Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 08:33 PM GMT

PDB ID	:	4TMR
Title	:	Crystal structure of ternary complex of Plasmodium vivax SHMT with glycine and a novel pyrazolopyran 99S: methyl 5-{3-[(4S)-6-amino-5-cyano-3-methyl-4-(propan-2-yl)-2,4-dihydropyrano[2,3-c]pyrazol-4-yl]-5-cyanophenyl}thiophene-2-carboxylate .
Authors	:	Chitnumsub, P.; Jaruwat, A.; Leartsakulpanich, U.; Witschel, M.C.
Deposited on	:	2014-06-02
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

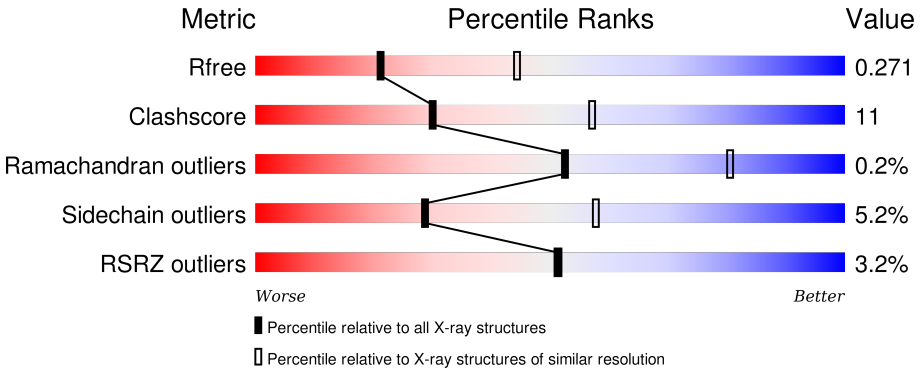
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	442	2% 76% 21%
1	B	442	3% 75% 24%
1	C	442	5% 74% 23%

2 Entry composition

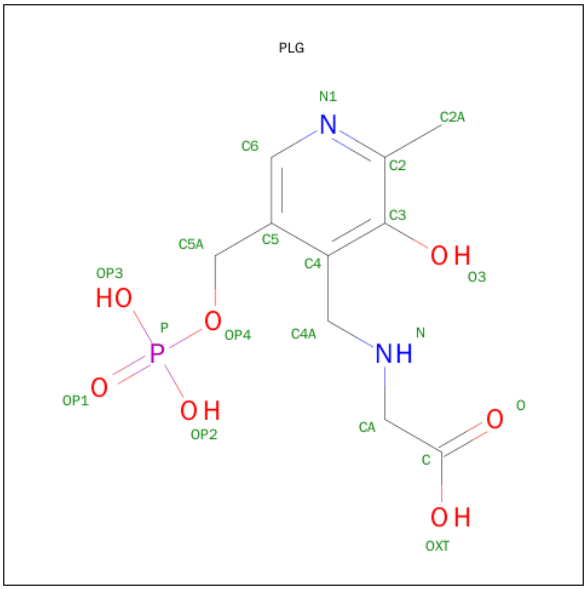
There are 5 unique types of molecules in this entry. The entry contains 10752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine hydroxymethyltransferase, putative.

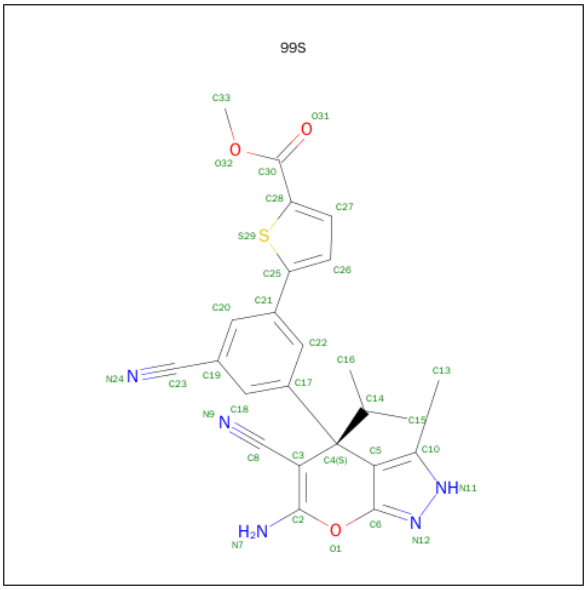
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			
1	B	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			
1	C	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: $C_{10}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is methyl 5-{3-[(4S)-6-amino-5-cyano-3-methyl-4-(propan-2-yl)-2,4-dihydropyrano[2,3-c]pyrazol-4-yl]-5-cyanophenyl}thiophene-2-carboxylate (three-letter code: 99S) (formula: $C_{24}H_{21}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			33	24	5	3	1		
3	B	1	Total	C	N	O	S	0	0
			33	24	5	3	1		
3	C	1	Total	C	N	O	S	0	0
			33	24	5	3	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

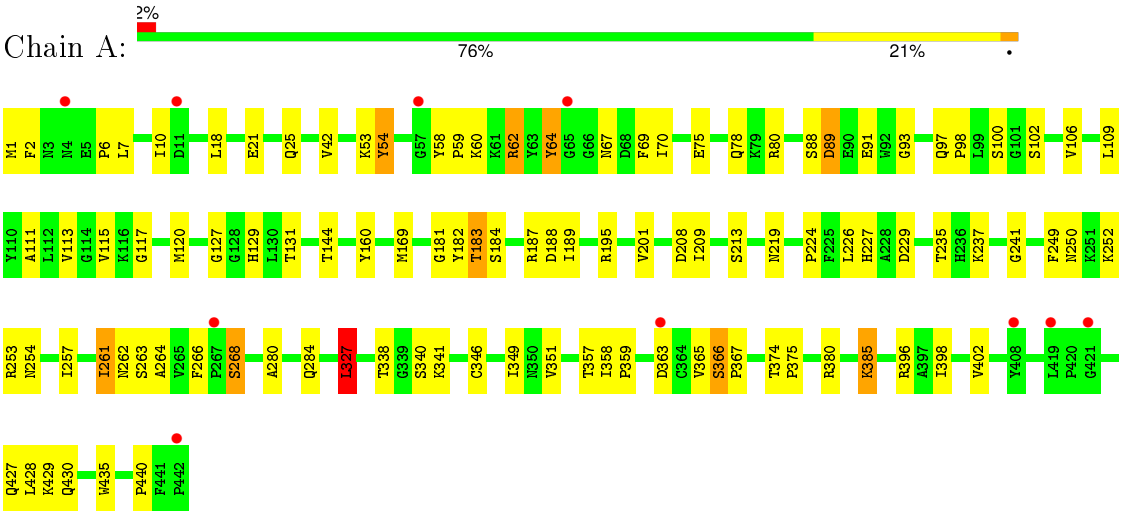
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		
5	B	69	Total	O	0	0
			69	69		
5	C	65	Total	O	0	0
			65	65		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

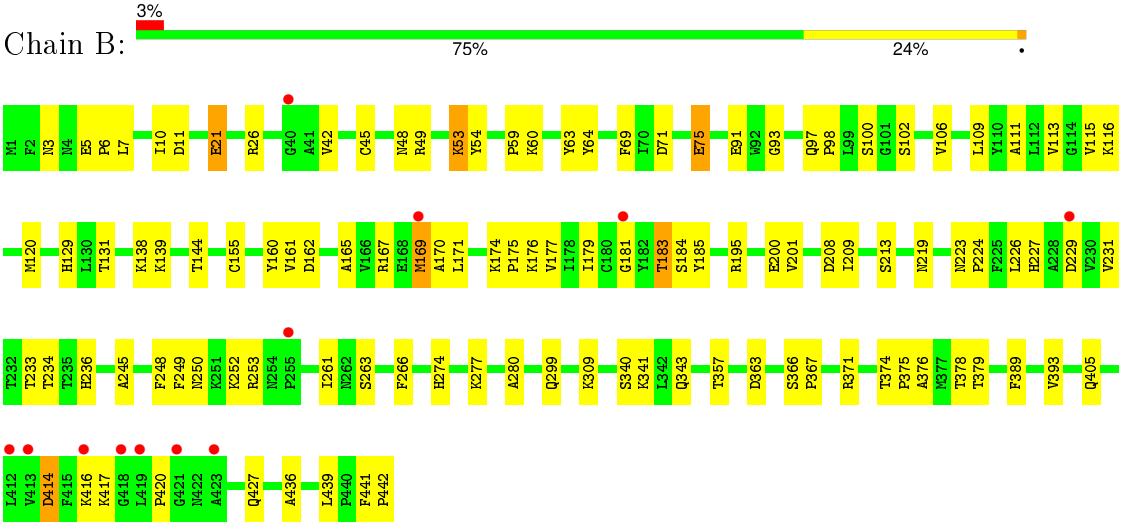
- Molecule 1: Serine hydroxymethyltransferase, putative

Chain A:



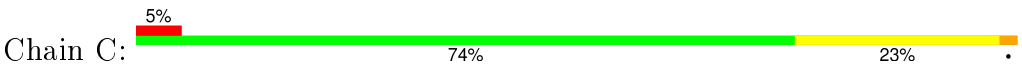
- Molecule 1: Serine hydroxymethyltransferase, putative

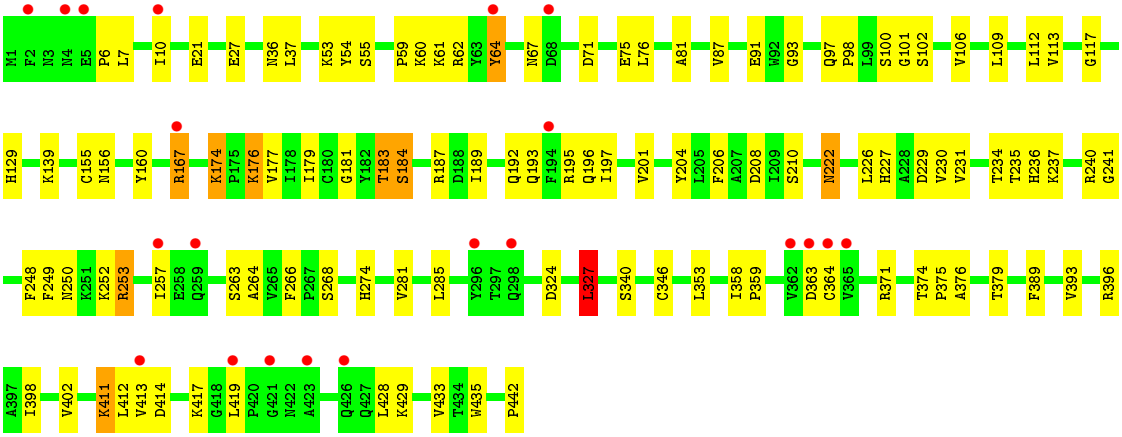
Chain B:



- Molecule 1: Serine hydroxymethyltransferase, putative

Chain C:




M1 F2 N3 N4 E5 P6 L7 I10 E21 E27 N36 L37 K53 Y54 S55 P59 K60 K61 R62 Y63 Y64 N67 D68 D71 E75 L76 A81 V87 E91 W92 G93 Q97 P98 L99 S100 G101 S102 V106 L109 L112 V113 G117
H129 K139 C155 N156 Y160 R167 K174 P175 K176 V177 I178 I179 C180 G181 Y182 T183 S184 R187 D188 I189 Q192 Q193 F194 R195 Q196 I197 V201 Y204 L205 F206 A207 D208 I209 S210 N222 L226 H227 A228 D229 V230 V231 T234 T235 H236 K237 R240 G241
F248 F249 N250 K251 K252 R253 I257 E258 Q259 S263 A264 V265 F266 P267 S268 H274 V281 L285 Y296 T297 Q298 D324 L327 S340 C346 L353 I358 P359 V362 D363 C364 V365 R371 T374 P375 A376 T379 F389 V393 R396
A397 I398 V402 K411 L412 V413 D414 K417 G418 L419 P420 G421 N422 A423 Q426 Q427 L428 K429 V433 T434 W435 P442

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.81Å 58.26Å 234.96Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.70) 92.0 (29.37-2.70)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	23.58 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.278 0.203 , 0.271	Depositor DCC
R_{free} test set	3462 reflections (11.04%)	DCC
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 7.1	EDS
Estimated twinning fraction	0.024 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.023 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.470 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.476 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.018 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 34824 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10752	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PLG, 99S, CL

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	0.51	1/3521 (0.0%)	0.62	1/4754 (0.0%)
1	B	0.51	0/3521	0.64	0/4754
1	C	0.51	1/3521 (0.0%)	0.66	2/4754 (0.0%)
All	All	0.51	2/10563 (0.0%)	0.64	3/14262 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	435	TRP	CD2-CE2	5.13	1.47	1.41
1	A	435	TRP	CD2-CE2	5.09	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	LEU	CA-CB-CG	5.83	128.71	115.30
1	C	327	LEU	CA-CB-CG	5.66	128.31	115.30
1	C	226	LEU	CA-CB-CG	5.03	126.87	115.30

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	3458	0	3477	77	0
1	B	3458	0	3477	85	0
1	C	3458	0	3477	67	0
2	A	20	0	11	3	0
2	B	20	0	10	0	0
2	C	20	0	11	2	0
3	A	33	0	21	4	0
3	B	33	0	21	4	0
3	C	33	0	21	5	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	83	0	0	0	0
5	B	69	0	0	2	0
5	C	65	0	0	3	0
All	All	10752	0	10526	234	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 11.

All (234) 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:385:LYS:H	1:A:385:LYS:HD3	1.14	1.07
3:B:502:99S:H19	3:B:502:99S:H12	1.45	0.98
1:A:385:LYS:N	1:A:385:LYS:HD3	1.79	0.97
3:A:502:99S:H19	3:A:502:99S:H12	1.55	0.87
1:B:91:GLU:HG3	1:B:252:LYS:HD2	1.62	0.81
1:C:6:PRO:O	1:C:10:ILE:HG22	1.81	0.81
1:C:109:LEU:HD21	1:C:179:ILE:HD11	1.61	0.80
1:C:363:ASP:HB3	5:C:645:HOH:O	1.83	0.78
1:B:120:MET:SD	1:B:169:MET:HE3	2.24	0.76
3:C:502:99S:H12	3:C:502:99S:H19	1.71	0.73
1:C:184:SER:HB3	1:C:371:ARG:HD3	1.71	0.73
1:A:6:PRO:O	1:A:10:ILE:HG22	1.88	0.72
1:C:113:VAL:HG12	1:C:176:LYS:HB2	1.71	0.71
1:A:250:ASN:OD1	1:A:253:ARG:HB2	1.90	0.70
1:A:21:GLU:HG2	1:B:69:PHE:HB2	1.75	0.69
1:A:183:THR:HB	2:A:501:PLG:O3	1.93	0.69
1:A:338:THR:HG23	1:A:341:LYS:NZ	2.08	0.68
1:C:263:SER:HA	1:C:266:PHE:O	1.92	0.68
1:A:338:THR:HG23	1:A:341:LYS:HZ2	1.56	0.67
1:A:7:LEU:HA	1:A:10:ILE:CG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:HB3	1:A:64:TYR:O	1.96	0.66
1:B:250:ASN:OD1	1:B:253:ARG:HB2	1.94	0.66
1:B:174:LYS:HE3	1:B:201:VAL:HG13	1.78	0.66
1:A:7:LEU:HA	1:A:10:ILE:HG22	1.79	0.65
1:B:167:ARG:HG2	1:B:171:LEU:HD12	1.80	0.64
1:B:195:ARG:HB2	1:B:227:HIS:HB3	1.78	0.64
3:B:502:99S:C13	3:B:502:99S:H12	2.24	0.63
3:B:502:99S:H19	3:B:502:99S:C16	2.26	0.63
1:C:64:TYR:CD1	1:C:64:TYR:N	2.66	0.62
1:B:184:SER:HB3	1:B:371:ARG:HD3	1.80	0.62
1:A:366:SER:N	1:A:367:PRO:CD	2.62	0.62
1:C:59:PRO:HA	1:C:71:ASP:OD1	2.00	0.62
1:B:299:GLN:HG3	1:B:378:THR:HG23	1.83	0.61
1:B:174:LYS:HG3	1:B:201:VAL:CG1	2.31	0.61
1:B:201:VAL:O	1:B:201:VAL:HG12	2.00	0.61
1:A:237:LYS:HE2	2:A:501:PLG:H4A2	1.83	0.61
1:B:167:ARG:NH1	1:B:200:GLU:OE2	2.34	0.61
1:B:26:ARG:CZ	1:B:441:PHE:HD2	2.14	0.60
1:B:174:LYS:HG3	1:B:201:VAL:HG13	1.82	0.60
1:C:234:THR:HB	1:C:236:HIS:CE1	2.37	0.60
1:B:111:ALA:CB	1:B:261:ILE:HD13	2.31	0.60
1:C:189:ILE:O	1:C:222:ASN:ND2	2.30	0.59
1:C:7:LEU:HA	1:C:10:ILE:CG2	2.32	0.59
1:A:398:ILE:O	1:A:402:VAL:HG23	2.04	0.58
1:A:363:ASP:OD2	1:A:365:VAL:HB	2.03	0.58
1:A:385:LYS:CD	1:A:385:LYS:N	2.53	0.58
1:A:129:HIS:HB2	1:A:183:THR:HG22	1.86	0.57
1:A:93:GLY:HA3	1:A:249:PHE:CE1	2.40	0.57
3:C:502:99S:C16	3:C:502:99S:H19	2.34	0.57
1:B:109:LEU:HD21	1:B:179:ILE:HD11	1.87	0.56
1:A:69:PHE:HB2	1:B:21:GLU:HG2	1.87	0.56
1:B:129:HIS:HA	1:B:183:THR:HG21	1.87	0.56
1:A:358:ILE:HB	1:A:359:PRO:CD	2.36	0.55
1:A:42:VAL:HG13	1:A:280:ALA:HB1	1.89	0.55
1:A:53:LYS:HG2	1:A:70:ILE:HG13	1.89	0.55
1:B:170:ALA:O	1:B:174:LYS:HA	2.06	0.55
1:A:97:GLN:N	1:A:98:PRO:CD	2.70	0.54
3:A:502:99S:C8	3:A:502:99S:C18	2.81	0.54
1:A:131:THR:O	1:A:144:THR:HG21	2.08	0.54
1:C:97:GLN:N	1:C:98:PRO:CD	2.71	0.54
1:A:129:HIS:HA	1:A:183:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLU:HA	1:C:252:LYS:HE3	1.89	0.54
1:A:396:ARG:CZ	1:A:428:LEU:HD13	2.38	0.54
1:B:389:PHE:O	1:B:393:VAL:HG23	2.08	0.54
1:B:414:ASP:OD1	1:B:414:ASP:N	2.40	0.53
1:C:53:LYS:HD2	1:C:67:ASN:OD1	2.07	0.53
1:B:10:ILE:HG23	1:B:11:ASP:H	1.73	0.53
1:C:327:LEU:HD22	1:C:371:ARG:HD2	1.91	0.53
1:C:346:CYS:SG	1:C:353:LEU:HD21	2.48	0.53
1:A:229:ASP:OD1	1:A:253:ARG:HD2	2.09	0.53
1:C:398:ILE:O	1:C:402:VAL:HG23	2.07	0.53
1:A:129:HIS:HB2	1:A:183:THR:CG2	2.39	0.53
1:B:59:PRO:O	1:B:60:LYS:HB2	2.09	0.53
1:A:366:SER:N	1:A:367:PRO:HD2	2.24	0.53
1:B:7:LEU:HA	1:B:10:ILE:HG22	1.91	0.52
1:B:111:ALA:HB3	1:B:261:ILE:HD13	1.91	0.52
1:C:112:LEU:HD11	1:C:230:VAL:HG21	1.92	0.52
1:B:263:SER:HA	1:B:266:PHE:O	2.09	0.52
1:B:131:THR:O	1:B:144:THR:HG21	2.10	0.52
3:A:502:99S:C13	3:A:502:99S:H12	2.34	0.52
1:C:192:GLN:HG3	5:C:607:HOH:O	2.09	0.52
1:B:64:TYR:CD1	1:B:64:TYR:N	2.77	0.52
1:C:358:ILE:HB	1:C:359:PRO:CD	2.40	0.52
1:A:109:LEU:O	1:A:113:VAL:HG22	2.10	0.51
1:A:127:GLY:O	1:A:182:TYR:HB3	2.11	0.51
1:B:113:VAL:HG12	1:B:176:LYS:HE3	1.91	0.51
1:A:263:SER:HA	1:A:266:PHE:O	2.10	0.51
1:B:7:LEU:HA	1:B:10:ILE:CG2	2.41	0.51
1:C:27:GLU:HG2	1:C:433:VAL:HG13	1.93	0.51
3:B:502:99S:C8	3:B:502:99S:C18	2.86	0.51
1:C:187:ARG:HA	1:C:324:ASP:HB2	1.92	0.51
1:C:183:THR:HB	2:C:501:PLG:O3	2.10	0.50
1:C:389:PHE:O	1:C:393:VAL:HG23	2.12	0.50
1:C:174:LYS:HE3	1:C:201:VAL:HG13	1.93	0.50
1:C:237:LYS:HE3	2:C:501:PLG:H4A2	1.93	0.50
1:C:93:GLY:HA3	1:C:249:PHE:CE2	2.46	0.50
1:B:374:THR:N	1:B:375:PRO:CD	2.75	0.50
1:A:209:ILE:HD12	1:A:213:SER:HA	1.94	0.50
1:B:120:MET:SD	1:B:175:PRO:HG3	2.51	0.49
1:A:184:SER:HA	1:A:327:LEU:HD21	1.94	0.49
1:B:6:PRO:O	1:B:10:ILE:HG22	2.12	0.49
1:B:376:ALA:O	1:B:379:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:CZ	1:B:441:PHE:CD2	2.94	0.49
1:A:18:LEU:HB3	1:B:48:ASN:HD21	1.75	0.49
1:A:188:ASP:OD1	1:A:189:ILE:N	2.42	0.49
1:C:264:ALA:HA	1:C:268:SER:HB2	1.94	0.49
1:C:396:ARG:NH2	1:C:428:LEU:HD13	2.28	0.49
1:A:374:THR:N	1:A:375:PRO:HD3	2.27	0.49
1:B:98:PRO:HB2	1:B:245:ALA:HB3	1.95	0.49
1:B:120:MET:SD	1:B:169:MET:CE	3.00	0.49
1:B:195:ARG:HD2	1:B:227:HIS:O	2.13	0.49
1:A:363:ASP:HB3	1:A:365:VAL:O	2.13	0.49
1:C:155:CYS:HB2	1:C:160:TYR:O	2.13	0.48
3:C:502:99S:C18	3:C:502:99S:C8	2.91	0.48
1:B:363:ASP:HB3	5:B:622:HOH:O	2.13	0.48
1:B:374:THR:N	1:B:375:PRO:HD3	2.28	0.48
1:B:416:LYS:O	1:B:420:PRO:HD3	2.12	0.48
1:C:36:ASN:CG	1:C:240:ARG:HG3	2.34	0.48
1:B:155:CYS:HB2	1:B:160:TYR:O	2.13	0.48
1:A:284:GLN:OE1	1:A:284:GLN:HA	2.14	0.47
1:A:62:ARG:HG3	1:A:67:ASN:ND2	2.29	0.47
1:C:181:GLY:HA3	1:C:208:ASP:O	2.14	0.47
1:B:115:VAL:O	1:B:116:LYS:HG2	2.14	0.47
1:C:250:ASN:OD1	1:C:253:ARG:HB2	2.14	0.47
1:B:226:LEU:HB2	1:B:227:HIS:CD2	2.50	0.47
1:B:341:LYS:NZ	5:B:635:HOH:O	2.48	0.47
1:B:102:SER:HA	1:B:131:THR:HG21	1.96	0.47
1:A:129:HIS:CA	1:A:183:THR:HG21	2.44	0.47
1:C:109:LEU:O	1:C:113:VAL:HG22	2.15	0.47
1:A:264:ALA:HA	1:A:268:SER:HB2	1.95	0.47
1:B:97:GLN:N	1:B:98:PRO:CD	2.78	0.47
1:A:75:GLU:HA	1:A:78:GLN:OE1	2.15	0.47
1:B:63:TYR:C	1:B:64:TYR:HD1	2.18	0.47
1:A:64:TYR:HA	1:B:343:GLN:NE2	2.30	0.46
1:B:91:GLU:CG	1:B:252:LYS:HD2	2.37	0.46
1:C:113:VAL:CG1	1:C:177:VAL:HG23	2.45	0.46
1:C:204:TYR:HA	1:C:229:ASP:OD2	2.15	0.46
1:C:235:THR:O	1:C:241:GLY:N	2.47	0.46
1:B:97:GLN:N	1:B:98:PRO:HD2	2.31	0.46
1:A:380:ARG:O	1:A:440:PRO:HD2	2.15	0.46
3:C:502:99S:H9	3:C:502:99S:H7	1.83	0.46
1:B:102:SER:O	1:B:106:VAL:HG23	2.16	0.46
1:B:26:ARG:NH2	1:B:441:PHE:HD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:O	1:A:106:VAL:HG23	2.15	0.46
1:C:197:ILE:O	1:C:201:VAL:HG23	2.15	0.46
1:A:358:ILE:HB	1:A:359:PRO:HD3	1.98	0.45
1:C:167:ARG:HB2	1:C:197:ILE:HD13	1.96	0.45
1:B:209:ILE:HD12	1:B:213:SER:HA	1.97	0.45
1:C:113:VAL:CG1	1:C:176:LYS:HB2	2.44	0.45
1:B:129:HIS:HB2	1:B:183:THR:HG22	1.98	0.45
1:A:2:PHE:CZ	1:B:442:PRO:HD3	2.51	0.45
1:C:59:PRO:O	1:C:60:LYS:HB2	2.17	0.45
1:A:54:TYR:HB3	1:A:64:TYR:HE2	1.82	0.45
1:B:162:ASP:OD2	1:B:165:ALA:HB2	2.17	0.45
1:A:160:TYR:CE1	1:A:187:ARG:HG3	2.51	0.45
1:B:129:HIS:HB2	1:B:183:THR:CG2	2.47	0.45
1:A:201:VAL:O	1:A:201:VAL:HG12	2.16	0.45
1:A:235:THR:O	1:A:241:GLY:N	2.49	0.45
1:A:349:ILE:HA	1:A:429:LYS:HB2	1.98	0.44
1:C:231:VAL:HB	1:C:248:PHE:HB2	1.98	0.44
1:B:48:ASN:OD1	1:B:49:ARG:N	2.50	0.44
1:A:2:PHE:CE1	1:B:442:PRO:HD3	2.52	0.44
1:C:37:LEU:HD22	1:C:442:PRO:HD2	1.99	0.44
1:B:10:ILE:HG23	1:B:11:ASP:N	2.32	0.44
1:A:120:MET:SD	1:A:169:MET:HE2	2.57	0.44
1:A:1:MET:N	1:B:379:THR:O	2.50	0.44
1:C:156:ASN:C	1:C:156:ASN:OD1	2.56	0.44
1:A:226:LEU:HB2	1:A:227:HIS:CD2	2.53	0.44
1:B:209:ILE:HG13	1:B:233:THR:HB	1.99	0.44
1:B:231:VAL:HB	1:B:248:PHE:HB2	1.98	0.44
1:C:174:LYS:HE3	1:C:201:VAL:CG1	2.48	0.43
1:A:346:CYS:HB3	1:A:351:VAL:HB	1.99	0.43
1:A:237:LYS:CE	2:A:501:PLG:H4A2	2.47	0.43
1:A:396:ARG:NH2	1:A:428:LEU:HD13	2.33	0.43
1:A:59:PRO:O	1:A:60:LYS:HB2	2.19	0.43
1:A:374:THR:N	1:A:375:PRO:CD	2.81	0.43
1:A:111:ALA:CB	1:A:261:ILE:HG12	2.48	0.43
1:C:101:GLY:HA3	1:C:234:THR:HG22	1.99	0.43
1:C:112:LEU:HD21	1:C:257:ILE:HD11	2.01	0.43
1:C:6:PRO:C	1:C:10:ILE:HG22	2.38	0.43
1:B:234:THR:HB	1:B:236:HIS:CE1	2.54	0.43
1:A:64:TYR:CD1	1:A:64:TYR:N	2.86	0.43
1:C:37:LEU:O	1:C:240:ARG:HD3	2.19	0.43
1:C:235:THR:O	1:C:241:GLY:CA	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:SER:N	1:B:367:PRO:CD	2.82	0.43
3:A:502:99S:C16	3:A:502:99S:H19	2.40	0.43
1:C:250:ASN:OD1	1:C:253:ARG:CB	2.67	0.43
1:A:346:CYS:HB3	1:A:351:VAL:O	2.19	0.43
1:B:181:GLY:HA3	1:B:208:ASP:O	2.18	0.43
1:C:195:ARG:HB2	1:C:227:HIS:HB3	2.00	0.43
1:C:129:HIS:HA	1:C:183:THR:HG21	2.00	0.42
1:B:3:ASN:OD1	1:B:5:GLU:HB2	2.19	0.42
1:A:58:TYR:OH	1:A:262:ASN:O	2.24	0.42
1:B:229:ASP:OD1	1:B:253:ARG:HD2	2.19	0.42
1:A:120:MET:CE	1:A:169:MET:HE2	2.48	0.42
1:B:223:ASN:HA	1:B:224:PRO:HD2	1.89	0.42
1:C:62:ARG:HB2	1:C:64:TYR:O	2.19	0.42
1:C:210:SER:HB3	1:C:234:THR:OG1	2.20	0.42
3:C:502:99S:H12	3:C:502:99S:C13	2.45	0.42
1:C:396:ARG:CZ	1:C:428:LEU:HD13	2.49	0.42
1:B:93:GLY:HA3	1:B:249:PHE:CE2	2.55	0.42
1:C:376:ALA:O	1:C:379:THR:HB	2.20	0.42
1:B:42:VAL:HG13	1:B:280:ALA:HB1	2.01	0.42
1:A:89:ASP:C	1:A:89:ASP:OD1	2.59	0.41
1:C:113:VAL:HB	1:C:117:GLY:HA3	2.02	0.41
1:A:7:LEU:CA	1:A:10:ILE:HG22	2.47	0.41
1:C:414:ASP:O	1:C:417:LYS:HB3	2.20	0.41
1:C:112:LEU:CD2	1:C:257:ILE:HD11	2.50	0.41
1:B:71:ASP:O	1:B:75:GLU:HB2	2.20	0.41
1:C:76:LEU:HD13	5:C:608:HOH:O	2.20	0.41
1:C:281:VAL:HG12	1:C:285:LEU:HD12	2.02	0.41
1:C:81:ALA:HA	1:C:285:LEU:HD22	2.02	0.41
1:C:374:THR:O	1:C:375:PRO:C	2.59	0.41
1:A:91:GLU:HG3	1:A:252:LYS:HB2	2.02	0.41
1:B:201:VAL:CG1	1:B:201:VAL:O	2.67	0.41
1:A:195:ARG:HB2	1:A:227:HIS:HB3	2.03	0.41
1:C:102:SER:O	1:C:106:VAL:HG23	2.21	0.41
1:A:21:GLU:OE1	1:A:25:GLN:NE2	2.54	0.41
1:B:129:HIS:CA	1:B:183:THR:HG21	2.50	0.41
1:B:53:LYS:HA	1:B:53:LYS:HD2	1.78	0.41
1:B:274:HIS:O	1:B:277:LYS:HB2	2.21	0.41
1:B:161:VAL:HG23	1:B:185:TYR:CZ	2.56	0.40
1:B:109:LEU:O	1:B:113:VAL:HG22	2.21	0.40
1:B:113:VAL:CG1	1:B:177:VAL:HG23	2.51	0.40
1:A:209:ILE:HG21	1:A:224:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:CYS:HB2	1:B:280:ALA:HB2	2.02	0.40
1:A:80:ARG:NH1	1:B:11:ASP:OD2	2.52	0.40
1:B:374:THR:H	1:B:375:PRO:HD3	1.87	0.40
1:B:436:ALA:HA	1:B:439:LEU:HD12	2.04	0.40
1:A:181:GLY:HA3	1:A:208:ASP:O	2.22	0.40
1:C:179:ILE:HA	1:C:206:PHE:HB3	2.03	0.40
1:A:102:SER:HA	1:A:131:THR:HG21	2.04	0.40
1:A:115:VAL:C	1:A:117:GLY:H	2.23	0.40
1:C:411:LYS:CE	1:C:411:LYS:HA	2.52	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	440/442 (100%)	423 (96%)	16 (4%)	1 (0%)	52 80
1	B	440/442 (100%)	421 (96%)	19 (4%)	0	100 100
1	C	440/442 (100%)	413 (94%)	25 (6%)	2 (0%)	34 63
All	All	1320/1326 (100%)	1257 (95%)	60 (4%)	3 (0%)	52 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	SER
1	C	222	ASN
1	C	174	LYS

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	381/381 (100%)	363 (95%)	18 (5%)	32	63
1	B	381/381 (100%)	364 (96%)	17 (4%)	34	65
1	C	381/381 (100%)	356 (93%)	25 (7%)	21	45
All	All	1143/1143 (100%)	1083 (95%)	60 (5%)	29	58

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	TYR
1	A	62	ARG
1	A	64	TYR
1	A	88	SER
1	A	89	ASP
1	A	100	SER
1	A	183	THR
1	A	219	ASN
1	A	254	ASN
1	A	257	ILE
1	A	261	ILE
1	A	268	SER
1	A	327	LEU
1	A	340	SER
1	A	357	THR
1	A	385	LYS
1	A	427	GLN
1	A	430	GLN
1	B	21	GLU
1	B	53	LYS
1	B	54	TYR
1	B	75	GLU
1	B	100	SER
1	B	138	LYS
1	B	139	LYS
1	B	169	MET

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Mol	Chain	Res	Type
1	B	183	THR
1	B	219	ASN
1	B	309	LYS
1	B	340	SER
1	B	357	THR
1	B	405	GLN
1	B	414	ASP
1	B	417	LYS
1	B	427	GLN
1	C	21	GLU
1	C	54	TYR
1	C	55	SER
1	C	61	LYS
1	C	64	TYR
1	C	75	GLU
1	C	87	VAL
1	C	100	SER
1	C	139	LYS
1	C	167	ARG
1	C	176	LYS
1	C	183	THR
1	C	184	SER
1	C	193	GLN
1	C	196	GLN
1	C	253	ARG
1	C	274	HIS
1	C	327	LEU
1	C	340	SER
1	C	364	CYS
1	C	411	LYS
1	C	412	LEU
1	C	413	VAL
1	C	419	LEU
1	C	429	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	HIS
1	B	86	ASN
1	B	227	HIS
1	B	424	GLN

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Mol	Chain	Res	Type
1	C	86	ASN
1	C	227	HIS
1	C	321	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
2	PLG	A	501	-	17,20,20	1.46	3 (17%)	23,28,28	2.98	9 (39%)
3	99S	A	502	-	27,36,36	2.98	4 (14%)	25,54,54	2.62	5 (20%)
2	PLG	B	501	-	17,20,20	1.51	3 (17%)	23,28,28	2.91	10 (43%)
3	99S	B	502	-	27,36,36	2.94	4 (14%)	25,54,54	2.75	9 (36%)
2	PLG	C	501	-	17,20,20	1.36	1 (5%)	23,28,28	3.00	11 (47%)
3	99S	C	502	-	27,36,36	3.10	5 (18%)	25,54,54	2.41	8 (32%)

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	PLG	A	501	-	-	0/10/12/12	0/1/1/1
3	99S	A	502	-	-	0/22/46/46	0/4/4/4
2	PLG	B	501	-	-	0/10/12/12	0/1/1/1
3	99S	B	502	-	-	0/22/46/46	0/4/4/4
2	PLG	C	501	-	-	0/10/12/12	0/1/1/1
3	99S	C	502	-	-	0/22/46/46	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	99S	C8-C3	-11.53	1.27	1.42
3	A	502	99S	C8-C3	-11.45	1.27	1.42
3	B	502	99S	C8-C3	-10.48	1.28	1.42
3	B	502	99S	C19-C23	-6.85	1.27	1.44
3	A	502	99S	C19-C23	-6.55	1.28	1.44
3	C	502	99S	C19-C23	-6.43	1.28	1.44
2	B	501	PLG	C4A-N	-4.19	1.26	1.45
2	A	501	PLG	C4A-N	-4.15	1.26	1.45
2	C	501	PLG	C4A-N	-4.00	1.27	1.45
2	B	501	PLG	C3-C2	-2.61	1.39	1.40
2	A	501	PLG	C4A-C4	-2.42	1.49	1.51
2	B	501	PLG	C4A-C4	-2.20	1.49	1.51
2	A	501	PLG	C3-C2	-2.18	1.39	1.40
3	C	502	99S	O1-C6	-2.05	1.35	1.37
3	A	502	99S	O32-C30	4.92	1.45	1.33
3	A	502	99S	O1-C2	5.36	1.44	1.36
3	B	502	99S	O32-C30	5.70	1.46	1.33
3	C	502	99S	O32-C30	5.70	1.46	1.33
3	B	502	99S	O1-C2	5.73	1.45	1.36
3	C	502	99S	O1-C2	6.08	1.45	1.36

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	99S	C3-C2-N7	-8.49	120.83	127.72
3	B	502	99S	C3-C2-N7	-8.08	121.17	127.72
3	C	502	99S	C3-C2-N7	-7.44	121.68	127.72
3	A	502	99S	C33-O32-C30	-3.37	108.91	115.84
3	B	502	99S	C18-C19-C23	-3.04	115.66	119.51
3	C	502	99S	C33-O32-C30	-3.02	109.63	115.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	99S	C33-O32-C30	-2.88	109.92	115.84
2	C	501	PLG	C5-C6-N1	-2.83	118.95	123.86
2	A	501	PLG	C5-C6-N1	-2.77	119.05	123.86
2	A	501	PLG	OP4-P-OP1	-2.69	100.31	107.14
2	B	501	PLG	OP2-P-OP4	-2.59	99.11	106.56
2	A	501	PLG	C5A-C5-C4	-2.50	117.06	121.89
2	C	501	PLG	C5A-C5-C4	-2.48	117.10	121.89
2	B	501	PLG	C5A-C5-C4	-2.41	117.24	121.89
2	C	501	PLG	OP4-P-OP1	-2.29	101.30	107.14
2	B	501	PLG	C2A-C2-C3	-2.22	118.36	121.04
3	C	502	99S	C20-C21-C25	-2.21	116.58	120.21
3	C	502	99S	C13-C10-N11	2.10	124.43	119.73
2	B	501	PLG	C4A-C4-C5	2.10	121.58	119.71
3	C	502	99S	C8-C3-C2	2.12	120.45	118.00
2	C	501	PLG	C4A-C4-C5	2.16	121.63	119.71
2	C	501	PLG	C-CA-N	2.17	115.37	111.66
2	B	501	PLG	C6-C5-C4	2.22	119.75	118.09
3	B	502	99S	C6-O1-C2	2.23	120.08	118.60
3	C	502	99S	C20-C21-C22	2.25	121.76	118.29
2	B	501	PLG	OP3-P-OP2	2.26	115.98	107.38
3	B	502	99S	C20-C21-C22	2.26	121.77	118.29
3	A	502	99S	O32-C30-C28	2.27	116.31	112.42
3	C	502	99S	C5-C4-C3	2.33	109.23	104.56
3	A	502	99S	C13-C10-N11	2.37	125.04	119.73
2	A	501	PLG	OP3-P-OP2	2.39	116.49	107.38
3	B	502	99S	C13-C10-N11	2.41	125.12	119.73
2	B	501	PLG	C-CA-N	2.45	115.84	111.66
2	A	501	PLG	O3-C3-C2	2.46	121.94	117.66
2	C	501	PLG	OP3-P-OP1	2.66	119.13	110.58
3	B	502	99S	C20-C19-C23	2.72	122.94	119.51
2	C	501	PLG	C4-C4A-N	3.02	116.81	111.66
3	B	502	99S	C5-C4-C3	3.06	110.70	104.56
2	C	501	PLG	O3-C3-C2	3.11	123.07	117.66
2	A	501	PLG	C4-C4A-N	3.13	117.00	111.66
2	A	501	PLG	C6-C5-C4	3.45	120.67	118.09
2	B	501	PLG	C4-C4A-N	3.58	117.78	111.66
2	C	501	PLG	C6-C5-C4	4.07	121.13	118.09
2	A	501	PLG	CA-N-C4A	6.13	124.59	112.03
2	B	501	PLG	CA-N-C4A	6.42	125.17	112.03
2	C	501	PLG	CA-N-C4A	6.74	125.83	112.03
3	C	502	99S	O1-C2-N7	6.92	115.42	110.13
3	B	502	99S	O1-C2-N7	7.73	116.03	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	99S	O1-C2-N7	7.96	116.21	110.13
2	C	501	PLG	OP4-C5A-C5	9.02	123.90	108.99
2	B	501	PLG	OP4-C5A-C5	9.24	124.27	108.99
2	A	501	PLG	OP4-C5A-C5	9.52	124.74	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLG	3	0
3	A	502	99S	4	0
3	B	502	99S	4	0
2	C	501	PLG	2	0
3	C	502	99S	5	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, 95^{th} 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	442/442 (100%)	0.30	10 (2%)	64	64	22, 31, 41, 51	0
1	B	442/442 (100%)	0.38	12 (2%)	58	58	23, 32, 42, 49	0
1	C	442/442 (100%)	0.39	21 (4%)	34	33	19, 32, 48, 64	0
All	All	1326/1326 (100%)	0.36	43 (3%)	51	51	19, 32, 44, 64	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	364	CYS	4.9
1	B	421	GLY	4.6
1	A	421	GLY	4.2
1	B	416	LYS	3.5
1	C	259	GLN	3.4
1	C	64	TYR	3.4
1	B	169	MET	3.4
1	C	167	ARG	3.2
1	B	419	LEU	3.0
1	B	423	ALA	3.0
1	C	421	GLY	3.0
1	B	181	GLY	2.9
1	C	419	LEU	2.9
1	C	2	PHE	2.9
1	C	296	TYR	2.8
1	B	40	GLY	2.8
1	A	419	LEU	2.7
1	B	255	PRO	2.7
1	C	423	ALA	2.7
1	C	365	VAL	2.7
1	C	194	PHE	2.6
1	C	298	GLN	2.6
1	C	68	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	363	ASP	2.6
1	C	5	GLU	2.5
1	C	426	GLN	2.5
1	A	11	ASP	2.5
1	B	229	ASP	2.5
1	C	4	ASN	2.5
1	B	413	VAL	2.4
1	B	412	LEU	2.4
1	A	65	GLY	2.4
1	A	4	ASN	2.3
1	C	257	ILE	2.2
1	A	267	PRO	2.2
1	C	413	VAL	2.2
1	C	362	VAL	2.1
1	A	57	GLY	2.1
1	B	418	GLY	2.1
1	A	442	PRO	2.1
1	C	363	ASP	2.1
1	A	408	TYR	2.1
1	C	10	ILE	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	99S	A	502	33/33	0.88	0.24	1.29	37,39,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	99S	C	502	33/33	0.88	0.24	0.51	34,39,46,47	0
3	99S	B	502	33/33	0.90	0.23	0.24	33,38,43,44	0
2	PLG	C	501	20/20	0.93	0.19	-0.24	22,23,24,25	0
2	PLG	A	501	20/20	0.95	0.16	-0.89	25,27,29,30	0
2	PLG	B	501	20/20	0.95	0.16	-1.16	22,24,25,26	0
4	CL	B	503	1/1	0.84	0.14	-3.78	33,33,33,33	0
4	CL	C	503	1/1	0.81	0.16	-	33,33,33,33	1

6.5 Other polymers

There are no such residues in this entry.