Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:58 am BST

PDB ID	:	4R5Z
Title	:	Crystal structure of Rv3772 encoded aminotransferase
Authors	:	Nasir, N.; Anant, A.; Vyas, R.; Biswal, B.K.
Deposited on	:	2014-08-22
Resolution	:	1.95 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 following versions of software and data (see references ⓘ) were used in the production of this report:

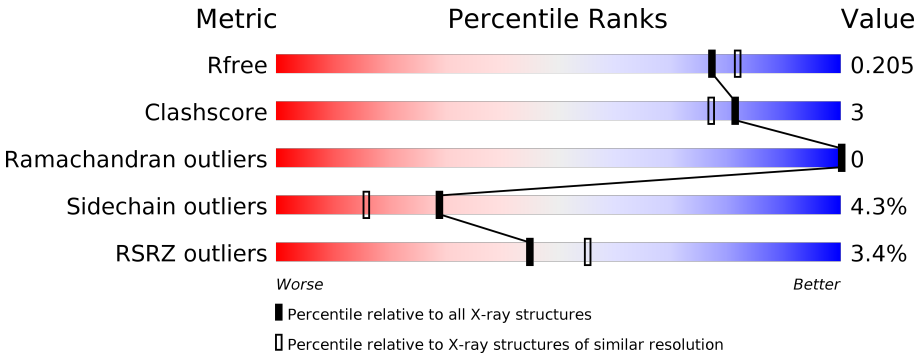
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	367	2% 88% 8%
1	B	367	3% 87% 8%
1	C	367	4% 89% 7%
1	D	367	4% 87% 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PMP	C	402	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12296 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 Putative phenylalanine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	4	0
			2706	1722	483	495	6			
1	B	353	Total	C	N	O	S	0	1	0
			2691	1710	481	494	6			
1	C	353	Total	C	N	O	S	0	1	0
			2691	1710	481	494	6			
1	D	353	Total	C	N	O	S	0	1	0
			2689	1709	479	495	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP I6Y4H4
A	1	VAL	-	EXPRESSION TAG	UNP I6Y4H4
A	354	LYS	-	EXPRESSION TAG	UNP I6Y4H4
A	355	LEU	-	EXPRESSION TAG	UNP I6Y4H4
A	356	ALA	-	EXPRESSION TAG	UNP I6Y4H4
A	357	ALA	-	EXPRESSION TAG	UNP I6Y4H4
A	358	ALA	-	EXPRESSION TAG	UNP I6Y4H4
A	359	LEU	-	EXPRESSION TAG	UNP I6Y4H4
A	360	GLU	-	EXPRESSION TAG	UNP I6Y4H4
A	361	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	362	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	363	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	364	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	365	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	366	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	0	MET	-	EXPRESSION TAG	UNP I6Y4H4
B	1	VAL	-	EXPRESSION TAG	UNP I6Y4H4
B	354	LYS	-	EXPRESSION TAG	UNP I6Y4H4
B	355	LEU	-	EXPRESSION TAG	UNP I6Y4H4
B	356	ALA	-	EXPRESSION TAG	UNP I6Y4H4
B	357	ALA	-	EXPRESSION TAG	UNP I6Y4H4

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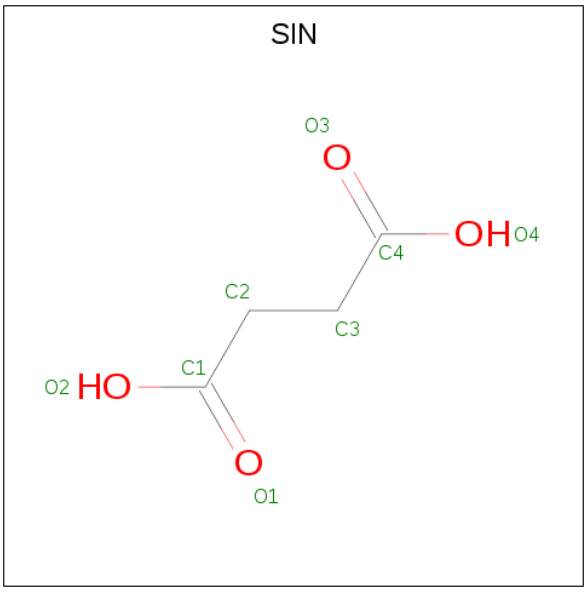
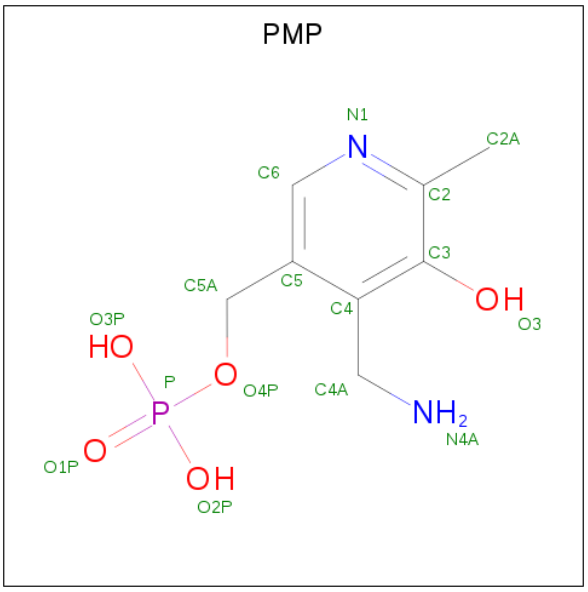
Chain	Residue	Modelled	Actual	Comment	Reference
B	358	ALA	-	EXPRESSION TAG	UNP I6Y4H4
B	359	LEU	-	EXPRESSION TAG	UNP I6Y4H4
B	360	GLU	-	EXPRESSION TAG	UNP I6Y4H4
B	361	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	362	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	363	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	364	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	365	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	366	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	0	MET	-	EXPRESSION TAG	UNP I6Y4H4
C	1	VAL	-	EXPRESSION TAG	UNP I6Y4H4
C	354	LYS	-	EXPRESSION TAG	UNP I6Y4H4
C	355	LEU	-	EXPRESSION TAG	UNP I6Y4H4
C	356	ALA	-	EXPRESSION TAG	UNP I6Y4H4
C	357	ALA	-	EXPRESSION TAG	UNP I6Y4H4
C	358	ALA	-	EXPRESSION TAG	UNP I6Y4H4
C	359	LEU	-	EXPRESSION TAG	UNP I6Y4H4
C	360	GLU	-	EXPRESSION TAG	UNP I6Y4H4
C	361	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	362	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	363	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	364	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	365	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	366	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	0	MET	-	EXPRESSION TAG	UNP I6Y4H4
D	1	VAL	-	EXPRESSION TAG	UNP I6Y4H4
D	354	LYS	-	EXPRESSION TAG	UNP I6Y4H4
D	355	LEU	-	EXPRESSION TAG	UNP I6Y4H4
D	356	ALA	-	EXPRESSION TAG	UNP I6Y4H4
D	357	ALA	-	EXPRESSION TAG	UNP I6Y4H4
D	358	ALA	-	EXPRESSION TAG	UNP I6Y4H4
D	359	LEU	-	EXPRESSION TAG	UNP I6Y4H4
D	360	GLU	-	EXPRESSION TAG	UNP I6Y4H4
D	361	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	362	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	363	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	364	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	365	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	366	HIS	-	EXPRESSION TAG	UNP I6Y4H4

- Molecule 2 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



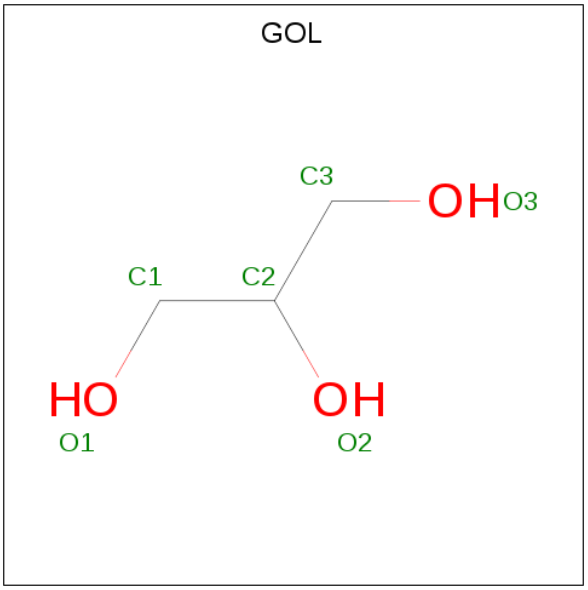
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 4 4	0	0
2	B	1	Total C O 8 4 4	0	0
2	C	1	Total C O 8 4 4	0	0
2	D	1	Total C O 8 4 4	0	0

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

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



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

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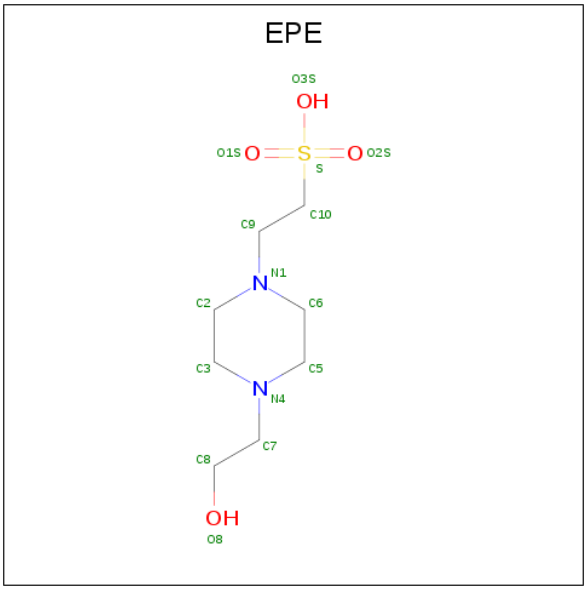
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

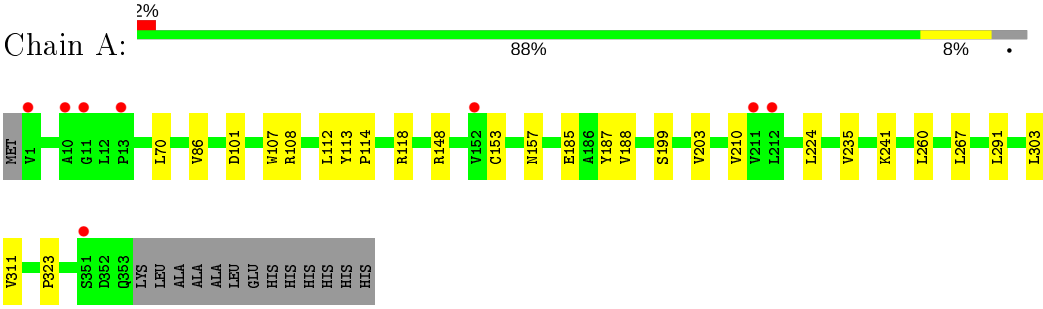
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	354	Total	O	0	0
			354	354		
6	B	302	Total	O	0	0
			302	302		
6	C	281	Total	O	0	0
			281	281		
6	D	306	Total	O	0	0
			306	306		

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 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.

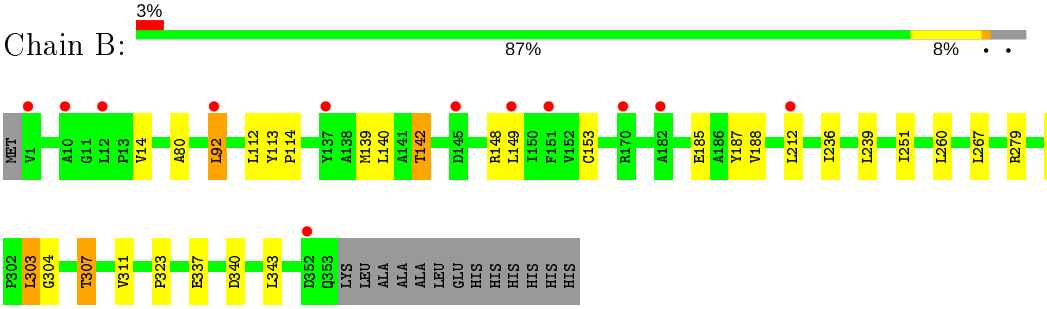
- Molecule 1: Putative phenylalanine aminotransferase

Chain A:



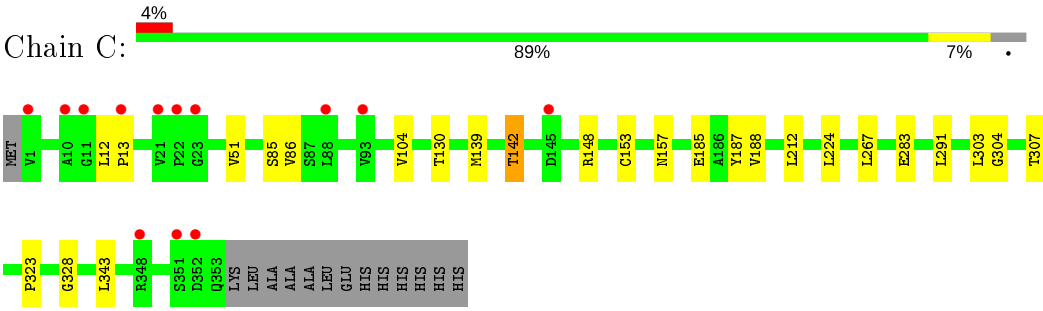
- Molecule 1: Putative phenylalanine aminotransferase

Chain B:



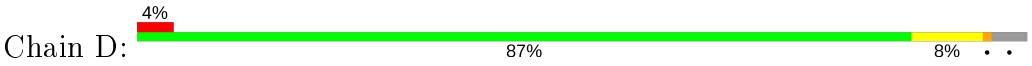
- Molecule 1: Putative phenylalanine aminotransferase

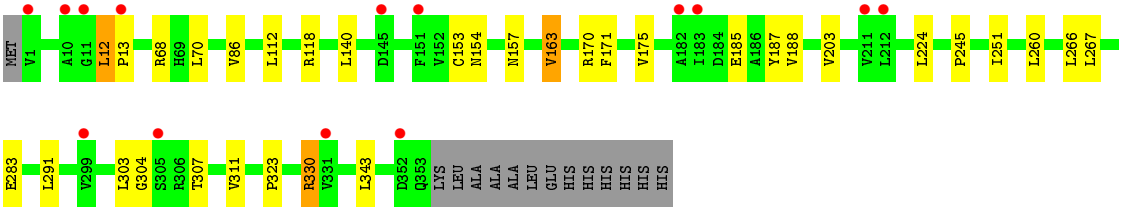
Chain C:



- Molecule 1: Putative phenylalanine aminotransferase

Chain D:




MET V1 A10 G11 L12 P13 R68 H69 L70 V86 L112 R118 L140 D145 F151 V152 C153 N154 N157 V163 R170 F171 V175 A182 I183 D184 E185 A186 Y187 V188 V203 V211 L212 L224 P245 I251 L260 L266 L267
E283 L291 V299 L303 G304 S305 R306 T307 V311 P323 R330 V331 L343 D352 Q353 LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	256.92Å 77.56Å 117.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.41 – 1.95 27.41 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.6 (27.41-1.95) 96.6 (27.41-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.203 0.184 , 0.205	Depositor DCC
R_{free} test set	8361 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12296	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EPE, PMP, SIN

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	0.33	0/2779	0.59	0/3805
1	B	0.32	0/2754	0.58	0/3770
1	C	0.31	0/2754	0.56	0/3770
1	D	0.31	0/2752	0.59	1/3768 (0.0%)
All	All	0.32	0/11039	0.58	1/15113 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	330	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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	2706	0	2733	15	0
1	B	2691	0	2710	15	0
1	C	2691	0	2710	14	0
1	D	2689	0	2705	14	0
2	A	8	0	4	0	0
2	B	8	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8	0	4	1	0
2	D	8	0	4	1	0
3	A	16	0	10	4	0
3	B	16	0	10	3	0
3	C	16	0	10	7	0
3	D	16	0	10	5	0
4	A	36	0	48	1	0
4	B	36	0	48	1	0
4	C	24	0	32	1	0
4	D	24	0	32	0	0
5	A	15	0	18	0	0
5	B	15	0	18	0	0
5	C	15	0	18	0	0
5	D	15	0	18	0	0
6	A	354	0	0	0	0
6	B	302	0	0	0	0
6	C	281	0	0	1	0
6	D	306	0	0	1	0
All	All	12296	0	11146	58	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 3.

All (58) 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:304:GLY:O	1:B:307:THR:HG23	1.81	0.79
1:A:304:GLY:O	1:A:307:THR:HG23	1.83	0.79
1:C:187:TYR:OH	3:C:402:PMP:N4A	2.20	0.73
1:B:92:LEU:HD13	1:B:239:LEU:HD21	1.70	0.71
1:D:154:ASN:HD21	1:D:163:VAL:H	1.41	0.67
1:C:224:LEU:HD21	1:D:251:ILE:HD12	1.76	0.66
1:C:157:ASN:ND2	3:C:402:PMP:O3	2.32	0.60
1:D:311:VAL:HG21	1:D:323:PRO:HB3	1.84	0.59
1:C:139:MET:O	1:C:142:THR:HG22	2.03	0.59
1:A:210[B]:VAL:HG21	1:A:235:VAL:HG11	1.85	0.58
1:B:279:ARG:NH2	1:B:340:ASP:OD1	2.31	0.57
1:A:86:VAL:HG13	3:A:402:PMP:H5A2	1.86	0.57
1:C:311:VAL:HG21	1:C:323:PRO:HB3	1.86	0.57
1:B:139:MET:O	1:B:142:THR:HG22	2.06	0.56
1:B:290:THR:HG22	4:B:408:GOL:H32	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TYR:OH	3:A:402:PMP:N4A	2.39	0.55
1:B:311:VAL:HG21	1:B:323:PRO:HB3	1.89	0.54
1:A:210[B]:VAL:CG2	1:A:235:VAL:HG11	2.38	0.53
1:D:187:TYR:OH	3:D:402:PMP:N4A	2.43	0.52
2:C:401:SIN:O1	3:C:402:PMP:N4A	2.43	0.50
1:A:101:ASP:HB3	1:A:148:ARG:HG3	1.94	0.50
1:B:153:CYS:SG	3:B:402:PMP:C2A	3.01	0.49
1:C:51:VAL:HG21	1:D:224:LEU:HD12	1.95	0.49
1:D:185:GLU:HB3	1:D:188:VAL:HB	1.95	0.49
1:C:86:VAL:HG13	3:C:402:PMP:H5A2	1.96	0.48
1:A:157:ASN:ND2	3:A:402:PMP:O3	2.39	0.47
1:D:86:VAL:HG13	3:D:402:PMP:H5A2	1.97	0.46
1:C:185:GLU:HB3	1:C:188:VAL:HB	1.97	0.46
1:A:311:VAL:HG21	1:A:323:PRO:HB3	1.97	0.46
1:C:85:SER:OG	3:C:402:PMP:H6	2.15	0.46
1:C:153:CYS:SG	3:C:402:PMP:C2A	3.03	0.46
1:B:187:TYR:OH	3:B:402:PMP:N4A	2.49	0.46
1:D:157:ASN:ND2	3:D:402:PMP:O3	2.46	0.45
1:B:185:GLU:HB3	1:B:188:VAL:HB	1.99	0.44
1:A:224:LEU:HD21	1:B:251:ILE:HD12	1.99	0.44
1:C:12:LEU:HD22	1:C:13:PRO:HD2	2.00	0.43
1:B:301:LEU:HB3	1:B:303:LEU:HD13	2.00	0.43
2:D:401:SIN:O3	3:D:402:PMP:N4A	2.51	0.43
3:B:402:PMP:N4A	3:B:402:PMP:O3	2.50	0.43
1:A:153:CYS:SG	3:A:402:PMP:C2A	3.07	0.43
1:B:113:TYR:HB2	1:B:114:PRO:HD3	2.00	0.42
1:D:304:GLY:O	1:D:307:THR:HG23	2.19	0.42
1:C:307:THR:HG21	1:C:328:GLY:CA	2.49	0.42
1:C:304:GLY:O	1:C:307:THR:HG23	2.19	0.42
1:A:107:TRP:CD2	1:A:108:ARG:HA	2.55	0.42
1:A:303:LEU:HD23	4:A:408:GOL:H31	2.00	0.42
3:C:402:PMP:O3	3:C:402:PMP:N4A	2.48	0.42
1:D:12:LEU:HD23	1:D:13:PRO:HD2	2.02	0.41
1:D:153:CYS:SG	3:D:402:PMP:C2A	3.08	0.41
1:C:130:THR:HG22	6:C:696:HOH:O	2.20	0.41
1:B:304:GLY:O	1:B:307:THR:CG2	2.62	0.41
1:A:241:LYS:HG2	1:B:14:VAL:HG21	2.03	0.41
1:A:113:TYR:HB2	1:A:114:PRO:HD3	2.03	0.41
1:B:80:ALA:HB2	1:B:236:ILE:HG23	2.03	0.41
1:D:171:PHE:O	1:D:175:VAL:HG23	2.21	0.40
4:C:404:GOL:C1	1:D:245:PRO:HD3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ARG:NH2	6:D:651:HOH:O	2.54	0.40
1:A:185:GLU:HB3	1:A:188:VAL:HB	2.02	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	355/367 (97%)	347 (98%)	8 (2%)	0	100	100
1	B	352/367 (96%)	345 (98%)	7 (2%)	0	100	100
1	C	352/367 (96%)	343 (97%)	9 (3%)	0	100	100
1	D	352/367 (96%)	342 (97%)	10 (3%)	0	100	100
All	All	1411/1468 (96%)	1377 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/293 (98%)	277 (97%)	9 (3%)	40	28
1	B	283/293 (97%)	269 (95%)	14 (5%)	25	12
1	C	283/293 (97%)	274 (97%)	9 (3%)	39	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	283/293 (97%)	267 (94%)	16 (6%)	20 9
All	All	1135/1172 (97%)	1087 (96%)	48 (4%)	29 17

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	112	LEU
1	A	118	ARG
1	A	199	SER
1	A	203	VAL
1	A	260	LEU
1	A	267	LEU
1	A	291	LEU
1	A	307	THR
1	B	92	LEU
1	B	112	LEU
1	B	140	LEU
1	B	142	THR
1	B	148	ARG
1	B	149	LEU
1	B	212	LEU
1	B	260	LEU
1	B	267	LEU
1	B	291	LEU
1	B	303	LEU
1	B	307	THR
1	B	337	GLU
1	B	343	LEU
1	C	104	VAL
1	C	142	THR
1	C	148	ARG
1	C	212	LEU
1	C	267	LEU
1	C	283	GLU
1	C	291	LEU
1	C	303	LEU
1	C	343	LEU
1	D	12	LEU
1	D	70	LEU
1	D	112	LEU
1	D	118	ARG

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Mol	Chain	Res	Type
1	D	140	LEU
1	D	163	VAL
1	D	170	ARG
1	D	203	VAL
1	D	260	LEU
1	D	266	LEU
1	D	267	LEU
1	D	283	GLU
1	D	291	LEU
1	D	303	LEU
1	D	330	ARG
1	D	343	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	61	GLN
1	A	116	GLN
1	A	156	ASN
1	A	232	HIS
1	B	30	ASN
1	B	116	GLN
1	B	154	ASN
1	B	156	ASN
1	B	232	HIS
1	C	30	ASN
1	C	116	GLN
1	C	154	ASN
1	C	156	ASN
1	C	232	HIS
1	D	30	ASN
1	D	116	GLN
1	D	154	ASN
1	D	156	ASN
1	D	232	HIS

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SIN	A	401	-	1,7,7	0.05	0	2,8,8	0.42	0
2	SIN	C	401	-	1,7,7	0.01	0	2,8,8	0.28	0
3	PMP	C	402	-	16,16,16	2.68	3 (18%)	21,23,23	1.40	3 (14%)
3	PMP	B	402	-	16,16,16	2.79	3 (18%)	21,23,23	1.44	4 (19%)
4	GOL	B	407	-	5,5,5	0.26	0	5,5,5	0.26	0
4	GOL	D	404	-	5,5,5	0.27	0	5,5,5	0.31	0
4	GOL	D	403	-	5,5,5	0.41	0	5,5,5	0.35	0
5	EPE	A	409	-	15,15,15	1.89	1 (6%)	18,20,20	2.69	9 (50%)
4	GOL	C	405	-	5,5,5	0.21	0	5,5,5	0.28	0
4	GOL	B	405	-	5,5,5	0.22	0	5,5,5	0.26	0
4	GOL	D	406	-	5,5,5	0.31	0	5,5,5	0.35	0
3	PMP	D	402	-	16,16,16	2.81	3 (18%)	21,23,23	1.40	4 (19%)
4	GOL	B	404	-	5,5,5	0.28	0	5,5,5	0.25	0
4	GOL	C	406	-	5,5,5	0.19	0	5,5,5	0.25	0
4	GOL	A	406	-	5,5,5	0.28	0	5,5,5	0.18	0
5	EPE	D	407	-	15,15,15	1.94	1 (6%)	18,20,20	2.70	9 (50%)
4	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.26	0
5	EPE	C	407	-	15,15,15	1.97	1 (6%)	18,20,20	2.68	9 (50%)
4	GOL	A	404	-	5,5,5	0.20	0	5,5,5	0.39	0
4	GOL	C	403	-	5,5,5	0.27	0	5,5,5	0.20	0
4	GOL	B	403	-	5,5,5	0.34	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SIN	B	401	-	1,7,7	0.09	0	2,8,8	0.26	0
2	SIN	D	401	-	1,7,7	0.06	0	2,8,8	0.16	0
4	GOL	B	408	-	5,5,5	0.32	0	5,5,5	0.36	0
4	GOL	A	408	-	5,5,5	0.32	0	5,5,5	0.25	0
4	GOL	A	405	-	5,5,5	0.22	0	5,5,5	0.30	0
3	PMP	A	402	-	16,16,16	2.65	3 (18%)	21,23,23	1.41	5 (23%)
4	GOL	C	404	-	5,5,5	0.34	0	5,5,5	0.55	0
4	GOL	A	403	-	5,5,5	0.48	0	5,5,5	0.39	0
4	GOL	A	407	-	5,5,5	0.25	0	5,5,5	0.25	0
4	GOL	D	405	-	5,5,5	0.31	0	5,5,5	0.26	0
5	EPE	B	409	-	15,15,15	1.92	1 (6%)	18,20,20	2.80	10 (55%)

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	SIN	A	401	-	-	0/1/5/5	-
2	SIN	C	401	-	-	0/1/5/5	-
3	PMP	C	402	-	-	2/8/8/8	0/1/1/1
3	PMP	B	402	-	-	5/8/8/8	0/1/1/1
4	GOL	B	407	-	-	2/4/4/4	-
4	GOL	D	404	-	-	3/4/4/4	-
4	GOL	D	403	-	-	2/4/4/4	-
5	EPE	A	409	-	-	5/9/19/19	0/1/1/1
4	GOL	C	405	-	-	1/4/4/4	-
4	GOL	B	405	-	-	0/4/4/4	-
4	GOL	D	406	-	-	2/4/4/4	-
3	PMP	D	402	-	-	7/8/8/8	0/1/1/1
4	GOL	B	404	-	-	2/4/4/4	-
4	GOL	C	406	-	-	2/4/4/4	-
4	GOL	A	406	-	-	1/4/4/4	-
5	EPE	D	407	-	-	6/9/19/19	0/1/1/1
4	GOL	B	406	-	-	1/4/4/4	-
5	EPE	C	407	-	-	2/9/19/19	0/1/1/1
4	GOL	A	404	-	-	0/4/4/4	-
4	GOL	C	403	-	-	0/4/4/4	-
4	GOL	B	403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIN	B	401	-	-	0/1/5/5	-
2	SIN	D	401	-	-	0/1/5/5	-
4	GOL	B	408	-	-	4/4/4/4	-
4	GOL	A	408	-	-	2/4/4/4	-
4	GOL	A	405	-	-	0/4/4/4	-
3	PMP	A	402	-	-	7/8/8/8	0/1/1/1
4	GOL	C	404	-	-	2/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
4	GOL	A	407	-	-	2/4/4/4	-
4	GOL	D	405	-	-	0/4/4/4	-
5	EPE	B	409	-	-	2/9/19/19	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	PMP	C3-C2	7.54	1.48	1.40
3	B	402	PMP	C3-C2	7.44	1.48	1.40
5	C	407	EPE	C10-S	-7.32	1.67	1.77
3	C	402	PMP	C3-C2	7.31	1.48	1.40
5	D	407	EPE	C10-S	-7.24	1.67	1.77
5	B	409	EPE	C10-S	-7.12	1.67	1.77
5	A	409	EPE	C10-S	-7.02	1.67	1.77
3	A	402	PMP	C3-C2	6.87	1.47	1.40
3	B	402	PMP	C5-C4	5.88	1.48	1.40
3	D	402	PMP	C5-C4	5.81	1.48	1.40
3	A	402	PMP	C5-C4	5.76	1.48	1.40
3	C	402	PMP	C5-C4	5.53	1.48	1.40
3	D	402	PMP	C3-C4	5.53	1.48	1.40
3	B	402	PMP	C3-C4	5.47	1.48	1.40
3	A	402	PMP	C3-C4	5.13	1.47	1.40
3	C	402	PMP	C3-C4	4.97	1.47	1.40

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	407	EPE	C5-N4-C3	5.40	120.99	108.83
5	D	407	EPE	C5-N4-C3	5.39	120.95	108.83
5	C	407	EPE	C6-N1-C2	5.31	120.77	108.83
5	D	407	EPE	C6-N1-C2	5.12	120.35	108.83
5	B	409	EPE	C6-N1-C2	5.07	120.24	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	409	EPE	C5-N4-C3	4.99	120.06	108.83
5	A	409	EPE	C6-N1-C2	4.84	119.73	108.83
5	A	409	EPE	C5-N4-C3	4.65	119.30	108.83
5	A	409	EPE	C7-N4-C3	3.80	120.95	111.23
5	B	409	EPE	C9-N1-C6	3.72	120.76	111.23
5	A	409	EPE	C9-N1-C6	3.69	120.67	111.23
5	D	407	EPE	C9-N1-C2	3.61	120.46	111.23
5	C	407	EPE	C7-N4-C5	3.59	120.42	111.23
5	B	409	EPE	C7-N4-C5	3.58	120.40	111.23
5	A	409	EPE	O1S-S-C10	3.53	111.17	106.92
5	D	407	EPE	C7-N4-C5	3.36	119.84	111.23
5	A	409	EPE	C7-N4-C5	3.32	119.73	111.23
5	B	409	EPE	O1S-S-C10	3.31	110.90	106.92
5	C	407	EPE	C9-N1-C6	3.29	119.64	111.23
5	C	407	EPE	C9-N1-C2	3.26	119.58	111.23
5	A	409	EPE	C9-N1-C2	3.26	119.57	111.23
5	B	409	EPE	C7-N4-C3	3.25	119.54	111.23
5	D	407	EPE	O1S-S-C10	3.14	110.70	106.92
5	D	407	EPE	C7-N4-C3	3.12	119.21	111.23
5	D	407	EPE	C9-N1-C6	3.11	119.18	111.23
5	B	409	EPE	C2-C3-N4	-3.08	104.31	110.64
3	C	402	PMP	C3-C4-C5	-3.08	115.77	118.72
5	B	409	EPE	C9-N1-C2	3.04	119.00	111.23
5	C	407	EPE	C7-N4-C3	2.88	118.59	111.23
3	A	402	PMP	C3-C4-C5	-2.73	116.10	118.72
5	C	407	EPE	O1S-S-C10	2.70	110.17	106.92
3	D	402	PMP	C6-C5-C4	2.64	119.99	118.12
3	B	402	PMP	C6-N1-C2	2.59	123.97	119.17
5	C	407	EPE	O3S-S-C10	2.57	109.92	105.77
3	B	402	PMP	O3P-P-O2P	2.54	117.34	107.64
3	B	402	PMP	C6-C5-C4	2.52	119.90	118.12
5	D	407	EPE	O3S-S-C10	2.51	109.82	105.77
3	A	402	PMP	C6-C5-C4	2.50	119.89	118.12
3	D	402	PMP	C3-C4-C5	-2.49	116.33	118.72
3	B	402	PMP	C3-C4-C5	-2.40	116.41	118.72
3	C	402	PMP	C6-C5-C4	2.29	119.74	118.12
5	A	409	EPE	O2S-S-C10	2.29	109.67	106.92
5	B	409	EPE	C3-C2-N1	-2.27	105.98	110.64
3	D	402	PMP	C6-N1-C2	2.27	123.37	119.17
3	C	402	PMP	O3P-P-O2P	2.27	116.31	107.64
5	B	409	EPE	O2S-S-C10	2.25	109.63	106.92
3	A	402	PMP	O3P-P-O4P	-2.23	100.81	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	PMP	O3P-P-O2P	2.19	116.02	107.64
3	A	402	PMP	C6-N1-C2	2.15	123.15	119.17
5	A	409	EPE	C5-C6-N1	-2.10	106.33	110.64
3	D	402	PMP	O3P-P-O2P	2.10	115.64	107.64
5	D	407	EPE	C3-C2-N1	-2.05	106.44	110.64
5	C	407	EPE	O2S-S-C10	2.03	109.36	106.92

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	PMP	C5A-O4P-P-O1P
3	B	402	PMP	C5A-O4P-P-O2P
3	B	402	PMP	C5A-O4P-P-O3P
4	D	404	GOL	C1-C2-C3-O3
5	A	409	EPE	C9-C10-S-O1S
3	D	402	PMP	C5A-O4P-P-O1P
3	D	402	PMP	C5A-O4P-P-O2P
3	D	402	PMP	C5A-O4P-P-O3P
4	B	404	GOL	C1-C2-C3-O3
4	B	404	GOL	O2-C2-C3-O3
5	D	407	EPE	C9-C10-S-O1S
4	B	408	GOL	O1-C1-C2-C3
3	A	402	PMP	C3-C4-C4A-N4A
3	A	402	PMP	C5-C4-C4A-N4A
3	A	402	PMP	C5A-O4P-P-O1P
3	A	402	PMP	C5A-O4P-P-O2P
3	A	402	PMP	C5A-O4P-P-O3P
4	C	404	GOL	C1-C2-C3-O3
4	C	404	GOL	O2-C2-C3-O3
3	C	402	PMP	C3-C4-C4A-N4A
3	B	402	PMP	C3-C4-C4A-N4A
3	D	402	PMP	C3-C4-C4A-N4A
5	D	407	EPE	N4-C7-C8-O8
5	D	407	EPE	C9-C10-S-O3S
4	D	404	GOL	O1-C1-C2-C3
4	D	403	GOL	O1-C1-C2-C3
4	D	406	GOL	O1-C1-C2-C3
4	C	406	GOL	C1-C2-C3-O3
4	B	403	GOL	O1-C1-C2-C3
4	B	408	GOL	C1-C2-C3-O3
4	A	408	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	403	GOL	O1-C1-C2-C3
4	A	407	GOL	O1-C1-C2-C3
3	C	402	PMP	C5-C4-C4A-N4A
3	B	402	PMP	C5-C4-C4A-N4A
3	D	402	PMP	C5-C4-C4A-N4A
4	D	404	GOL	O2-C2-C3-O3
4	C	406	GOL	O2-C2-C3-O3
4	B	408	GOL	O1-C1-C2-O2
4	A	407	GOL	O1-C1-C2-O2
4	D	406	GOL	O1-C1-C2-O2
4	A	408	GOL	O1-C1-C2-O2
5	A	409	EPE	C8-C7-N4-C5
5	A	409	EPE	C10-C9-N1-C6
5	D	407	EPE	C10-C9-N1-C6
4	B	407	GOL	O1-C1-C2-O2
3	D	402	PMP	C4-C5-C5A-O4P
3	A	402	PMP	C4-C5-C5A-O4P
5	D	407	EPE	C8-C7-N4-C3
5	A	409	EPE	C9-C10-S-O2S
5	D	407	EPE	C9-C10-S-O2S
5	B	409	EPE	C8-C7-N4-C5
4	B	408	GOL	O2-C2-C3-O3
5	C	407	EPE	N4-C7-C8-O8
5	C	407	EPE	C10-C9-N1-C6
5	B	409	EPE	C10-C9-N1-C6
4	B	406	GOL	O2-C2-C3-O3
3	D	402	PMP	C6-C5-C5A-O4P
3	A	402	PMP	C6-C5-C5A-O4P
4	C	405	GOL	O1-C1-C2-C3
4	B	403	GOL	O1-C1-C2-O2
4	A	403	GOL	O1-C1-C2-O2
5	A	409	EPE	C9-C10-S-O3S
4	D	403	GOL	O1-C1-C2-O2
4	B	407	GOL	O1-C1-C2-C3
4	A	406	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	SIN	1	0
3	C	402	PMP	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	PMP	3	0
3	D	402	PMP	5	0
2	D	401	SIN	1	0
4	B	408	GOL	1	0
4	A	408	GOL	1	0
3	A	402	PMP	4	0
4	C	404	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	353/367 (96%)	-0.06	8 (2%) 60 69	18, 25, 36, 57	0
1	B	353/367 (96%)	0.02	12 (3%) 45 55	20, 27, 38, 57	0
1	C	353/367 (96%)	0.06	14 (3%) 38 48	21, 29, 46, 67	0
1	D	353/367 (96%)	0.11	14 (3%) 38 48	23, 30, 42, 59	0
All	All	1412/1468 (96%)	0.03	48 (3%) 45 55	18, 28, 42, 67	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	TYR	5.2
1	C	22	PRO	4.0
1	C	1	VAL	4.0
1	D	1	VAL	3.8
1	C	318	ARG	3.4
1	A	1	VAL	3.0
1	B	149	LEU	3.0
1	B	10	ALA	2.9
1	D	352	ASP	2.8
1	C	352	ASP	2.7
1	C	145	ASP	2.7
1	B	151	PHE	2.7
1	C	10	ALA	2.7
1	C	11	GLY	2.7
1	D	13	PRO	2.6
1	A	10	ALA	2.6
1	D	211	VAL	2.6
1	B	1	VAL	2.6
1	C	351	SER	2.5
1	A	11	GLY	2.5
1	D	212	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	10	ALA	2.4
1	A	211	VAL	2.4
1	D	331	VAL	2.4
1	B	212	LEU	2.4
1	A	152	VAL	2.4
1	A	351	SER	2.3
1	B	12	LEU	2.3
1	B	352	ASP	2.3
1	D	145	ASP	2.3
1	D	151	PHE	2.3
1	B	145	ASP	2.3
1	C	21	VAL	2.3
1	A	212	LEU	2.3
1	B	170	ARG	2.3
1	D	11	GLY	2.2
1	A	13	PRO	2.2
1	C	348	ARG	2.2
1	D	183	ILE	2.1
1	B	92	LEU	2.1
1	C	23	GLY	2.1
1	B	182	ALA	2.1
1	C	93	VAL	2.0
1	D	182	ALA	2.0
1	D	305	SER	2.0
1	C	13	PRO	2.0
1	D	299	VAL	2.0
1	C	88	LEU	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 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. 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	B-factors(Å^2)	Q<0.9
4	GOL	B	408	6/6	0.65	0.31	48,50,51,53	0
4	GOL	A	406	6/6	0.76	0.39	50,59,62,65	0
4	GOL	B	406	6/6	0.80	0.30	59,59,60,61	0
4	GOL	D	406	6/6	0.80	0.33	48,52,53,53	0
4	GOL	A	407	6/6	0.82	0.26	60,61,61,62	0
4	GOL	C	406	6/6	0.83	0.29	73,74,75,76	0
4	GOL	A	408	6/6	0.85	0.26	52,53,54,56	0
4	GOL	B	405	6/6	0.87	0.21	49,51,51,51	0
4	GOL	C	403	6/6	0.88	0.23	46,48,48,49	0
4	GOL	B	404	6/6	0.88	0.16	46,48,49,50	0
4	GOL	B	407	6/6	0.90	0.16	62,62,63,63	0
4	GOL	A	404	6/6	0.90	0.17	37,40,41,42	0
5	EPE	D	407	15/15	0.90	0.26	56,66,68,68	0
4	GOL	D	405	6/6	0.90	0.20	55,56,57,57	0
3	PMP	A	402	16/16	0.91	0.19	29,36,38,38	16
4	GOL	A	403	6/6	0.91	0.12	29,31,32,32	0
4	GOL	D	403	6/6	0.91	0.14	33,35,36,36	0
4	GOL	A	405	6/6	0.91	0.15	41,41,42,42	0
3	PMP	D	402	16/16	0.92	0.20	34,41,43,44	16
3	PMP	B	402	16/16	0.92	0.21	30,39,41,41	16
5	EPE	C	407	15/15	0.92	0.30	51,62,66,66	0
5	EPE	A	409	15/15	0.93	0.27	47,54,57,57	0
4	GOL	C	405	6/6	0.93	0.18	42,45,46,46	0
4	GOL	D	404	6/6	0.93	0.13	43,48,48,49	0
3	PMP	C	402	16/16	0.93	0.18	34,38,41,43	16
5	EPE	B	409	15/15	0.93	0.29	52,61,64,64	0
4	GOL	B	403	6/6	0.94	0.12	27,30,30,30	0
4	GOL	C	404	6/6	0.94	0.13	35,36,37,37	0
2	SIN	D	401	8/8	0.95	0.11	26,28,32,34	0
2	SIN	C	401	8/8	0.96	0.09	30,32,34,37	0
2	SIN	A	401	8/8	0.98	0.07	25,27,30,32	0
2	SIN	B	401	8/8	0.98	0.09	24,27,30,32	0

6.5 Other polymers (i)

There are no such residues in this entry.