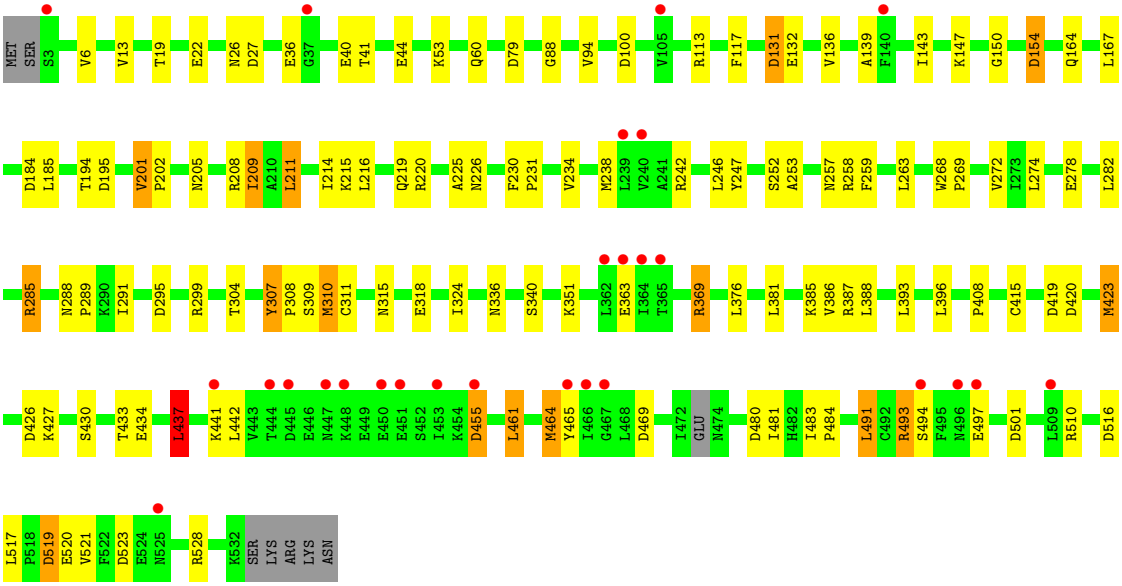
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	92	Total O 92 92	0	0
5	C	6	Total O 6 6	0	0
5	D	2	Total O 2 2	0	0

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.

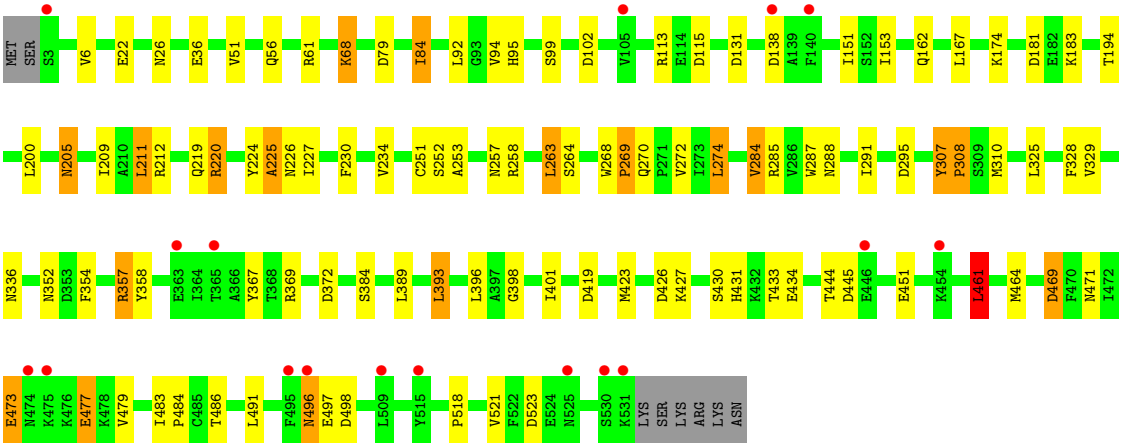
- Molecule 1: Poly(A) polymerase

Chain A:



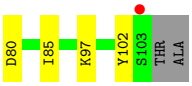
- Molecule 1: Poly(A) polymerase

Chain B:



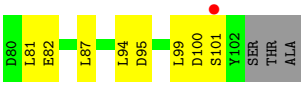
• Molecule 2: Pre-mRNA polyadenylation factor FIP1

Chain C:



• Molecule 2: Pre-mRNA polyadenylation factor FIP1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.12Å 184.21Å 73.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.87 – 2.60 28.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.87-2.60) 99.3 (28.86-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.197 , 0.258 0.196 , 0.258	Depositor DCC
R_{free} test set	2383 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9172	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, MES

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	0.54	1/4371 (0.0%)	0.81	21/5919 (0.4%)
1	B	0.52	0/4354	0.79	14/5905 (0.2%)
2	C	0.84	1/178 (0.6%)	0.90	0/243
2	D	0.43	0/180	1.08	2/245 (0.8%)
All	All	0.54	2/9083 (0.0%)	0.81	37/12312 (0.3%)

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	3
1	B	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	80	ASP	N-CA	8.11	1.62	1.46
1	A	22	GLU	CD-OE1	6.44	1.32	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	LEU	CA-CB-CG	7.60	132.79	115.30
1	A	523	ASP	CB-CG-OD2	7.39	124.95	118.30
1	B	115	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	131	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	469	ASP	CB-CG-OD2	6.60	124.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	426	ASP	CB-CG-OD2	6.40	124.06	118.30
2	D	100	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	195	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	461	LEU	CA-CB-CG	6.23	129.63	115.30
2	D	95	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	419	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	79	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	519	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	419	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	455	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	100	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	154	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	498	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	420	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	131	ASP	CB-CG-OD2	5.91	123.61	118.30
1	A	295	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	79	ASP	CB-CG-OD2	5.79	123.52	118.30
1	A	501	ASP	CB-CG-OD2	5.53	123.27	118.30
1	B	295	ASP	CB-CG-OD2	5.53	123.27	118.30
1	B	102	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	426	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	19	THR	OG1-CB-CG2	-5.25	97.91	110.00
1	A	516	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	461	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	480	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	372[A]	ASP	CB-CG-OD2	5.13	122.91	118.30
1	B	372[B]	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	27	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	469	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	184	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	523	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	TRP	Mainchain,Peptide
1	A	307	TYR	Peptide
1	B	268	TRP	Peptide
1	B	307	TYR	Mainchain,Peptide

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	4259	0	4276	74	0
1	B	4247	0	4228	56	0
2	C	176	0	177	1	0
2	D	178	0	181	1	0
3	A	12	0	12	1	0
3	B	24	0	24	2	0
4	A	30	0	40	5	0
4	B	36	0	48	9	0
5	A	110	0	0	8	0
5	B	92	0	0	2	0
5	C	6	0	0	0	0
5	D	2	0	0	0	0
All	All	9172	0	8986	130	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 7.

All (130) 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:B:310[A]:MET:SD	4:B:544:GOL:H11	2.07	0.94
1:A:285:ARG:HG2	1:A:285:ARG:HH11	1.30	0.93
1:A:167:LEU:HG	4:A:540:GOL:H31	1.55	0.87
1:A:258[B]:ARG:NH1	5:A:601:HOH:O	2.08	0.86
1:B:352:ASN:HD22	1:B:354:PHE:H	1.24	0.81
1:A:26:ASN:HD22	1:A:253:ALA:H	1.35	0.74
1:A:40:GLU:HB2	1:A:44:GLU:HG3	1.69	0.73
1:B:444:THR:HG22	1:B:445:ASP:H	1.53	0.73
1:B:287:TRP:HZ2	4:B:545:GOL:H31	1.53	0.71
1:B:234:VAL:H	4:B:541:GOL:H11	1.57	0.69
1:A:494:SER:HB3	1:A:497:GLU:O	1.92	0.68
1:A:408:PRO:HB3	1:A:464:MET:CE	2.23	0.68
1:B:352:ASN:ND2	1:B:354:PHE:H	1.91	0.68
1:A:26:ASN:HD21	1:A:252:SER:HB2	1.59	0.67
1:B:94:VAL:HG21	1:B:211:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:TRP:CZ2	4:B:545:GOL:H31	2.31	0.64
1:B:269:PRO:HB2	4:B:545:GOL:H2	1.78	0.64
1:A:299:ARG:HE	1:A:318[A]:GLU:CD	2.00	0.64
1:A:517:LEU:O	1:A:528:ARG:NH2	2.22	0.64
1:B:427:LYS:HD3	1:B:433:THR:HB	1.80	0.63
1:A:234:VAL:H	4:A:543:GOL:H31	1.64	0.62
1:A:94:VAL:HG11	1:A:211:LEU:HD13	1.80	0.62
1:B:56:GLN:HE22	1:B:84:ILE:H	1.46	0.62
1:B:257:ASN:HD21	1:B:336:ASN:ND2	1.98	0.61
1:A:289:PRO:HB2	1:B:284:VAL:CG2	2.32	0.60
1:A:315:ASN:HB3	1:A:387:ARG:HD2	1.82	0.59
1:A:408:PRO:HB3	1:A:464:MET:HE2	1.83	0.59
1:A:257:ASN:HD21	1:A:336:ASN:HD21	1.50	0.59
1:A:483:ILE:HB	1:A:484:PRO:HD3	1.84	0.59
1:A:285:ARG:HG2	1:A:285:ARG:NH1	2.08	0.59
1:B:227:ILE:HD11	1:B:384:SER:HA	1.84	0.58
1:A:36:GLU:HG2	1:A:216:LEU:HD21	1.85	0.58
1:A:363:GLU:HG2	1:A:465:TYR:CE2	2.39	0.58
1:B:444:THR:HG22	1:B:445:ASP:N	2.19	0.57
1:A:351:LYS:NZ	5:A:605:HOH:O	2.36	0.57
1:B:205:ASN:H	1:B:205:ASN:HD22	1.52	0.57
1:A:205:ASN:HB3	1:A:208[B]:ARG:HH21	1.71	0.56
1:B:285:ARG:HD3	4:B:544:GOL:O3	2.07	0.55
1:B:205:ASN:H	1:B:205:ASN:ND2	2.05	0.55
1:A:205:ASN:HA	1:A:208[B]:ARG:HE	1.71	0.54
1:B:26:ASN:HD22	1:B:253:ALA:H	1.55	0.54
1:A:289:PRO:HB2	1:B:284:VAL:HG22	1.88	0.54
1:A:147:LYS:HE3	1:A:150:GLY:HA2	1.90	0.53
1:B:357:ARG:HD3	1:B:358:TYR:CE1	2.44	0.53
1:B:26:ASN:HD21	1:B:252:SER:HB2	1.74	0.52
1:A:387:ARG:HB2	5:A:559:HOH:O	2.07	0.52
1:A:282:LEU:HD12	1:A:307:TYR:HE2	1.75	0.51
1:B:401:ILE:HG22	1:B:469:ASP:HB3	1.92	0.51
1:A:88:GLY:H	1:A:194:THR:HG21	1.76	0.51
1:A:53:LYS:HE3	5:A:631:HOH:O	2.10	0.51
1:A:164:GLN:OE1	4:A:541:GOL:H31	2.10	0.51
1:B:398:GLY:H	1:B:471:ASN:HD22	1.57	0.51
1:A:257:ASN:HD21	1:A:336:ASN:ND2	2.08	0.50
1:B:431:HIS:HD2	1:B:434:GLU:OE2	1.93	0.50
1:B:226:ASN:HA	1:B:230:PHE:O	2.11	0.50
1:A:481:ILE:HD11	2:C:85:ILE:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG23	1:A:246:LEU:HD22	1.94	0.50
1:A:285:ARG:HH11	1:A:285:ARG:CG	2.13	0.50
1:B:308:PRO:HG2	4:B:544:GOL:O1	2.11	0.50
1:A:234:VAL:HG23	4:A:543:GOL:H12	1.94	0.49
1:B:307:TYR:CD2	1:B:308:PRO:HD3	2.48	0.49
1:B:483:ILE:N	1:B:484:PRO:HD2	2.28	0.48
1:B:56:GLN:NE2	1:B:84:ILE:H	2.11	0.48
1:B:451:GLU:HB3	5:B:621:HOH:O	2.14	0.48
1:B:200:LEU:HD13	1:B:274:LEU:HB3	1.95	0.48
1:B:209:ILE:HD11	3:B:539:MES:H82	1.96	0.48
1:B:285:ARG:HD3	4:B:544:GOL:C3	2.44	0.48
1:A:387:ARG:HH11	1:A:387:ARG:HG2	1.79	0.48
1:B:518:PRO:O	1:B:521:VAL:HG22	2.13	0.48
1:B:264:SER:HB3	1:B:328:PHE:HB3	1.95	0.48
1:A:136:VAL:HG13	1:A:143:ILE:HG22	1.96	0.47
2:D:87:LEU:HD23	2:D:87:LEU:H	1.79	0.47
1:A:136:VAL:HG13	1:A:143:ILE:CG2	2.43	0.47
1:A:26:ASN:ND2	1:A:253:ALA:H	2.08	0.47
1:A:231:PRO:HD3	1:A:324:ILE:HD11	1.97	0.46
1:A:136:VAL:HG22	1:A:139:ALA:HB2	1.97	0.46
1:A:226:ASN:HA	1:A:230:PHE:O	2.15	0.46
1:A:278:GLU:HG2	5:A:625:HOH:O	2.15	0.46
1:A:299:ARG:NE	1:A:318[A]:GLU:OE2	2.42	0.46
1:A:238:MET:SD	1:A:304:THR:HA	2.56	0.46
1:A:299:ARG:NE	1:A:318[A]:GLU:CD	2.68	0.46
1:A:285:ARG:NH1	1:A:285:ARG:CG	2.78	0.45
1:A:423:MET:HE2	1:A:427:LYS:HB2	1.98	0.45
1:B:51:VAL:HG11	1:B:153:ILE:HD11	1.98	0.45
1:A:143:ILE:HD11	1:A:154:ASP:HB3	1.97	0.45
1:A:385:LYS:O	1:A:386:VAL:C	2.55	0.45
1:A:434:GLU:O	1:A:437:LEU:HD22	2.17	0.45
3:B:539:MES:H51	3:B:539:MES:H81	1.76	0.45
1:B:389:LEU:HG	1:B:393:LEU:HD22	1.99	0.45
1:A:242:ARG:NH1	3:A:538:MES:O2S	2.50	0.44
1:B:22:GLU:HB3	1:B:251:CYS:SG	2.57	0.44
1:B:95:HIS:HB2	1:B:99:SER:OG	2.17	0.44
1:B:224:TYR:O	1:B:225:ALA:HB2	2.16	0.44
1:B:496:ASN:O	1:B:497:GLU:HG3	2.16	0.44
1:A:209:ILE:HG22	1:A:252:SER:CB	2.48	0.44
1:A:369:ARG:NH2	1:A:415:CYS:O	2.51	0.43
1:A:408:PRO:HB3	1:A:464:MET:HE3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HG	1:B:194:THR:HG23	2.01	0.43
1:A:234:VAL:HB	4:A:543:GOL:H31	2.01	0.43
1:A:60:GLN:NE2	5:A:632:HOH:O	2.52	0.43
1:A:202:PRO:HD2	5:A:602:HOH:O	2.19	0.43
1:B:51:VAL:HG21	1:B:151:ILE:HD12	2.00	0.42
1:B:325:LEU:HD23	1:B:325:LEU:HA	1.86	0.42
1:B:288:ASN:ND2	1:B:291:ILE:HD12	2.35	0.42
1:B:211:LEU:O	1:B:212:ARG:C	2.57	0.42
1:A:36:GLU:CD	1:A:220:ARG:HH22	2.22	0.42
1:B:473:GLU:OE2	1:B:477:GLU:CB	2.68	0.42
1:A:427:LYS:HD2	1:A:433:THR:HB	2.02	0.41
1:A:310:MET:HG2	1:A:311:CYS:N	2.34	0.41
1:A:519:ASP:O	1:A:521:VAL:N	2.53	0.41
1:B:234:VAL:HB	4:B:541:GOL:H12	2.01	0.41
1:A:113:ARG:O	1:A:117:PHE:HD1	2.03	0.41
1:A:491:LEU:HD12	1:A:491:LEU:HA	1.91	0.41
1:B:36:GLU:OE1	1:B:220:ARG:NH2	2.51	0.41
1:A:288:ASN:ND2	1:A:291:ILE:HD12	2.36	0.41
1:A:211:LEU:HD22	1:A:215:LYS:HG3	2.03	0.41
1:B:113:ARG:NH2	1:B:183:LYS:HB2	2.35	0.41
1:B:263:LEU:HD12	1:B:263:LEU:HA	1.97	0.41
1:A:491:LEU:C	1:A:493:ARG:H	2.23	0.41
1:A:41:THR:OG1	1:A:44:GLU:HG2	2.21	0.41
1:A:201:VAL:HA	1:A:202:PRO:HD3	1.88	0.41
1:A:387:ARG:HG2	1:A:387:ARG:NH1	2.36	0.41
1:A:510:ARG:HB2	5:A:621:HOH:O	2.21	0.41
1:A:247:TYR:CZ	1:A:258[B]:ARG:HG3	2.56	0.41
1:B:68:LYS:HA	1:B:68:LYS:HE3	2.03	0.40
1:B:162:GLN:NE2	5:B:636:HOH:O	2.53	0.40
1:A:430:SER:O	1:A:434:GLU:HB2	2.21	0.40
1:A:214:ILE:HD13	1:A:214:ILE:HA	1.92	0.40
1:B:367:TYR:CE2	1:B:461:LEU:HD13	2.56	0.40
1:B:473:GLU:OE2	1:B:477:GLU:HB3	2.21	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	532/537 (99%)	508 (96%)	19 (4%)	5 (1%)	17	35
1	B	531/537 (99%)	503 (95%)	25 (5%)	3 (1%)	25	47
2	C	22/26 (85%)	20 (91%)	1 (4%)	1 (4%)	2	3
2	D	21/26 (81%)	21 (100%)	0	0	100	100
All	All	1106/1126 (98%)	1052 (95%)	45 (4%)	9 (1%)	19	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	PRO
1	B	225	ALA
1	A	269	PRO
1	A	225	ALA
1	A	455	ASP
1	A	520	GLU
1	B	269	PRO
1	B	308	PRO
2	C	102	TYR

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	465/479 (97%)	435 (94%)	30 (6%)	17	34
1	B	465/479 (97%)	432 (93%)	33 (7%)	14	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	19/23 (83%)	18 (95%)	1 (5%)	22 45
2	D	21/23 (91%)	16 (76%)	5 (24%)	0 1
All	All	970/1004 (97%)	901 (93%)	69 (7%)	14 29

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	131	ASP
1	A	132	GLU
1	A	185	LEU
1	A	201	VAL
1	A	209	ILE
1	A	211	LEU
1	A	219	GLN
1	A	259	PHE
1	A	263	LEU
1	A	272	VAL
1	A	274	LEU
1	A	285	ARG
1	A	309	SER
1	A	310	MET
1	A	340	SER
1	A	369	ARG
1	A	376	LEU
1	A	381	LEU
1	A	388	LEU
1	A	393	LEU
1	A	396	LEU
1	A	423	MET
1	A	437	LEU
1	A	441	LYS
1	A	442	LEU
1	A	461	LEU
1	A	464	MET
1	A	491	LEU
1	A	493	ARG
1	B	6	VAL
1	B	61	ARG
1	B	68	LYS
1	B	84	ILE

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Mol	Chain	Res	Type
1	B	167	LEU
1	B	174	LYS
1	B	181	ASP
1	B	205	ASN
1	B	211	LEU
1	B	219	GLN
1	B	220	ARG
1	B	258	ARG
1	B	263	LEU
1	B	270[A]	GLN
1	B	270[B]	GLN
1	B	272	VAL
1	B	274	LEU
1	B	284	VAL
1	B	329	VAL
1	B	357	ARG
1	B	369	ARG
1	B	393	LEU
1	B	396	LEU
1	B	423	MET
1	B	430	SER
1	B	461	LEU
1	B	464	MET
1	B	473	GLU
1	B	477	GLU
1	B	479	VAL
1	B	486	THR
1	B	491	LEU
1	B	496	ASN
2	C	97	LYS
2	D	81	LEU
2	D	82	GLU
2	D	94	LEU
2	D	99	LEU
2	D	101	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	60	GLN
1	A	162	GLN

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Mol	Chain	Res	Type
1	A	189	ASN
1	A	249	ASN
1	A	336	ASN
1	A	425	GLN
1	A	431	HIS
1	A	490	ASN
1	B	23	ASN
1	B	26	ASN
1	B	56	GLN
1	B	162	GLN
1	B	205	ASN
1	B	245	GLN
1	B	333	GLN
1	B	336	ASN
1	B	352	ASN
1	B	431	HIS
1	B	438	ASN
1	B	471	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
4	GOL	B	544	-	5,5,5	0.34	0	5,5,5	0.42	0
4	GOL	A	540	-	5,5,5	0.40	0	5,5,5	0.25	0
3	MES	B	538	-	12,12,12	1.99	1 (8%)	14,16,16	7.47	10 (71%)
4	GOL	B	541	-	5,5,5	0.40	0	5,5,5	0.42	0
4	GOL	A	542	-	5,5,5	0.40	0	5,5,5	0.25	0
4	GOL	B	542	-	5,5,5	0.48	0	5,5,5	0.47	0
3	MES	A	538	-	12,12,12	1.96	1 (8%)	14,16,16	7.06	10 (71%)
4	GOL	B	545	-	5,5,5	0.30	0	5,5,5	0.91	0
4	GOL	A	539	-	5,5,5	0.28	0	5,5,5	0.34	0
4	GOL	A	541	-	5,5,5	0.40	0	5,5,5	0.47	0
4	GOL	B	540	-	5,5,5	0.36	0	5,5,5	0.31	0
4	GOL	B	543	-	5,5,5	0.33	0	5,5,5	0.28	0
3	MES	B	539	-	12,12,12	1.99	1 (8%)	14,16,16	7.18	10 (71%)
4	GOL	A	543	-	5,5,5	0.45	0	5,5,5	0.35	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
4	GOL	B	544	-	-	2/4/4/4	-
4	GOL	A	540	-	-	4/4/4/4	-
3	MES	B	538	-	-	1/6/14/14	0/1/1/1
4	GOL	B	541	-	-	2/4/4/4	-
4	GOL	A	542	-	-	2/4/4/4	-
4	GOL	B	542	-	-	4/4/4/4	-
3	MES	A	538	-	-	4/6/14/14	0/1/1/1
4	GOL	B	545	-	-	4/4/4/4	-
4	GOL	A	539	-	-	2/4/4/4	-
4	GOL	A	541	-	-	4/4/4/4	-
4	GOL	B	540	-	-	2/4/4/4	-
4	GOL	B	543	-	-	2/4/4/4	-
3	MES	B	539	-	-	2/6/14/14	0/1/1/1
4	GOL	A	543	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	538	MES	C8-S	-6.41	1.68	1.77
3	B	539	MES	C8-S	-6.38	1.68	1.77
3	A	538	MES	C8-S	-6.31	1.68	1.77

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	538	MES	O1S-S-C8	-18.04	85.20	106.92
3	A	538	MES	O1S-S-C8	-17.91	85.35	106.92
3	B	539	MES	O2S-S-C8	-16.16	87.45	106.92
3	B	538	MES	O2S-S-C8	-15.27	88.53	106.92
3	B	539	MES	O1S-S-C8	-14.06	89.98	106.92
3	B	539	MES	O3S-S-C8	-12.97	84.79	105.77
3	A	538	MES	O3S-S-C8	-11.93	86.47	105.77
3	B	538	MES	O3S-S-C8	-11.20	87.66	105.77
3	A	538	MES	O2S-S-C8	-11.15	93.49	106.92
3	B	539	MES	C5-N4-C3	5.35	120.88	108.83
3	B	538	MES	C5-N4-C3	4.98	120.03	108.83
3	A	538	MES	C6-C5-N4	-4.43	103.38	110.10
3	A	538	MES	C7-N4-C3	4.23	122.06	111.23
3	A	538	MES	C5-N4-C3	4.22	118.32	108.83
3	B	539	MES	C7-N4-C5	3.89	121.19	111.23
3	A	538	MES	O3S-S-O2S	3.73	120.39	111.27
3	B	539	MES	O3S-S-O1S	3.72	120.37	111.27
3	A	538	MES	C2-C3-N4	-3.69	104.51	110.10
3	B	538	MES	C7-N4-C5	3.64	120.55	111.23
3	B	538	MES	O3S-S-O1S	3.53	119.89	111.27
3	B	538	MES	C6-C5-N4	-3.44	104.88	110.10
3	B	538	MES	O3S-S-O2S	3.36	119.48	111.27
3	B	539	MES	O3S-S-O2S	3.36	119.47	111.27
3	A	538	MES	C7-N4-C5	3.27	119.60	111.23
3	B	538	MES	C7-N4-C3	3.20	119.41	111.23
3	A	538	MES	O3S-S-O1S	3.08	118.80	111.27
3	B	538	MES	C2-C3-N4	-2.75	105.93	110.10
3	B	539	MES	C2-C3-N4	-2.68	106.04	110.10
3	B	539	MES	C7-N4-C3	2.61	117.92	111.23
3	B	539	MES	C6-C5-N4	-2.54	106.26	110.10

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	538	MES	C7-C8-S-O1S
3	A	538	MES	C7-C8-S-O3S
3	B	539	MES	C8-C7-N4-C5
4	A	540	GOL	O1-C1-C2-O2
4	A	540	GOL	O1-C1-C2-C3
4	A	540	GOL	C1-C2-C3-O3
4	A	541	GOL	O1-C1-C2-C3
4	A	541	GOL	C1-C2-C3-O3
4	A	542	GOL	O1-C1-C2-C3
4	B	542	GOL	O1-C1-C2-C3
4	B	542	GOL	C1-C2-C3-O3
4	B	543	GOL	O1-C1-C2-O2
4	B	543	GOL	O1-C1-C2-C3
4	B	545	GOL	O1-C1-C2-C3
4	B	545	GOL	C1-C2-C3-O3
4	A	539	GOL	O1-C1-C2-O2
4	B	541	GOL	O2-C2-C3-O3
4	A	539	GOL	O1-C1-C2-C3
4	B	540	GOL	O1-C1-C2-C3
4	B	541	GOL	C1-C2-C3-O3
4	B	544	GOL	C1-C2-C3-O3
4	A	540	GOL	O2-C2-C3-O3
4	A	541	GOL	O1-C1-C2-O2
4	A	541	GOL	O2-C2-C3-O3
4	A	542	GOL	O1-C1-C2-O2
4	B	542	GOL	O1-C1-C2-O2
4	B	542	GOL	O2-C2-C3-O3
4	B	544	GOL	O2-C2-C3-O3
4	B	545	GOL	O1-C1-C2-O2
3	A	538	MES	C8-C7-N4-C5
3	B	539	MES	C8-C7-N4-C3
3	A	538	MES	C7-C8-S-O2S
4	B	545	GOL	O2-C2-C3-O3
4	B	540	GOL	O1-C1-C2-O2
3	B	538	MES	C8-C7-N4-C3

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	544	GOL	4	0
4	A	540	GOL	1	0
4	B	541	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	538	MES	1	0
4	B	545	GOL	3	0
4	A	541	GOL	1	0
3	B	539	MES	2	0
4	A	543	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	529/537 (98%)	0.14	27 (5%)	28	22	37, 53, 68, 90	0
1	B	529/537 (98%)	0.01	17 (3%)	47	40	28, 54, 69, 77	0
2	C	24/26 (92%)	0.22	1 (4%)	36	29	54, 57, 62, 64	0
2	D	23/26 (88%)	0.68	1 (4%)	35	28	63, 71, 77, 77	0
All	All	1105/1126 (98%)	0.09	46 (4%)	36	29	28, 54, 70, 90	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	ASN	5.9
1	A	453	ILE	5.4
1	A	450	GLU	4.5
1	B	3	SER	4.4
1	B	515	TYR	4.2
1	A	445	ASP	4.2
1	A	451	GLU	4.0
2	C	103	SER	3.9
1	A	364	ILE	3.6
1	A	494	SER	3.6
1	A	465	TYR	3.3
1	A	240	VAL	3.2
1	A	140	PHE	3.0
1	A	455	ASP	2.9
1	A	447	ASN	2.9
1	B	138	ASP	2.9
1	B	140	PHE	2.9
1	A	509	LEU	2.8
1	B	525	ASN	2.7
1	A	444	THR	2.7
1	B	454	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	466	ILE	2.5
1	B	105	VAL	2.5
1	A	467	GLY	2.5
1	A	365	THR	2.4
1	A	239	LEU	2.4
1	A	105	VAL	2.4
1	B	530	SER	2.4
1	B	496	ASN	2.4
1	B	495	PHE	2.3
1	B	509	LEU	2.3
1	A	448	LYS	2.3
1	B	475	LYS	2.2
1	A	362	LEU	2.2
1	B	363	GLU	2.2
1	A	525	ASN	2.2
1	A	3	SER	2.2
1	A	37	GLY	2.2
1	A	441	LYS	2.1
1	A	363	GLU	2.1
2	D	101	SER	2.1
1	B	531	LYS	2.1
1	B	365	THR	2.1
1	B	474	ASN	2.1
1	A	497	GLU	2.1
1	B	446	GLU	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 monosaccharides 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
4	GOL	A	541	6/6	0.34	0.58	87,89,89,89	0
4	GOL	A	540	6/6	0.54	0.65	82,85,85,86	0
4	GOL	A	539	6/6	0.67	0.35	78,80,81,81	0
4	GOL	B	540	6/6	0.67	0.32	86,88,88,88	0
4	GOL	A	542	6/6	0.71	0.24	82,83,83,84	0
3	MES	B	539	12/12	0.77	0.32	93,94,97,97	12
4	GOL	B	543	6/6	0.78	0.25	77,78,78,79	0
4	GOL	B	544	6/6	0.81	0.47	86,88,89,89	0
4	GOL	B	542	6/6	0.82	0.44	57,61,61,62	0
3	MES	B	538	12/12	0.84	0.30	85,87,91,91	12
4	GOL	B	545	6/6	0.84	0.55	58,59,60,61	0
4	GOL	A	543	6/6	0.90	0.25	76,78,79,79	0
4	GOL	B	541	6/6	0.90	0.16	69,71,72,72	0
3	MES	A	538	12/12	0.96	0.14	52,54,54,54	12

6.5 Other polymers (i)

There are no such residues in this entry.