



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:48 PM GMT

PDB ID : 2QRY  
Title : Periplasmic thiamin binding protein  
Authors : Ealick, S.E.; Soriano, E.V.  
Deposited on : 2007-07-30  
Resolution : 2.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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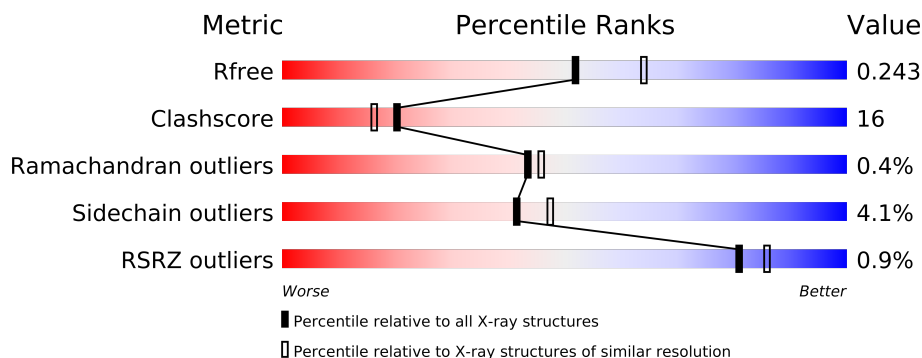
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.25 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))
$R_{free}$	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	330	
1	B	330	
1	C	330	
1	D	330	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	TPS	A	400	-	X
2	TPS	B	400	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10279 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Thiamine-binding periplasmic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	Se	0	0	0
			2395	1546	393	450	2	4			
1	B	309	Total	C	N	O	S	Se	0	0	0
			2412	1554	398	454	2	4			
1	C	318	Total	C	N	O	S	Se	0	0	0
			2470	1590	411	462	2	5			
1	D	310	Total	C	N	O	S	Se	0	0	0
			2414	1556	397	454	2	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	EXPRESSION TAG	UNP P31550
A	-1	GLY	-	EXPRESSION TAG	UNP P31550
A	0	SER	-	EXPRESSION TAG	UNP P31550
A	1	SER	-	EXPRESSION TAG	UNP P31550
A	2	HIS	-	EXPRESSION TAG	UNP P31550
A	3	HIS	-	EXPRESSION TAG	UNP P31550
A	4	HIS	-	EXPRESSION TAG	UNP P31550
A	5	HIS	-	EXPRESSION TAG	UNP P31550
A	6	HIS	-	EXPRESSION TAG	UNP P31550
A	7	HIS	-	EXPRESSION TAG	UNP P31550
A	8	SER	-	EXPRESSION TAG	UNP P31550
A	9	SER	-	EXPRESSION TAG	UNP P31550
A	10	GLY	-	EXPRESSION TAG	UNP P31550
A	11	LEU	-	EXPRESSION TAG	UNP P31550
A	12	VAL	-	EXPRESSION TAG	UNP P31550
A	13	PRO	-	EXPRESSION TAG	UNP P31550
A	14	ARG	-	EXPRESSION TAG	UNP P31550
A	15	GLY	-	EXPRESSION TAG	UNP P31550
A	16	SER	-	EXPRESSION TAG	UNP P31550
A	17	HIS	-	EXPRESSION TAG	UNP P31550
A	18	MSE	-	EXPRESSION TAG	UNP P31550

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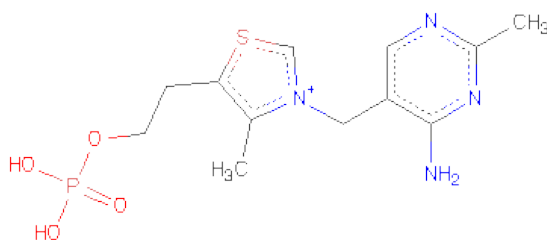
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MSE	-	EXPRESSION TAG	UNP P31550
B	-1	GLY	-	EXPRESSION TAG	UNP P31550
B	0	SER	-	EXPRESSION TAG	UNP P31550
B	1	SER	-	EXPRESSION TAG	UNP P31550
B	2	HIS	-	EXPRESSION TAG	UNP P31550
B	3	HIS	-	EXPRESSION TAG	UNP P31550
B	4	HIS	-	EXPRESSION TAG	UNP P31550
B	5	HIS	-	EXPRESSION TAG	UNP P31550
B	6	HIS	-	EXPRESSION TAG	UNP P31550
B	7	HIS	-	EXPRESSION TAG	UNP P31550
B	8	SER	-	EXPRESSION TAG	UNP P31550
B	9	SER	-	EXPRESSION TAG	UNP P31550
B	10	GLY	-	EXPRESSION TAG	UNP P31550
B	11	LEU	-	EXPRESSION TAG	UNP P31550
B	12	VAL	-	EXPRESSION TAG	UNP P31550
B	13	PRO	-	EXPRESSION TAG	UNP P31550
B	14	ARG	-	EXPRESSION TAG	UNP P31550
B	15	GLY	-	EXPRESSION TAG	UNP P31550
B	16	SER	-	EXPRESSION TAG	UNP P31550
B	17	HIS	-	EXPRESSION TAG	UNP P31550
B	18	MSE	-	EXPRESSION TAG	UNP P31550
C	-2	MSE	-	EXPRESSION TAG	UNP P31550
C	-1	GLY	-	EXPRESSION TAG	UNP P31550
C	0	SER	-	EXPRESSION TAG	UNP P31550
C	1	SER	-	EXPRESSION TAG	UNP P31550
C	2	HIS	-	EXPRESSION TAG	UNP P31550
C	3	HIS	-	EXPRESSION TAG	UNP P31550
C	4	HIS	-	EXPRESSION TAG	UNP P31550
C	5	HIS	-	EXPRESSION TAG	UNP P31550
C	6	HIS	-	EXPRESSION TAG	UNP P31550
C	7	HIS	-	EXPRESSION TAG	UNP P31550
C	8	SER	-	EXPRESSION TAG	UNP P31550
C	9	SER	-	EXPRESSION TAG	UNP P31550
C	10	GLY	-	EXPRESSION TAG	UNP P31550
C	11	LEU	-	EXPRESSION TAG	UNP P31550
C	12	VAL	-	EXPRESSION TAG	UNP P31550
C	13	PRO	-	EXPRESSION TAG	UNP P31550
C	14	ARG	-	EXPRESSION TAG	UNP P31550
C	15	GLY	-	EXPRESSION TAG	UNP P31550
C	16	SER	-	EXPRESSION TAG	UNP P31550
C	17	HIS	-	EXPRESSION TAG	UNP P31550
C	18	MSE	-	EXPRESSION TAG	UNP P31550

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MSE	-	EXPRESSION TAG	UNP P31550
D	-1	GLY	-	EXPRESSION TAG	UNP P31550
D	0	SER	-	EXPRESSION TAG	UNP P31550
D	1	SER	-	EXPRESSION TAG	UNP P31550
D	2	HIS	-	EXPRESSION TAG	UNP P31550
D	3	HIS	-	EXPRESSION TAG	UNP P31550
D	4	HIS	-	EXPRESSION TAG	UNP P31550
D	5	HIS	-	EXPRESSION TAG	UNP P31550
D	6	HIS	-	EXPRESSION TAG	UNP P31550
D	7	HIS	-	EXPRESSION TAG	UNP P31550
D	8	SER	-	EXPRESSION TAG	UNP P31550
D	9	SER	-	EXPRESSION TAG	UNP P31550
D	10	GLY	-	EXPRESSION TAG	UNP P31550
D	11	LEU	-	EXPRESSION TAG	UNP P31550
D	12	VAL	-	EXPRESSION TAG	UNP P31550
D	13	PRO	-	EXPRESSION TAG	UNP P31550
D	14	ARG	-	EXPRESSION TAG	UNP P31550
D	15	GLY	-	EXPRESSION TAG	UNP P31550
D	16	SER	-	EXPRESSION TAG	UNP P31550
D	17	HIS	-	EXPRESSION TAG	UNP P31550
D	18	MSE	-	EXPRESSION TAG	UNP P31550

- Molecule 2 is THIAMIN PHOSPHATE (three-letter code: TPS) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>4</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			22	12	4	4	1	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	0
			22	12	4	4	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			22	12	4	4	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			22	12	4	4	1	1		

- Molecule 3 is water.

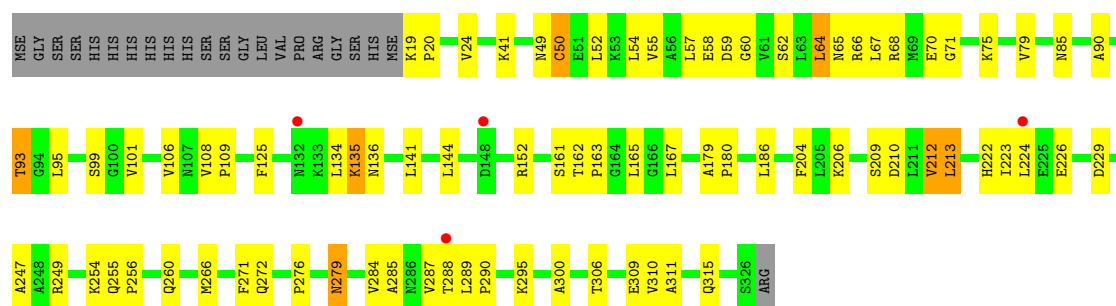
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	138	Total	O	0	0
			138	138		
3	C	127	Total	O	0	0
			127	127		
3	D	132	Total	O	0	0
			132	132		

### 3 Residue-property plots

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.

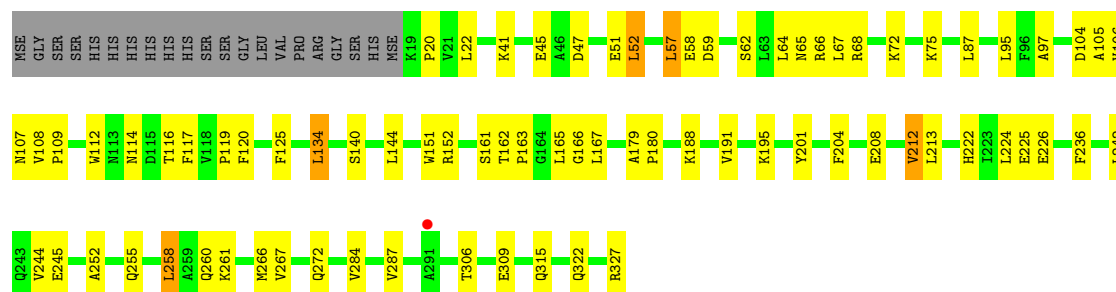
- Molecule 1: Thiamine-binding periplasmic protein

Chain A: 



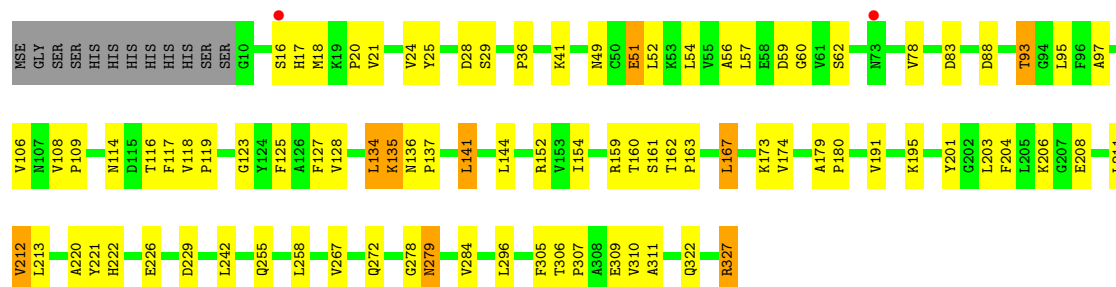
- Molecule 1: Thiamine-binding periplasmic protein

Chain B: 



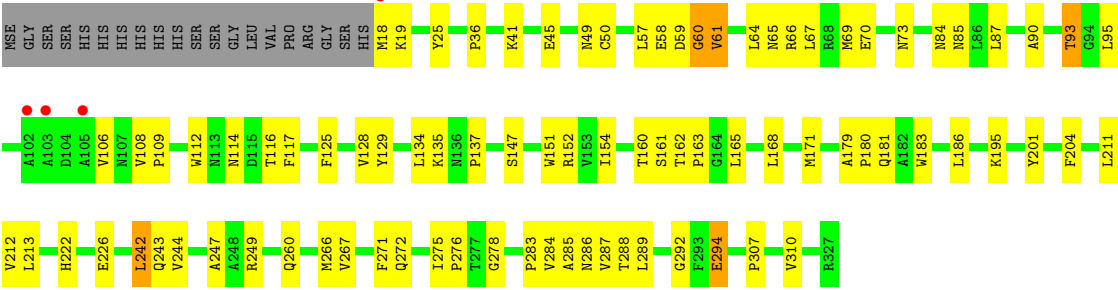
- Molecule 1: Thiamine-binding periplasmic protein

Chain C: 



- Molecule 1: Thiamine-binding periplasmic protein

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.04Å 118.07Å 90.33Å 90.00° 93.74° 90.00°	Depositor
Resolution (Å)	49.39 – 2.25 49.39 – 2.24	Depositor EDS
% Data completeness (in resolution range)	90.1 (49.39-2.25) 89.7 (49.39-2.24)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 2.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.198 , 0.241 0.201 , 0.243	Depositor DCC
$R_{free}$ test set	3076 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 25.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 62014 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: TPS

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	0.34	0/2455	0.59	0/3341
1	B	0.36	0/2472	0.58	0/3363
1	C	0.35	0/2531	0.58	0/3442
1	D	0.35	0/2474	0.59	1/3366 (0.0%)
All	All	0.35	0/9932	0.58	1/13512 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	213	LEU	CA-CB-CG	-5.04	103.71	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2395	0	2345	90	0
1	B	2412	0	2364	68	0
1	C	2470	0	2418	80	0
1	D	2414	0	2364	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	22	0	16	1	0
2	B	22	0	16	2	0
2	C	22	0	16	2	0
2	D	22	0	16	3	0
3	A	103	0	0	5	0
3	B	138	0	0	5	0
3	C	127	0	0	3	0
3	D	132	0	0	3	0
All	All	10279	0	9555	306	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (306) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:LYS:HD3	1:A:135:LYS:H	1.14	1.11
1:A:62:SER:HA	1:A:65:ASN:ND2	1.74	1.02
1:C:135:LYS:HD3	1:C:135:LYS:H	1.26	0.97
1:A:272:GLN:NE2	1:A:284:VAL:H	1.64	0.94
1:C:93:THR:HG23	1:C:95:LEU:HD13	1.49	0.94
1:A:272:GLN:HE22	1:A:284:VAL:H	1.01	0.92
1:D:18:MSE:HG2	1:D:19:LYS:H	1.35	0.92
1:C:272:GLN:HE22	1:C:284:VAL:H	1.18	0.90
1:C:114:ASN:HD22	1:C:116:THR:H	1.20	0.88
1:D:204:PHE:HB2	1:D:212:VAL:HG11	1.56	0.86
1:A:19:LYS:HB3	1:C:221:TYR:OH	1.77	0.85
1:C:59:ASP:HB3	2:C:400:TPS:O2	1.79	0.83
1:A:135:LYS:H	1:A:135:LYS:CD	1.93	0.82
1:A:161:SER:OG	1:A:163:PRO:HD2	1.80	0.81
1:A:135:LYS:HD3	1:A:135:LYS:N	1.92	0.81
1:D:114:ASN:ND2	1:D:117:PHE:H	1.77	0.81
1:C:93:THR:HG22	1:C:95:LEU:H	1.45	0.80
1:D:204:PHE:HB2	1:D:212:VAL:CG1	2.11	0.80
1:C:204:PHE:HB2	1:C:212:VAL:HG11	1.62	0.80
1:C:161:SER:OG	1:C:163:PRO:HD2	1.83	0.79
1:D:106:VAL:HG13	1:D:284:VAL:HG22	1.64	0.78
1:A:93:THR:HG23	1:A:95:LEU:H	1.47	0.78
1:A:167:LEU:HB2	1:A:213:LEU:HD13	1.66	0.78
1:A:152:ARG:HH11	1:A:152:ARG:HG3	1.50	0.77
1:B:75:LYS:NZ	1:B:75:LYS:HB2	1.99	0.77
1:A:67:LEU:HG	1:A:95:LEU:HD23	1.66	0.76
1:A:223:ILE:HD13	1:A:295:LYS:HD3	1.69	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:204:PHE:HB2	1:B:212:VAL:CG1	2.17	0.74
1:C:272:GLN:NE2	1:C:284:VAL:H	1.86	0.74
1:C:327:ARG:HG2	3:C:510:HOH:O	1.86	0.74
1:B:167:LEU:HB2	1:B:213:LEU:HD22	1.69	0.73
1:D:59:ASP:HB3	2:D:400:TPS:O2	1.89	0.73
1:A:247:ALA:HB3	1:A:266:MSE:HE1	1.71	0.73
1:B:272:GLN:HE22	1:B:284:VAL:H	1.36	0.72
1:C:204:PHE:HB2	1:C:212:VAL:CG1	2.18	0.72
1:D:106:VAL:HG13	1:D:284:VAL:CG2	2.20	0.72
1:C:93:THR:CG2	1:C:95:LEU:H	2.02	0.72
1:D:181:GLN:HG3	3:D:480:HOH:O	1.89	0.72
1:A:59:ASP:HB3	2:A:400:TPS:O2	1.91	0.71
1:A:106:VAL:HG13	1:A:284:VAL:CG2	2.21	0.71
1:B:22:LEU:HB2	1:B:258:LEU:HD13	1.73	0.71
1:C:106:VAL:HG13	1:C:284:VAL:CG2	2.20	0.70
1:D:18:MSE:HG2	1:D:19:LYS:N	2.06	0.70
1:C:108:VAL:HG22	1:C:109:PRO:HD2	1.73	0.70
1:D:272:GLN:HE22	1:D:284:VAL:H	1.35	0.70
1:D:114:ASN:HD22	1:D:116:THR:H	1.39	0.69
1:B:152:ARG:HD2	3:B:439:HOH:O	1.90	0.69
1:C:114:ASN:ND2	1:C:116:THR:H	1.90	0.69
1:A:62:SER:HA	1:A:65:ASN:HD22	1.57	0.69
1:D:93:THR:HG23	1:D:95:LEU:H	1.58	0.69
1:D:249:ARG:NH1	1:D:260:GLN:HG3	2.09	0.68
1:C:24:VAL:HG22	1:C:78:VAL:HB	1.75	0.68
1:B:306:THR:OG1	1:B:309:GLU:HG3	1.94	0.68
1:B:272:GLN:NE2	1:B:284:VAL:H	1.92	0.67
1:A:272:GLN:NE2	1:A:284:VAL:N	2.39	0.67
1:C:306:THR:OG1	1:C:309:GLU:HG3	1.96	0.66
1:A:144:LEU:C	1:A:144:LEU:HD23	2.16	0.66
1:A:93:THR:CG2	1:A:95:LEU:H	2.08	0.65
1:D:161:SER:OG	1:D:163:PRO:HD2	1.95	0.65
1:B:204:PHE:HB2	1:B:212:VAL:HG11	1.78	0.65
1:D:114:ASN:ND2	1:D:116:THR:H	1.94	0.65
1:B:161:SER:OG	1:B:163:PRO:HD2	1.96	0.65
1:A:55:VAL:CG1	1:A:57:LEU:HD13	2.27	0.65
1:C:21:VAL:HG22	1:C:51:GLU:HG2	1.76	0.65
1:A:287:VAL:HG22	1:A:288:THR:N	2.12	0.65
1:A:272:GLN:HE22	1:A:284:VAL:N	1.86	0.64
1:C:135:LYS:HD3	1:C:135:LYS:N	2.07	0.64
1:C:201:TYR:OH	1:C:222:HIS:HE1	1.79	0.64
1:A:272:GLN:NE2	1:A:284:VAL:HG12	2.13	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:58:GLU:OE1	1:B:195:LYS:HE2	1.97	0.63
1:A:152:ARG:HG2	1:A:210:ASP:OD2	1.97	0.63
1:C:167:LEU:HG	1:C:213:LEU:HD13	1.79	0.63
1:B:20:PRO:HB2	1:B:255:GLN:HE22	1.64	0.62
1:B:204:PHE:HB2	1:B:212:VAL:HG13	1.81	0.62
1:C:162:THR:OG1	1:C:163:PRO:HD3	1.99	0.62
1:B:59:ASP:HB3	2:B:400:TPS:O2	1.98	0.62
1:D:85:ASN:O	1:D:310:VAL:HG21	1.99	0.62
1:D:272:GLN:NE2	1:D:284:VAL:H	1.97	0.61
1:C:167:LEU:HB2	1:C:213:LEU:HD22	1.80	0.61
1:C:152:ARG:HG3	1:C:152:ARG:HH11	1.64	0.61
1:A:162:THR:OG1	1:A:163:PRO:HD3	1.99	0.61
1:D:201:TYR:OH	1:D:222:HIS:HE1	1.83	0.61
1:D:93:THR:CG2	1:D:95:LEU:H	2.13	0.61
1:C:106:VAL:HG13	1:C:284:VAL:HG22	1.82	0.61
1:D:114:ASN:HD22	1:D:117:PHE:H	1.48	0.60
1:D:272:GLN:HG3	1:D:285:ALA:HB3	1.81	0.60
1:A:204:PHE:HB2	1:A:212:VAL:CG1	2.30	0.60
1:D:18:MSE:CG	1:D:19:LYS:H	2.11	0.60
1:B:106:VAL:HG22	1:B:284:VAL:HG21	1.83	0.60
1:A:106:VAL:HG13	1:A:284:VAL:HG22	1.82	0.60
1:B:106:VAL:HG13	1:B:284:VAL:CG2	2.32	0.60
1:B:57:LEU:HD21	1:B:66:ARG:HD3	1.84	0.60
1:B:188:LYS:HE3	3:B:465:HOH:O	2.00	0.60
1:D:61:VAL:HG22	1:D:160:THR:CA	2.32	0.59
1:D:61:VAL:HG22	1:D:160:THR:HA	1.85	0.59
1:C:272:GLN:HE22	1:C:284:VAL:N	1.97	0.59
1:B:75:LYS:HZ3	1:B:75:LYS:HB2	1.67	0.58
1:A:306:THR:OG1	1:A:309:GLU:HG3	2.04	0.57
1:B:315:GLN:HG3	3:B:471:HOH:O	2.04	0.57
1:C:222:HIS:HD2	1:C:226:GLU:OE1	1.86	0.57
1:C:267:VAL:HG12	1:C:267:VAL:O	2.02	0.57
1:B:224:LEU:HD23	1:B:224:LEU:C	2.24	0.57
1:A:152:ARG:NH1	1:A:152:ARG:HG3	2.18	0.57
1:B:201:TYR:OH	1:B:222:HIS:HE1	1.88	0.56
1:A:55:VAL:HG12	1:A:57:LEU:HD13	1.86	0.56
1:B:144:LEU:C	1:B:144:LEU:HD23	2.26	0.56
1:A:279:ASN:ND2	3:A:402:HOH:O	2.39	0.56
1:C:60:GLY:HA3	1:C:162:THR:HG23	1.88	0.55
1:D:125:PHE:CE1	1:D:163:PRO:HA	2.41	0.55
1:A:90:ALA:O	1:A:93:THR:HG22	2.07	0.55
1:B:114:ASN:HD22	1:B:116:THR:H	1.54	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:LEU:O	1:A:68:ARG:HG3	2.07	0.55
1:C:141:LEU:HD12	1:C:174:VAL:HG21	1.89	0.55
1:A:93:THR:CG2	1:A:95:LEU:HB2	2.36	0.55
1:A:108:VAL:HG13	1:A:109:PRO:HD2	1.87	0.54
1:D:108:VAL:HG22	1:D:109:PRO:HD2	1.89	0.54
1:A:108:VAL:CG2	1:A:284:VAL:HG23	2.36	0.54
1:A:204:PHE:HB2	1:A:212:VAL:HG11	1.88	0.54
1:D:25:TYR:CD2	1:D:57:LEU:HD22	2.42	0.54
1:C:272:GLN:NE2	1:C:284:VAL:N	2.55	0.54
1:A:272:GLN:CD	1:A:284:VAL:HG12	2.29	0.54
1:A:108:VAL:HG23	1:A:284:VAL:HG23	1.89	0.54
1:A:49:ASN:O	1:A:50:CYS:HB3	2.08	0.53
1:D:267:VAL:HG12	1:D:267:VAL:O	2.08	0.53
1:C:135:LYS:H	1:C:135:LYS:CD	2.08	0.53
1:C:167:LEU:HB2	1:C:213:LEU:CD2	2.39	0.53
1:C:41:LYS:HA	1:C:52:LEU:HD23	1.91	0.53
1:C:203:LEU:HB3	1:C:208:GLU:HG3	1.91	0.53
1:C:195:LYS:HE2	1:D:58:GLU:OE1	2.09	0.53
1:A:24:VAL:HB	1:A:54:LEU:HD23	1.90	0.53
1:B:106:VAL:HG13	1:B:284:VAL:HG21	1.90	0.53
1:B:224:LEU:HD22	1:B:225:GLU:OE2	2.09	0.52
1:A:272:GLN:HE21	1:A:285:ALA:H	1.58	0.52
1:B:108:VAL:HG23	1:B:284:VAL:HG23	1.92	0.52
1:A:179:ALA:N	1:A:180:PRO:HD2	2.24	0.52
1:C:307:PRO:O	1:C:310:VAL:HG22	2.09	0.52
1:B:114:ASN:ND2	1:B:117:PHE:H	2.08	0.52
1:D:36:PRO:HD3	1:D:278:GLY:C	2.30	0.52
1:C:134:LEU:HD13	1:C:137:PRO:HB3	1.91	0.52
1:B:272:GLN:NE2	1:B:284:VAL:N	2.57	0.52
1:D:90:ALA:O	1:D:93:THR:HG22	2.10	0.52
1:B:162:THR:OG1	1:B:163:PRO:HD3	2.09	0.51
1:A:55:VAL:HG11	1:A:57:LEU:HD13	1.92	0.51
1:A:249:ARG:HE	1:A:260:GLN:NE2	2.08	0.51
1:C:93:THR:CG2	1:C:95:LEU:HB2	2.41	0.51
1:D:272:GLN:HG3	1:D:285:ALA:CB	2.40	0.51
1:D:162:THR:OG1	1:D:163:PRO:HD3	2.11	0.51
1:D:168:LEU:HD13	1:D:168:LEU:C	2.31	0.51
1:D:87:LEU:HD11	1:D:112:TRP:CH2	2.46	0.50
1:B:107:ASN:H	1:B:284:VAL:HG22	1.75	0.50
1:C:20:PRO:HB2	1:C:255:GLN:NE2	2.26	0.50
1:B:167:LEU:HB2	1:B:213:LEU:CD2	2.41	0.50
1:B:119:PRO:HA	1:B:245:GLU:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:THR:HG23	1:A:95:LEU:N	2.24	0.50
1:B:144:LEU:HD23	1:B:144:LEU:O	2.12	0.50
1:C:106:VAL:HG13	1:C:284:VAL:HG21	1.93	0.49
1:A:161:SER:HG	1:A:163:PRO:HD2	1.75	0.49
1:A:266:MSE:HG3	1:A:271:PHE:CZ	2.47	0.49
1:A:287:VAL:HG22	1:A:288:THR:H	1.75	0.49
1:B:75:LYS:HZ2	1:B:75:LYS:HB2	1.76	0.49
1:B:114:ASN:HD22	1:B:117:PHE:H	1.60	0.49
1:D:275:ILE:HB	1:D:276:PRO:HD3	1.93	0.49
1:D:204:PHE:HB2	1:D:212:VAL:HG13	1.91	0.49
1:A:41:LYS:HA	1:A:52:LEU:HD23	1.93	0.49
1:C:62:SER:OG	1:C:160:THR:HG22	2.13	0.49
1:B:140:SER:HA	1:B:236:PHE:HB3	1.95	0.49
1:B:161:SER:HA	2:B:400:TPS:O2	2.13	0.49
1:C:322:GLN:NE2	3:C:410:HOH:O	2.45	0.49
1:C:154:ILE:HB	1:C:212:VAL:HG12	1.95	0.49
1:C:206:LYS:HG3	1:C:208:GLU:HG2	1.95	0.49
1:A:66:ARG:O	1:A:70:GLU:HG3	2.12	0.49
1:D:70:GLU:O	1:D:73:ASN:HB2	2.13	0.49
1:A:180:PRO:HG2	3:A:413:HOH:O	2.13	0.48
1:C:114:ASN:ND2	1:C:117:PHE:H	2.11	0.48
1:A:249:ARG:HD3	1:A:260:GLN:HG2	1.96	0.48
1:C:125:PHE:CE1	1:C:163:PRO:HA	2.49	0.48
1:D:60:GLY:N	2:D:400:TPS:O2	2.47	0.48
1:A:167:LEU:HB2	1:A:213:LEU:CD1	2.41	0.48
1:C:203:LEU:HA	1:C:206:LYS:HG2	1.94	0.48
1:B:65:ASN:ND2	3:B:448:HOH:O	2.47	0.48
1:C:161:SER:HA	2:C:400:TPS:O2	2.13	0.47
1:A:125:PHE:CE1	1:A:163:PRO:HA	2.49	0.47
3:C:448:HOH:O	1:D:195:LYS:HE2	2.14	0.47
1:B:67:LEU:HG	1:B:95:LEU:HD23	1.95	0.47
1:D:307:PRO:O	1:D:310:VAL:HG22	2.15	0.47
1:D:292:GLY:N	1:D:294:GLU:OE1	2.25	0.47
1:B:179:ALA:HB3	1:B:180:PRO:HD3	1.97	0.47
1:C:36:PRO:HD3	1:C:278:GLY:O	2.14	0.47
1:A:206:LYS:HG3	3:A:469:HOH:O	2.14	0.47
1:A:287:VAL:CG2	1:A:288:THR:N	2.77	0.47
1:B:114:ASN:ND2	1:B:116:THR:H	2.13	0.47
1:B:64:LEU:O	1:B:68:ARG:HG3	2.15	0.47
1:A:75:LYS:HE2	1:B:208:GLU:OE2	2.15	0.46
1:B:242:LEU:HD11	1:B:244:VAL:HG23	1.97	0.46
1:A:300:ALA:HB3	3:A:422:HOH:O	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:24:VAL:HB	1:C:54:LEU:HD23	1.97	0.46
1:D:168:LEU:HD13	1:D:168:LEU:O	2.15	0.46
1:D:66:ARG:O	1:D:70:GLU:HG3	2.16	0.46
1:B:105:ALA:HB1	1:B:267:VAL:HG11	1.97	0.46
1:A:95:LEU:HD11	1:B:327:ARG:HG3	1.98	0.46
1:D:60:GLY:HA3	1:D:162:THR:HG23	1.97	0.46
1:C:28:ASP:HA	1:C:56:ALA:HB1	1.96	0.46
1:A:67:LEU:HD22	1:A:79:VAL:HG21	1.97	0.46
1:B:97:ALA:O	1:B:116:THR:HG23	2.16	0.46
1:B:87:LEU:HD11	1:B:112:TRP:CH2	2.51	0.46
1:A:272:GLN:HG3	1:A:285:ALA:HB3	1.97	0.46
1:D:93:THR:HG23	1:D:95:LEU:N	2.29	0.45
1:D:179:ALA:N	1:D:180:PRO:CD	2.80	0.45
1:D:128:VAL:O	1:D:211:LEU:HA	2.16	0.45
1:C:203:LEU:HD22	1:C:208:GLU:HG3	1.97	0.45
1:D:285:ALA:O	1:D:287:VAL:N	2.49	0.45
1:B:72:LYS:HD2	1:B:252:ALA:HB2	1.99	0.45
1:D:242:LEU:HD22	1:D:243:GLN:N	2.31	0.45
1:D:129:TYR:CZ	1:D:137:PRO:HG3	2.52	0.45
1:A:62:SER:HA	1:A:65:ASN:HD21	1.71	0.45
1:D:93:THR:CG2	1:D:95:LEU:HB2	2.47	0.45
1:A:99:SER:HB2	1:A:101:VAL:HG23	1.99	0.45
1:A:19:LYS:N	1:A:20:PRO:HD2	2.32	0.45
1:A:255:GLN:N	1:A:256:PRO:HD3	2.32	0.45
1:A:204:PHE:HB2	1:A:212:VAL:HG13	2.00	0.44
1:A:224:LEU:HD21	1:A:290:PRO:HB2	1.99	0.44
1:C:25:TYR:CD2	1:C:57:LEU:HD22	2.52	0.44
1:D:41:LYS:NZ	1:D:45:GLU:OE2	2.50	0.44
1:C:97:ALA:O	1:C:116:THR:HG23	2.17	0.44
1:B:75:LYS:NZ	1:B:75:LYS:CB	2.77	0.44
1:D:287:VAL:HG22	1:D:288:THR:N	2.33	0.44
1:C:108:VAL:HG22	1:C:109:PRO:CD	2.45	0.44
1:D:266:MSE:HG3	1:D:271:PHE:CE1	2.52	0.44
1:B:222:HIS:HD2	1:B:226:GLU:OE1	2.00	0.44
1:B:125:PHE:CE2	1:B:166:GLY:HA3	2.53	0.44
1:A:93:THR:HG23	1:A:95:LEU:HB2	1.98	0.44
1:C:20:PRO:HD2	1:C:49:ASN:O	2.18	0.44
1:A:315:GLN:HA	1:A:315:GLN:NE2	2.32	0.44
1:B:58:GLU:HB3	1:B:62:SER:HB2	2.00	0.43
1:C:173:LYS:HE2	1:C:305:PHE:CD2	2.52	0.43
1:D:84:ASN:HA	1:D:87:LEU:HG	1.99	0.43
1:A:144:LEU:O	1:A:144:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:159:ARG:NH2	1:D:69:MSE:HE1	2.33	0.43
1:B:163:PRO:O	1:B:213:LEU:HD21	2.19	0.43
1:D:222:HIS:HD2	1:D:226:GLU:OE1	2.01	0.43
1:D:49:ASN:O	1:D:50:CYS:HB3	2.18	0.43
1:B:120:PHE:HB3	1:B:266:MSE:HE3	2.00	0.43
1:D:67:LEU:HG	1:D:95:LEU:HD13	2.01	0.43
1:D:161:SER:HA	2:D:400:TPS:O2	2.19	0.43
1:C:152:ARG:HB3	1:C:191:VAL:CG2	2.49	0.42
1:C:118:VAL:HA	1:C:119:PRO:HD3	1.89	0.42
1:D:147:SER:HB3	1:D:151:TRP:CZ3	2.54	0.42
1:A:272:GLN:NE2	1:A:285:ALA:H	2.16	0.42
1:A:152:ARG:HB2	1:A:210:ASP:H	1.85	0.42
1:D:267:VAL:CG1	1:D:267:VAL:O	2.67	0.42
1:C:123:GLY:O	1:C:242:LEU:HD12	2.20	0.42
1:B:204:PHE:CB	1:B:212:VAL:HG11	2.47	0.42
1:A:152:ARG:HB2	1:A:209:SER:HA	2.02	0.42
1:D:65:ASN:OD1	1:D:69:MSE:HE3	2.20	0.42
1:B:261:LYS:HG3	3:B:477:HOH:O	2.19	0.42
1:C:93:THR:HG21	1:C:95:LEU:HD22	2.02	0.42
1:A:310:VAL:HG23	1:A:311:ALA:N	2.35	0.42
1:D:283:PRO:HD2	1:D:289:LEU:HD21	2.02	0.42
1:B:57:LEU:HD23	1:B:58:GLU:HG2	2.02	0.42
1:C:310:VAL:HG23	1:C:311:ALA:N	2.34	0.42
1:C:179:ALA:N	1:C:180:PRO:CD	2.83	0.42
1:A:85:ASN:O	1:A:310:VAL:HG21	2.20	0.42
1:A:135:LYS:HG2	1:A:136:ASN:ND2	2.35	0.41
1:A:254:LYS:C	1:A:256:PRO:HD3	2.41	0.41
1:C:128:VAL:O	1:C:211:LEU:HA	2.19	0.41
1:B:58:GLU:HB3	1:B:62:SER:CB	2.50	0.41
1:D:171:MSE:HG3	1:D:183:TRP:CZ2	2.55	0.41
1:B:106:VAL:HG22	1:B:284:VAL:CG2	2.49	0.41
1:D:108:VAL:HG22	1:D:109:PRO:CD	2.50	0.41
1:B:134:LEU:HD21	1:B:151:TRP:HE1	1.84	0.41
1:A:256:PRO:O	1:A:260:GLN:HG3	2.20	0.41
1:C:28:ASP:OD1	1:C:29:SER:N	2.52	0.41
1:A:229:ASP:HA	3:A:492:HOH:O	2.20	0.41
1:C:135:LYS:HG2	1:C:136:ASN:N	2.35	0.41
1:A:71:GLY:HA3	1:B:327:ARG:HE	1.85	0.41
1:D:154:ILE:HB	1:D:212:VAL:HG12	2.01	0.41
1:D:272:GLN:NE2	1:D:284:VAL:N	2.65	0.41
1:B:140:SER:HA	1:B:236:PHE:CB	2.50	0.41
1:B:41:LYS:HE2	1:B:52:LEU:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:87:LEU:HD22	1:D:117:PHE:CG	2.56	0.41
1:B:152:ARG:HB3	1:B:191:VAL:CG2	2.50	0.41
1:D:108:VAL:HG21	1:D:244:VAL:HG22	2.03	0.41
1:C:279:ASN:HD22	1:C:279:ASN:HA	1.71	0.41
1:B:108:VAL:HG13	1:B:109:PRO:HD2	2.03	0.41
1:D:247:ALA:HB3	1:D:266:MSE:HE1	2.03	0.41
1:C:173:LYS:HG2	1:C:305:PHE:CE1	2.56	0.41
1:C:204:PHE:HB2	1:C:212:VAL:HG13	2.01	0.41
1:C:127:PHE:HA	1:C:212:VAL:O	2.21	0.41
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.74	0.41
1:D:294:GLU:HG3	3:D:414:HOH:O	2.21	0.41
1:A:289:LEU:HA	1:A:290:PRO:HD3	1.96	0.41
1:C:179:ALA:HB3	1:C:180:PRO:HD3	2.03	0.41
1:C:83:ASP:C	1:C:83:ASP:OD1	2.59	0.41
1:A:222:HIS:HD2	1:A:226:GLU:OE1	2.04	0.41
1:A:62:SER:CA	1:A:65:ASN:ND2	2.65	0.41
1:A:272:GLN:O	1:A:276:PRO:HD3	2.21	0.41
1:A:287:VAL:CG2	1:A:288:THR:H	2.33	0.41
1:C:159:ARG:HH22	1:D:65:ASN:HD21	1.69	0.40
1:D:152:ARG:NH2	3:D:505:HOH:O	2.54	0.40
1:A:60:GLY:HA3	1:A:162:THR:HG23	2.03	0.40
1:C:41:LYS:HE2	1:C:52:LEU:O	2.20	0.40
1:D:135:LYS:HA	1:D:135:LYS:HE2	2.04	0.40
1:C:162:THR:N	1:C:163:PRO:CD	2.84	0.40
1:C:17:HIS:O	1:C:18:MSE:HB2	2.21	0.40
1:C:220:ALA:HB2	1:C:296:LEU:HD11	2.03	0.40
1:B:45:GLU:OE2	1:B:51:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	306/330 (93%)	293 (96%)	12 (4%)	1 (0%)	50 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	307/330 (93%)	297 (97%)	9 (3%)	1 (0%)	50	54
1	C	316/330 (96%)	305 (96%)	10 (3%)	1 (0%)	50	54
1	D	308/330 (93%)	289 (94%)	17 (6%)	2 (1%)	33	33
All	All	1237/1320 (94%)	1184 (96%)	48 (4%)	5 (0%)	43	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	60	GLY
1	C	16	SER
1	D	286	ASN
1	A	50	CYS
1	B	47	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/266 (94%)	239 (96%)	10 (4%)	42	49
1	B	252/266 (95%)	242 (96%)	10 (4%)	42	49
1	C	257/266 (97%)	244 (95%)	13 (5%)	33	35
1	D	252/266 (95%)	244 (97%)	8 (3%)	51	60
All	All	1010/1064 (95%)	969 (96%)	41 (4%)	41	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	93	THR
1	A	134	LEU
1	A	135	LYS
1	A	141	LEU
1	A	165	LEU
1	A	186	LEU

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Mol	Chain	Res	Type
1	A	212	VAL
1	A	213	LEU
1	A	279	ASN
1	B	52	LEU
1	B	57	LEU
1	B	104	ASP
1	B	134	LEU
1	B	165	LEU
1	B	212	VAL
1	B	258	LEU
1	B	260	GLN
1	B	287	VAL
1	B	322	GLN
1	C	51	GLU
1	C	88	ASP
1	C	93	THR
1	C	134	LEU
1	C	135	LYS
1	C	141	LEU
1	C	144	LEU
1	C	167	LEU
1	C	212	VAL
1	C	229	ASP
1	C	258	LEU
1	C	279	ASN
1	C	327	ARG
1	D	61	VAL
1	D	64	LEU
1	D	93	THR
1	D	134	LEU
1	D	165	LEU
1	D	186	LEU
1	D	242	LEU
1	D	294	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	136	ASN
1	A	172	GLN
1	A	222	HIS

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Mol	Chain	Res	Type
1	A	260	GLN
1	A	272	GLN
1	A	279	ASN
1	A	315	GLN
1	B	65	ASN
1	B	114	ASN
1	B	172	GLN
1	B	222	HIS
1	B	255	GLN
1	B	260	GLN
1	B	272	GLN
1	B	286	ASN
1	C	65	ASN
1	C	107	ASN
1	C	114	ASN
1	C	222	HIS
1	C	255	GLN
1	C	272	GLN
1	C	279	ASN
1	C	286	ASN
1	D	73	ASN
1	D	113	ASN
1	D	114	ASN
1	D	172	GLN
1	D	222	HIS
1	D	272	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	TPS	A	400	-	23,23,23	1.54	2 (8%)	33,33,33	3.63	15 (45%)
2	TPS	B	400	-	23,23,23	1.80	2 (8%)	33,33,33	3.41	15 (45%)
2	TPS	C	400	-	23,23,23	1.66	3 (13%)	33,33,33	3.52	14 (42%)
2	TPS	D	400	-	23,23,23	1.66	2 (8%)	33,33,33	3.63	14 (42%)

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	TPS	A	400	-	-	0/11/11/11	0/2/2/2
2	TPS	B	400	-	-	0/11/11/11	0/2/2/2
2	TPS	C	400	-	-	0/11/11/11	0/2/2/2
2	TPS	D	400	-	-	0/11/11/11	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	TPS	C5-S1	5.77	1.78	1.73
2	D	400	TPS	C5-S1	5.26	1.77	1.73
2	C	400	TPS	C5-S1	4.92	1.77	1.73
2	A	400	TPS	C5-S1	4.88	1.77	1.73
2	B	400	TPS	C4-N3	-4.50	1.34	1.39
2	D	400	TPS	C4-N3	-3.99	1.35	1.39
2	C	400	TPS	C4-N3	-3.87	1.35	1.39
2	A	400	TPS	C4-N3	-2.48	1.36	1.39
2	C	400	TPS	C6A-C5A	2.03	1.42	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	TPS	C4-C5-S1	-10.12	101.66	109.93
2	A	400	TPS	C4-C5-S1	-9.94	101.81	109.93
2	C	400	TPS	C4-C5-S1	-9.92	101.82	109.93
2	B	400	TPS	C4-C5-S1	-9.57	102.12	109.93
2	A	400	TPS	C2-S1-C5	9.23	97.80	91.63
2	C	400	TPS	C2-S1-C5	9.21	97.79	91.63
2	A	400	TPS	C6-C5-C4	9.17	134.11	127.44
2	D	400	TPS	C2-S1-C5	9.04	97.68	91.63
2	D	400	TPS	C6-C5-C4	9.04	134.02	127.44
2	B	400	TPS	C2-S1-C5	8.56	97.36	91.63
2	C	400	TPS	C6-C5-C4	8.43	133.57	127.44
2	B	400	TPS	C6-C5-C4	7.60	132.97	127.44
2	D	400	TPS	S1-C2-N3	-5.76	104.00	112.62
2	A	400	TPS	S1-C2-N3	-5.62	104.21	112.62
2	C	400	TPS	S1-C2-N3	-5.58	104.27	112.62
2	B	400	TPS	S1-C2-N3	-5.55	104.31	112.62
2	D	400	TPS	C5-C4-N3	4.66	117.00	107.53
2	A	400	TPS	C5-C4-N3	4.62	116.91	107.53
2	B	400	TPS	C5-C4-N3	4.47	116.62	107.53
2	C	400	TPS	C5-C4-N3	4.46	116.59	107.53
2	D	400	TPS	C7-C6-C5	-4.35	100.80	112.48
2	A	400	TPS	C7-C6-C5	-4.32	100.89	112.48
2	A	400	TPS	P1-O7-C7	-4.09	106.35	118.19
2	B	400	TPS	C7-C6-C5	-3.94	101.90	112.48
2	B	400	TPS	P1-O7-C7	-3.88	106.96	118.19
2	D	400	TPS	P1-O7-C7	-3.88	106.98	118.19
2	C	400	TPS	C7-C6-C5	-3.63	102.74	112.48
2	C	400	TPS	P1-O7-C7	-3.55	107.91	118.19
2	D	400	TPS	C2-N3-C4	3.39	119.66	110.82
2	A	400	TPS	CM4-C4-C5	-3.39	120.64	129.10
2	B	400	TPS	CM4-C4-C5	-3.39	120.64	129.10
2	B	400	TPS	C2-N3-C4	3.37	119.59	110.82
2	A	400	TPS	C6A-N1A-C2A	3.37	121.59	115.68
2	C	400	TPS	C2-N3-C4	3.34	119.52	110.82
2	B	400	TPS	C6A-N1A-C2A	3.30	121.47	115.68
2	D	400	TPS	CM4-C4-C5	-3.26	120.95	129.10
2	D	400	TPS	C6A-N1A-C2A	3.25	121.39	115.68
2	C	400	TPS	CM4-C4-C5	-3.24	121.00	129.10
2	A	400	TPS	C2-N3-C4	3.24	119.26	110.82
2	C	400	TPS	C6A-N1A-C2A	3.03	121.00	115.68
2	C	400	TPS	C7A-N3-C2	-2.79	119.14	125.05
2	B	400	TPS	C7A-N3-C2	-2.74	119.23	125.05
2	A	400	TPS	C7A-N3-C2	-2.72	119.28	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	TPS	N1A-C2A-N3A	-2.56	121.02	125.65
2	D	400	TPS	N1A-C2A-N3A	-2.56	121.04	125.65
2	D	400	TPS	C7A-N3-C2	-2.51	119.72	125.05
2	B	400	TPS	N1A-C2A-N3A	-2.43	121.27	125.65
2	C	400	TPS	N4A-C4A-N3A	2.39	120.34	116.88
2	B	400	TPS	N4A-C4A-N3A	2.37	120.33	116.88
2	C	400	TPS	N1A-C2A-N3A	-2.35	121.41	125.65
2	D	400	TPS	N4A-C4A-N3A	2.31	120.24	116.88
2	B	400	TPS	C5A-C6A-N1A	-2.31	119.69	123.86
2	A	400	TPS	N4A-C4A-N3A	2.24	120.12	116.88
2	C	400	TPS	C5A-C6A-N1A	-2.22	119.85	123.86
2	A	400	TPS	C5A-C6A-N1A	-2.16	119.96	123.86
2	A	400	TPS	CM2-C2A-N1A	2.01	119.42	117.02
2	D	400	TPS	C5A-C6A-N1A	-2.01	120.23	123.86
2	B	400	TPS	CM2-C2A-N1A	2.01	119.41	117.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	308/330 (93%)	-0.13	4 (1%) 74 80	14, 28, 44, 60	0
1	B	309/330 (93%)	-0.26	1 (0%) 91 95	12, 24, 41, 59	0
1	C	318/330 (96%)	-0.26	2 (0%) 86 91	14, 25, 41, 49	0
1	D	310/330 (93%)	-0.24	4 (1%) 74 80	11, 25, 42, 69	0
All	All	1245/1320 (94%)	-0.22	11 (0%) 81 86	11, 26, 43, 69	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	ALA	3.2
1	C	16	SER	3.2
1	D	18	MSE	3.1
1	B	291	ALA	3.0
1	A	224	LEU	2.4
1	A	132	ASN	2.4
1	D	102	ALA	2.3
1	D	103	ALA	2.2
1	A	288	THR	2.1
1	C	73	ASN	2.1
1	A	148	ASP	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	TPS	A	400	22/22	0.14	2.50	15,21,27,31	0
2	TPS	B	400	22/22	0.14	2.05	14,16,23,27	0
2	TPS	C	400	22/22	0.13	1.90	13,19,20,24	0
2	TPS	D	400	22/22	0.13	1.35	13,19,24,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.