Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 09:17 PM EST

PDB ID	:	4KC8
Title	:	Crystal Structure of Endo-1,5-alpha-L-arabinanase from Thermotoga petrophila RKU-1 in complex with TRIS
Authors	:	Nascimento, A.F.Z.; Polo, C.C.; Santos, C.R.; Costa, M.C.M.F.; Mesa, A.N.; Prade, R.A.; Ruller, R.; Squina, F.M.; Murakami, M.T.
Deposited on	:	2013-04-24
Resolution	:	1.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

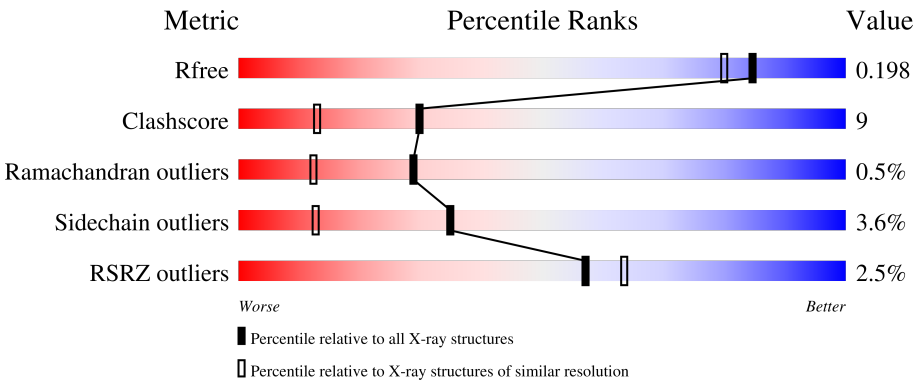
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	% 75% 19% • 5%
1	B	474	72% 21% • 5%
1	C	474	6% 69% 21% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRS	B	501	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11549 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 Glycoside hydrolase, family 43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	449	3625	2338	602	675	10	0	6	0
1	B	449	3631	2342	602	677	10	0	8	0
1	C	443	3575	2310	595	660	10	0	4	0

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A5IKD4
A	-1	GLY	-	expression tag	UNP A5IKD4
A	0	SER	-	expression tag	UNP A5IKD4
A	1	SER	-	expression tag	UNP A5IKD4
A	2	HIS	-	expression tag	UNP A5IKD4
A	3	HIS	-	expression tag	UNP A5IKD4
A	4	HIS	-	expression tag	UNP A5IKD4
A	5	HIS	-	expression tag	UNP A5IKD4
A	6	HIS	-	expression tag	UNP A5IKD4
A	7	HIS	-	expression tag	UNP A5IKD4
A	8	SER	-	expression tag	UNP A5IKD4
A	9	SER	-	expression tag	UNP A5IKD4
A	10	GLY	-	expression tag	UNP A5IKD4
A	11	LEU	-	expression tag	UNP A5IKD4
A	12	VAL	-	expression tag	UNP A5IKD4
A	13	PRO	-	expression tag	UNP A5IKD4
A	14	ARG	-	expression tag	UNP A5IKD4
A	15	GLY	-	expression tag	UNP A5IKD4
A	16	SER	-	expression tag	UNP A5IKD4
A	17	HIS	-	expression tag	UNP A5IKD4
A	18	MET	-	expression tag	UNP A5IKD4
A	19	ALA	-	expression tag	UNP A5IKD4
A	20	SER	-	expression tag	UNP A5IKD4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	initiating methionine	UNP A5IKD4
B	-1	GLY	-	expression tag	UNP A5IKD4
B	0	SER	-	expression tag	UNP A5IKD4
B	1	SER	-	expression tag	UNP A5IKD4
B	2	HIS	-	expression tag	UNP A5IKD4
B	3	HIS	-	expression tag	UNP A5IKD4
B	4	HIS	-	expression tag	UNP A5IKD4
B	5	HIS	-	expression tag	UNP A5IKD4
B	6	HIS	-	expression tag	UNP A5IKD4
B	7	HIS	-	expression tag	UNP A5IKD4
B	8	SER	-	expression tag	UNP A5IKD4
B	9	SER	-	expression tag	UNP A5IKD4
B	10	GLY	-	expression tag	UNP A5IKD4
B	11	LEU	-	expression tag	UNP A5IKD4
B	12	VAL	-	expression tag	UNP A5IKD4
B	13	PRO	-	expression tag	UNP A5IKD4
B	14	ARG	-	expression tag	UNP A5IKD4
B	15	GLY	-	expression tag	UNP A5IKD4
B	16	SER	-	expression tag	UNP A5IKD4
B	17	HIS	-	expression tag	UNP A5IKD4
B	18	MET	-	expression tag	UNP A5IKD4
B	19	ALA	-	expression tag	UNP A5IKD4
B	20	SER	-	expression tag	UNP A5IKD4
C	-2	MET	-	initiating methionine	UNP A5IKD4
C	-1	GLY	-	expression tag	UNP A5IKD4
C	0	SER	-	expression tag	UNP A5IKD4
C	1	SER	-	expression tag	UNP A5IKD4
C	2	HIS	-	expression tag	UNP A5IKD4
C	3	HIS	-	expression tag	UNP A5IKD4
C	4	HIS	-	expression tag	UNP A5IKD4
C	5	HIS	-	expression tag	UNP A5IKD4
C	6	HIS	-	expression tag	UNP A5IKD4
C	7	HIS	-	expression tag	UNP A5IKD4
C	8	SER	-	expression tag	UNP A5IKD4
C	9	SER	-	expression tag	UNP A5IKD4
C	10	GLY	-	expression tag	UNP A5IKD4
C	11	LEU	-	expression tag	UNP A5IKD4
C	12	VAL	-	expression tag	UNP A5IKD4
C	13	PRO	-	expression tag	UNP A5IKD4
C	14	ARG	-	expression tag	UNP A5IKD4
C	15	GLY	-	expression tag	UNP A5IKD4
C	16	SER	-	expression tag	UNP A5IKD4

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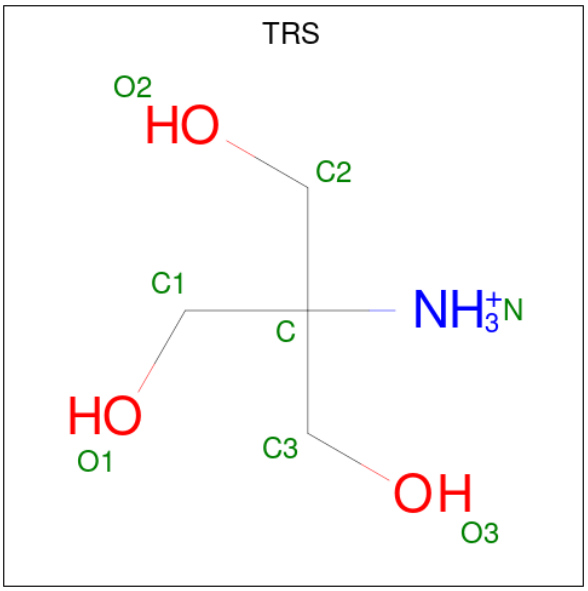
Chain	Residue	Modelled	Actual	Comment	Reference
C	17	HIS	-	expression tag	UNP A5IKD4
C	18	MET	-	expression tag	UNP A5IKD4
C	19	ALA	-	expression tag	UNP A5IKD4
C	20	SER	-	expression tag	UNP A5IKD4

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0
2	B	1	8	4	1	3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is water.

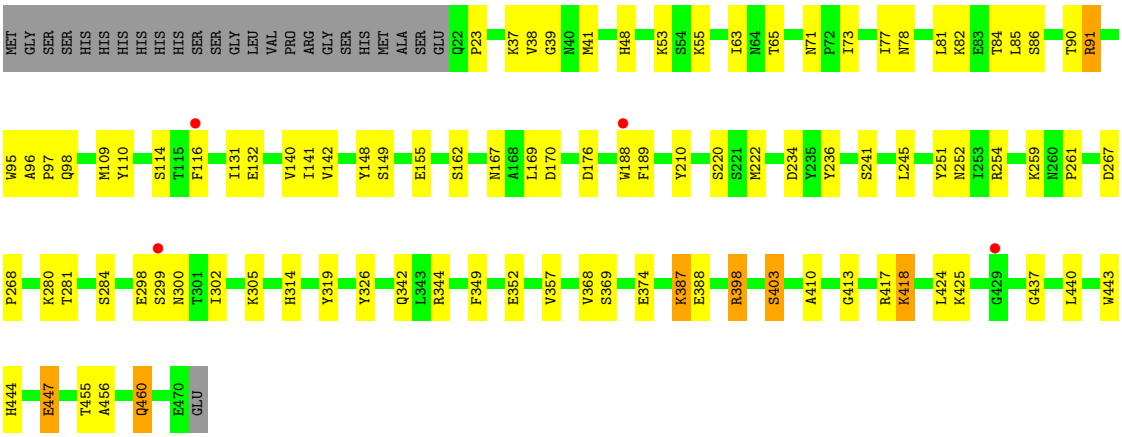
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	241	241	241	0	0
			Total	O		
4	B	316	316	316	0	0
			Total	O		
4	C	142	142	142	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

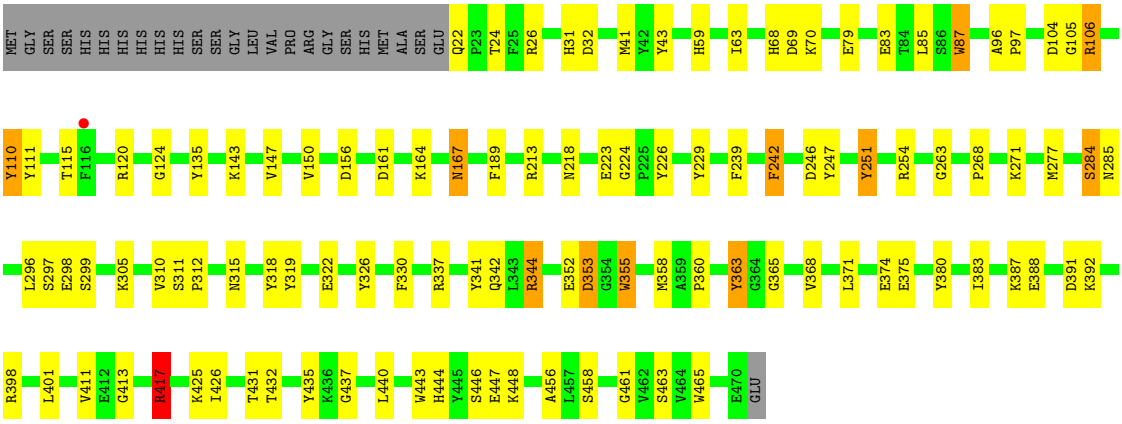
• Molecule 1: Glycoside hydrolase, family 43

Chain A:



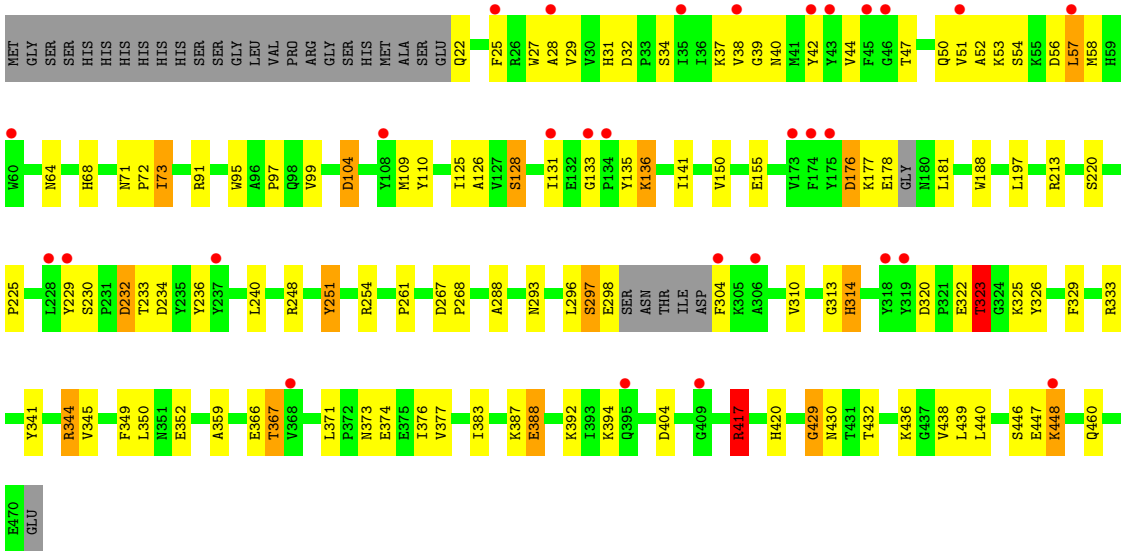
• Molecule 1: Glycoside hydrolase, family 43

Chain B:



• Molecule 1: Glycoside hydrolase, family 43

Chain C:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER GLU Q22 F25 R26 W27 A28 V29 V30 H31 D32 P33 S34 I35 I36 K37 V38 G39 N40 M41 Y42 Y43 V44 F45 G46 T47 Q50 V51 A52 K53 S54 K55 D56 L57 M58 H59
W60 N64 H68 N71 P72 I73 R91 W95 A96 P97 Q98 V99 D104 Y108 M109 Y110 I125 A126 V127 S128 I131 E132 G133 P134 Y135 K136 I141 V150 E155 V173 F174 Y175 D176 K177 E178 GLY N180 L181 W188 L197 R213 S220
P225 L228 Y229 S230 P231 D232 T233 D234 Y235 Y236 Y237 L240 R248 Y251 R254 P261 D267 P268 A288 N293 L296 S297 E298 SER ASN THR ILE ASP F304 K305 A306 V310 G313 H314 Y318 Y319 D320 P321 E322 T323 G324 K325 Y326 F329 R333
Y341 R344 V345 F349 L350 N351 E352 A359 E366 T367 V368 L371 P372 N373 E374 E375 I376 V377 I383 K387 E388 K392 I393 K394 Q395 D404 G409 R417 H420 G429 N430 T431 T432 K436 G437 V438 L439 L440 S446 E447 K448 Q460
E470 GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.67Å 86.77Å 194.37Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	43.38 – 1.76 43.38 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.38-1.76) 99.2 (43.38-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.153 , 0.197 0.161 , 0.198	Depositor DCC
R_{free} test set	6836 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.527 for H, K, L 0.473 for -h,-k,l	Depositor
Outliers	0 of 135737 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11549	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, CA

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	0.95	0/3768	1.03	6/5119 (0.1%)
1	B	1.53	30/3781 (0.8%)	1.38	27/5137 (0.5%)
1	C	0.86	0/3707	0.97	6/5033 (0.1%)
All	All	1.15	30/11256 (0.3%)	1.14	39/15289 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
All	All	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	GLY	N-CA	-9.72	1.31	1.46
1	B	226	TYR	CG-CD2	7.20	1.48	1.39
1	B	330	PHE	CG-CD2	-6.95	1.28	1.38
1	B	135	TYR	CD1-CE1	-6.94	1.28	1.39
1	B	458	SER	CB-OG	6.83	1.51	1.42
1	B	360	PRO	C-O	6.45	1.36	1.23
1	B	111	TYR	CE1-CZ	6.34	1.46	1.38
1	B	284	SER	CA-CB	-6.24	1.43	1.52
1	B	363	TYR	CG-CD1	6.18	1.47	1.39
1	B	461	GLY	N-CA	6.16	1.55	1.46
1	B	43	TYR	CE1-CZ	-6.10	1.30	1.38
1	B	135	TYR	CE1-CZ	-5.96	1.30	1.38
1	B	465	TRP	CD1-NE1	5.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	GLY	C-O	5.91	1.33	1.23
1	B	226	TYR	CB-CG	-5.58	1.43	1.51
1	B	355	TRP	CE3-CZ3	5.56	1.47	1.38
1	B	224	GLY	N-CA	-5.46	1.37	1.46
1	B	344	ARG	NE-CZ	-5.42	1.26	1.33
1	B	105	GLY	N-CA	-5.42	1.38	1.46
1	B	115	THR	C-O	-5.39	1.13	1.23
1	B	167	ASN	C-O	5.25	1.33	1.23
1	B	229	TYR	CZ-OH	5.24	1.46	1.37
1	B	229	TYR	CB-CG	-5.22	1.43	1.51
1	B	318	TYR	CB-CG	-5.22	1.43	1.51
1	B	247	TYR	CD2-CE2	5.14	1.47	1.39
1	B	223	GLU	CD-OE1	5.14	1.31	1.25
1	B	326	TYR	CA-C	-5.13	1.39	1.52
1	B	319	TYR	CE1-CZ	-5.10	1.31	1.38
1	B	87	TRP	CG-CD1	5.08	1.43	1.36
1	B	239	PHE	CE1-CZ	5.00	1.46	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	106	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	C	213	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	106	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	B	213	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	B	344	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	C	213	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	B	254	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	B	330	PHE	CB-CG-CD1	-7.09	115.84	120.80
1	B	213	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	111	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	C	91	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	344	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	246	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	91	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	91	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	85	LEU	CB-CG-CD2	-6.05	100.71	111.00
1	B	110	TYR	CZ-CE2-CD2	5.98	125.18	119.80
1	A	170	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	41	MET	CG-SD-CE	5.92	109.67	100.20
1	A	398	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	156	ASP	CB-CG-OD1	5.76	123.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	120	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	B	437	GLY	N-CA-C	5.55	126.98	113.10
1	B	110	TYR	CG-CD1-CE1	5.53	125.72	121.30
1	B	353	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	391	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	B	26	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	234	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	A	234	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	169	LEU	CA-CB-CG	5.34	127.57	115.30
1	B	417	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	32	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	242	PHE	CB-CG-CD1	5.14	124.40	120.80
1	B	417	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	C	417	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	B	189	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	B	310	VAL	CG1-CB-CG2	-5.02	102.86	110.90
1	B	358	MET	CG-SD-CE	-5.01	92.19	100.20
1	B	239	PHE	CB-CG-CD2	-5.01	117.30	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	315	ASN	Peptide
1	C	297	SER	Peptide
1	C	322	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3625	0	3478	61	0
1	B	3631	0	3486	60	1
1	C	3575	0	3436	86	1
2	A	8	0	12	0	0
2	B	8	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	241	0	0	7	0
4	B	316	0	0	17	0
4	C	142	0	0	13	1
All	All	11549	0	10424	201	2

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 9.

All (201) 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:90:THR:O	1:A:91:ARG:HD2	1.53	1.08
1:B:341:TYR:CG	4:B:795:HOH:O	2.06	1.06
1:B:31:HIS:CD2	4:B:795:HOH:O	2.17	0.95
1:C:377:VAL:HB	4:C:681:HOH:O	1.70	0.92
1:C:27:TRP:NE1	4:C:730:HOH:O	2.04	0.91
1:C:38:VAL:HG21	1:C:131:ILE:HG12	1.51	0.90
1:C:125:ILE:HD11	1:C:141:ILE:HD13	1.54	0.87
1:B:31:HIS:HD2	4:B:795:HOH:O	1.52	0.83
1:B:296:LEU:CD2	1:B:383:ILE:HD11	2.09	0.82
1:C:373:ASN:HB3	4:C:651:HOH:O	1.78	0.81
1:C:73:ILE:N	1:C:73:ILE:HD12	1.95	0.81
1:C:323:THR:HG23	1:C:325:LYS:HG3	1.64	0.79
1:C:229:TYR:OH	1:C:234:ASP:OD1	1.99	0.79
1:A:342:GLN:OE1	1:A:344:ARG:NH1	2.16	0.78
1:A:300:ASN:OD1	1:A:302:ILE:O	2.04	0.75
1:C:344:ARG:NH2	4:C:730:HOH:O	2.18	0.74
1:B:104:ASP:OD2	1:B:106:ARG:HD3	1.87	0.74
1:C:430:ASN:OD1	1:C:430:ASN:O	2.06	0.73
1:B:104:ASP:OD2	1:B:106:ARG:CD	2.37	0.73
1:B:24[B]:THR:HG22	1:B:59:HIS:NE2	2.04	0.72
1:A:90:THR:O	1:A:91:ARG:CD	2.34	0.72
1:C:27:TRP:CD1	4:C:730:HOH:O	2.39	0.72
1:A:78:ASN:O	1:A:91:ARG:NH2	2.22	0.71
1:A:298[B]:GLU:OE2	1:A:398:ARG:NH2	2.17	0.71
1:C:323:THR:HG23	1:C:325:LYS:CG	2.20	0.71
1:C:310:VAL:N	1:C:333:ARG:O	2.23	0.70
1:C:371:LEU:O	1:C:417:ARG:NH1	2.21	0.70
1:C:64:ASN:ND2	1:C:73:ILE:HD13	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:HIS:O	1:C:71:ASN:ND2	2.26	0.69
1:B:426:ILE:HD12	1:B:435:TYR:CE1	2.28	0.69
1:B:79:GLU:HG3	4:B:793:HOH:O	1.95	0.67
1:C:230:SER:OG	1:C:326:TYR:OH	2.05	0.67
1:B:68:HIS:HD2	4:B:767:HOH:O	1.80	0.65
1:A:444:HIS:CD2	1:A:447:GLU:HB2	2.33	0.64
1:B:22:GLN:OE1	1:C:436:LYS:NZ	2.23	0.64
1:B:375:GLU:OE2	4:B:765:HOH:O	2.15	0.63
1:B:401:LEU:HD23	1:B:401:LEU:N	2.14	0.62
1:B:426:ILE:HD12	1:B:435:TYR:CD1	2.33	0.62
1:B:22:GLN:HG2	4:B:912:HOH:O	2.00	0.62
1:A:357:VAL:HG12	4:A:681:HOH:O	2.00	0.62
1:C:181:LEU:HB3	1:C:197:LEU:HB2	1.81	0.61
1:A:41:MET:SD	1:A:55:LYS:HG2	2.41	0.61
1:C:430:ASN:HA	4:C:635:HOH:O	2.02	0.60
1:C:73:ILE:N	1:C:73:ILE:CD1	2.65	0.60
1:C:323:THR:CG2	1:C:325:LYS:H	2.15	0.59
1:C:22:GLN:N	4:C:674:HOH:O	2.35	0.59
1:C:323:THR:HG22	1:C:325:LYS:H	1.69	0.58
1:B:296:LEU:HD23	1:B:383:ILE:HD11	1.86	0.58
1:C:39:GLY:N	4:C:726:HOH:O	2.29	0.58
4:A:767:HOH:O	1:C:374:GLU:HG2	2.03	0.58
1:A:162:SER:HB2	1:A:189:PHE:CD1	2.38	0.57
1:A:82:LYS:O	1:A:86:SER:OG	2.14	0.57
1:B:69:ASP:OD1	4:B:914:HOH:O	2.17	0.57
1:B:444:HIS:CD2	1:B:447:GLU:H	2.23	0.57
1:B:440:LEU:HD23	1:B:440:LEU:N	2.20	0.56
1:A:252:ASN:ND2	1:A:254:ARG:HE	2.04	0.56
1:C:267:ASP:HB2	1:C:268:PRO:HD2	1.89	0.55
1:A:188:TRP:HA	1:A:220:SER:O	2.07	0.54
1:C:104:ASP:N	1:C:104:ASP:OD1	2.39	0.54
1:C:349:PHE:CE1	1:C:359:ALA:HB2	2.42	0.53
1:B:97:PRO:HA	1:B:110:TYR:O	2.07	0.53
1:C:225:PRO:HA	1:C:240:LEU:HD23	1.89	0.53
1:C:47:THR:HG23	1:C:95:TRP:HA	1.90	0.53
1:C:126:ALA:HB1	1:C:135:TYR:HB3	1.90	0.53
1:A:252:ASN:HD21	1:A:254:ARG:HE	1.57	0.53
1:B:322:GLU:HG3	4:B:771:HOH:O	2.09	0.53
1:C:29:VAL:O	1:C:29:VAL:HG12	2.09	0.53
1:C:97:PRO:HA	1:C:110:TYR:O	2.09	0.53
1:B:342:GLN:OE1	1:B:344:ARG:NH1	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PHE:CD2	1:C:345:VAL:HG22	2.44	0.52
1:C:56:ASP:O	1:C:57:LEU:HG	2.09	0.52
1:C:349:PHE:HE1	1:C:359:ALA:HB2	1.74	0.52
1:C:25:PHE:CD2	1:C:58:MET:HB3	2.45	0.52
1:A:437:GLY:HA3	1:A:456:ALA:HA	1.92	0.51
1:C:37:LYS:N	4:C:725:HOH:O	2.16	0.51
1:B:147:VAL:HB	1:B:150:VAL:HG22	1.91	0.51
1:A:245:LEU:HD12	1:A:245:LEU:C	2.30	0.51
1:B:363:TYR:CZ	1:B:365:GLY:HA2	2.46	0.51
1:B:218:ASN:OD1	1:B:277:MET:CE	2.59	0.51
1:C:42:TYR:N	1:C:54:SER:O	2.34	0.51
1:B:104:ASP:OD2	1:B:106:ARG:HD2	2.10	0.51
1:A:53:LYS:HE2	1:A:63:ILE:HD11	1.93	0.51
1:A:300:ASN:OD1	1:A:302:ILE:C	2.50	0.50
1:A:77:ILE:HG13	1:A:81:LEU:CD1	2.41	0.50
1:A:437:GLY:HA3	1:A:455:THR:O	2.11	0.50
1:C:176:ASP:OD1	1:C:176:ASP:C	2.50	0.50
1:A:387:LYS:NZ	1:A:460:GLN:O	2.34	0.50
1:B:444:HIS:HE1	4:B:876:HOH:O	1.95	0.50
1:A:23:PRO:HG2	1:A:443:TRP:CD2	2.46	0.50
1:A:403:SER:OG	1:B:374:GLU:OE1	2.28	0.50
1:C:367:THR:HG22	4:C:731:HOH:O	2.12	0.50
1:B:70:LYS:O	4:B:775:HOH:O	2.20	0.49
1:B:271:LYS:HE3	1:B:285:ASN:O	2.12	0.49
1:A:155:GLU:HG3	1:A:210:TYR:CE1	2.47	0.48
1:A:368:VAL:HG12	1:A:369:SER:N	2.28	0.48
1:C:128:SER:OG	1:C:133:GLY:HA2	2.14	0.48
1:A:444:HIS:CG	1:A:447:GLU:HB2	2.48	0.48
1:C:420:HIS:HD2	1:C:438[B]:VAL:HG23	1.78	0.48
1:C:267:ASP:HB2	1:C:268:PRO:CD	2.44	0.47
1:A:65:THR:HG23	4:A:796:HOH:O	2.13	0.47
1:A:85:LEU:HD22	1:A:90:THR:HG23	1.96	0.47
4:A:767:HOH:O	1:C:374:GLU:CG	2.59	0.47
1:A:398:ARG:HG3	1:C:404:ASP:HA	1.96	0.47
1:C:31:HIS:N	1:C:50:GLN:OE1	2.45	0.47
1:C:232:ASP:N	1:C:232:ASP:OD1	2.48	0.47
1:B:296:LEU:HD21	1:B:383:ILE:CD1	2.44	0.47
1:B:341:TYR:CD2	4:B:795:HOH:O	2.52	0.47
1:A:84:THR:HG22	1:A:140:VAL:HG22	1.96	0.47
1:B:444:HIS:HD2	1:B:446:SER:H	1.63	0.47
1:C:72:PRO:HB2	1:C:73:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ARG:CZ	4:C:730:HOH:O	2.58	0.47
1:A:413:GLY:HA3	1:A:425:LYS:O	2.15	0.47
1:B:311:SER:N	1:B:312:PRO:CD	2.78	0.46
1:B:413:GLY:HA3	1:B:425:LYS:O	2.15	0.46
1:A:71:ASN:OD1	1:A:73:ILE:N	2.49	0.46
1:A:280:LYS:HD2	4:A:740:HOH:O	2.14	0.46
1:C:387:LYS:NZ	1:C:460:GLN:O	2.38	0.46
1:A:77:ILE:HG23	1:A:78:ASN:N	2.31	0.46
1:C:176:ASP:OD1	1:C:176:ASP:O	2.32	0.46
1:B:63:ILE:HD12	4:B:778:HOH:O	2.15	0.46
1:C:29:VAL:HG13	1:C:341:TYR:CE1	2.50	0.46
1:B:352:GLU:OE1	4:B:874:HOH:O	2.20	0.46
1:C:366:GLU:HA	4:C:612:HOH:O	2.16	0.45
1:A:77:ILE:HG13	1:A:81:LEU:HD12	1.98	0.45
1:A:368:VAL:CG1	1:A:369:SER:N	2.80	0.45
1:B:277:MET:HE3	1:B:277:MET:HB2	1.89	0.45
1:B:296:LEU:HD21	1:B:383:ILE:HD11	1.95	0.45
1:C:126:ALA:HA	1:C:136:LYS:O	2.17	0.45
1:A:176:ASP:HB2	1:A:236:TYR:OH	2.17	0.45
1:C:430:ASN:CA	4:C:635:HOH:O	2.64	0.45
1:C:323:THR:CG2	1:C:325:LYS:HB2	2.46	0.44
1:B:218:ASN:OD1	1:B:277:MET:HE1	2.18	0.44
1:C:73:ILE:HD12	1:C:73:ILE:H	1.76	0.44
1:C:251:TYR:CD2	1:C:313:GLY:HA3	2.53	0.44
1:C:446:SER:O	1:C:448:LYS:HG2	2.17	0.44
1:A:281:THR:O	1:A:284:SER:OG	2.36	0.44
1:C:293:ASN:HB2	1:C:392:LYS:O	2.18	0.44
1:C:373:ASN:HA	1:C:376:ILE:HD12	2.00	0.44
1:A:267:ASP:HB2	1:A:268:PRO:CD	2.49	0.43
1:B:218:ASN:OD1	1:B:277:MET:HE2	2.18	0.43
1:B:371:LEU:O	1:B:417:ARG:NH1	2.47	0.43
1:B:161:ASP:HB3	1:B:164:LYS:HE3	1.99	0.43
1:A:352:GLU:OE2	1:A:418:LYS:NZ	2.50	0.43
1:B:284:SER:O	1:B:387:LYS:HG3	2.18	0.43
1:B:448:LYS:HD2	1:C:432:THR:O	2.19	0.43
1:B:63:ILE:O	1:B:63:ILE:CG2	2.67	0.43
1:B:443:TRP:CZ2	1:B:448:LYS:HA	2.54	0.42
1:A:95:TRP:CZ3	1:A:114:SER:HB3	2.53	0.42
1:C:37:LYS:HE3	1:C:42:TYR:CZ	2.54	0.42
1:C:296:LEU:CD2	1:C:383:ILE:HD11	2.48	0.42
1:C:32:ASP:HB3	1:C:314:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ASP:O	1:C:57:LEU:CG	2.66	0.42
1:C:236:TYR:CZ	1:C:261:PRO:HD3	2.54	0.42
1:B:297:SER:HG	1:B:299[B]:SER:HG	1.63	0.42
1:C:320:ASP:O	1:C:323:THR:HG22	2.19	0.42
1:A:97:PRO:HA	1:A:110:TYR:O	2.19	0.42
1:B:298[B]:GLU:OE1	1:B:398:ARG:NH2	2.46	0.42
1:B:380:TYR:CE1	1:B:401:LEU:HG	2.54	0.42
1:A:222:MET:HA	1:A:241:SER:O	2.20	0.42
1:A:236:TYR:CE1	1:A:261:PRO:HD3	2.54	0.42
1:C:177:LYS:CG	1:C:178:GLU:N	2.82	0.42
1:A:77:ILE:CG1	1:A:81:LEU:HD12	2.50	0.42
1:A:38:VAL:HG21	1:A:131:ILE:HD13	2.02	0.42
1:A:252:ASN:HD21	1:A:254:ARG:HH21	1.68	0.41
1:A:319:TYR:HD1	1:A:326:TYR:CE1	2.38	0.41
1:A:23:PRO:HG2	1:A:443:TRP:CE2	2.55	0.41
1:A:37:LYS:HE2	1:A:39:GLY:O	2.20	0.41
1:A:82:LYS:C	4:A:648:HOH:O	2.59	0.41
1:B:392:LYS:NZ	4:B:881:HOH:O	2.54	0.41
1:B:268:PRO:HD3	1:B:355:TRP:CH2	2.56	0.41
1:C:388:GLU:OE2	1:C:394:LYS:NZ	2.51	0.41
1:C:73:ILE:CD1	1:C:73:ILE:H	2.33	0.41
1:A:131:ILE:HG23	1:A:132:GLU:N	2.36	0.41
1:A:148:TYR:C	1:A:148:TYR:CD1	2.93	0.41
1:B:456:ALA:O	1:B:463:SER:HA	2.21	0.41
1:B:305:LYS:HE3	1:C:429:GLY:O	2.20	0.41
1:A:98:GLN:O	1:A:109:MET:HA	2.20	0.41
1:A:141:ILE:HG13	1:A:142:VAL:HG23	2.03	0.41
1:C:188:TRP:HA	1:C:220:SER:O	2.20	0.41
1:C:233:THR:HG21	1:C:350:LEU:HD22	2.02	0.41
1:C:254:ARG:HA	1:C:288:ALA:O	2.21	0.41
1:C:323:THR:HG23	1:C:325:LYS:CB	2.51	0.41
1:A:96:ALA:N	1:A:97:PRO:CD	2.84	0.41
1:A:349:PHE:CE1	1:A:368:VAL:HG23	2.56	0.41
1:B:87:TRP:CD2	1:B:143:LYS:HD2	2.55	0.41
1:B:242:PHE:O	1:B:251:TYR:HA	2.22	0.40
1:B:368:VAL:HG13	1:B:440:LEU:HB3	2.02	0.40
1:C:439:LEU:O	1:C:440:LEU:HB3	2.21	0.40
1:C:99:VAL:HG22	1:C:109:MET:HG3	2.03	0.40
1:C:297:SER:HA	1:C:298:GLU:HB3	2.02	0.40
1:A:410:ALA:O	1:C:373:ASN:ND2	2.45	0.40
1:C:44:VAL:HG23	1:C:44:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:VAL:N	1:C:64:ASN:O	2.51	0.40
1:A:37:LYS:NZ	4:A:837:HOH:O	2.31	0.40
1:B:96:ALA:HB1	4:B:908:HOH:O	2.21	0.40
1:B:353:ASP:OD2	4:B:853:HOH:O	2.22	0.40
1:C:28:ALA:CB	1:C:52:ALA:HB2	2.51	0.40
1:A:374:GLU:H	1:A:374:GLU:CD	2.24	0.40
1:B:426:ILE:O	1:B:432:THR:HA	2.21	0.40
1:C:344:ARG:HD3	1:C:344:ARG:HA	1.67	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:THR:O	1:C:248:ARG:NH2[1_455]	1.82	0.38
1:B:83[B]:GLU:OE1	4:C:737:HOH:O[2_648]	2.01	0.19

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	453/474 (96%)	428 (94%)	24 (5%)	1 (0%)	47 29
1	B	455/474 (96%)	440 (97%)	15 (3%)	0	100 100
1	C	441/474 (93%)	403 (91%)	32 (7%)	6 (1%)	11 2
All	All	1349/1422 (95%)	1271 (94%)	71 (5%)	7 (0%)	29 12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	323	THR
1	C	57	LEU
1	C	429	GLY

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Mol	Chain	Res	Type
1	C	448	LYS
1	C	155	GLU
1	A	314	HIS
1	C	314	HIS

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	391/406 (96%)	375 (96%)	16 (4%)	30 10
1	B	393/406 (97%)	386 (98%)	7 (2%)	59 40
1	C	384/406 (95%)	366 (95%)	18 (5%)	26 7
All	All	1168/1218 (96%)	1127 (96%)	41 (4%)	35 13

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

Mol	Chain	Res	Type
1	A	116	PHE
1	A	149	SER
1	A	167	ASN
1	A	251	TYR
1	A	259	LYS
1	A	299	SER
1	A	305	LYS
1	A	387	LYS
1	A	388	GLU
1	A	403	SER
1	A	417	ARG
1	A	418	LYS
1	A	424	LEU
1	A	440	LEU
1	A	447	GLU
1	A	460	GLN
1	B	167	ASN
1	B	251	TYR

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Mol	Chain	Res	Type
1	B	337	ARG
1	B	388	GLU
1	B	411	VAL
1	B	417	ARG
1	B	431	THR
1	C	34	SER
1	C	40	ASN
1	C	53	LYS
1	C	73	ILE
1	C	104	ASP
1	C	128	SER
1	C	136	LYS
1	C	150	VAL
1	C	176	ASP
1	C	232	ASP
1	C	251	TYR
1	C	304	PHE
1	C	323	THR
1	C	352	GLU
1	C	367	THR
1	C	388	GLU
1	C	417	ARG
1	C	447	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	200	ASN
1	A	252	ASN
1	A	260	ASN
1	A	444	HIS
1	B	68	HIS
1	B	167	ASN
1	B	430	ASN
1	B	444	HIS
1	C	167	ASN
1	C	200	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	TRS	B	501	-	7,7,7	2.39	3 (42%)	9,9,9	2.63	5 (55%)
2	TRS	A	501	-	7,7,7	0.34	0	9,9,9	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	B	501	-	-	4/9/9/9	-
2	TRS	A	501	-	-	3/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	TRS	C-N	3.94	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	TRS	O3-C3	3.52	1.54	1.42
2	B	501	TRS	C1-C	-2.88	1.44	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	TRS	O3-C3-C	4.52	125.32	111.00
2	B	501	TRS	O1-C1-C	-3.72	99.19	111.00
2	B	501	TRS	O2-C2-C	3.23	121.23	111.00
2	B	501	TRS	C2-C-C1	-2.68	102.50	110.81
2	B	501	TRS	C2-C-N	2.66	115.93	107.98

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	TRS	N-C-C2-O2
2	B	501	TRS	C1-C-C2-O2
2	B	501	TRS	C2-C-C3-O3
2	A	501	TRS	N-C-C1-O1
2	B	501	TRS	C3-C-C2-O2
2	A	501	TRS	C2-C-C1-O1
2	A	501	TRS	C3-C-C1-O1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	449/474 (94%)	0.05	4 (0%)	84	89	20, 30, 41, 55	0
1	B	449/474 (94%)	-0.06	1 (0%)	95	96	10, 17, 30, 59	0
1	C	443/474 (93%)	0.64	29 (6%)	18	24	22, 38, 54, 64	1 (0%)
All	All	1341/1422 (94%)	0.21	34 (2%)	57	63	10, 29, 49, 64	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	TYR	5.6
1	B	116	PHE	5.0
1	C	318	TYR	5.0
1	C	42	TYR	3.9
1	C	35	ILE	3.7
1	C	237	TYR	3.5
1	C	133	GLY	3.2
1	C	173	VAL	3.2
1	A	429	GLY	3.1
1	C	45	PHE	3.1
1	C	46	GLY	3.1
1	C	134	PRO	3.1
1	C	174	PHE	3.0
1	C	51	VAL	3.0
1	C	38	VAL	3.0
1	C	304	PHE	2.9
1	C	368	VAL	2.9
1	C	229	TYR	2.9
1	C	57	LEU	2.8
1	C	175	TYR	2.8
1	A	116	PHE	2.6
1	C	43	TYR	2.5
1	A	299	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	25	PHE	2.3
1	C	60	TRP	2.3
1	C	448	LYS	2.3
1	C	306	ALA	2.2
1	C	28	ALA	2.2
1	C	131	ILE	2.1
1	C	395	GLN	2.1
1	C	108	TYR	2.1
1	C	228	LEU	2.1
1	A	188	TRP	2.0
1	C	409	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRS	A	501	8/8	0.89	0.12	32,36,38,53	0
2	TRS	B	501	8/8	0.96	0.09	14,18,22,28	0
3	CA	A	502	1/1	0.96	0.11	53,53,53,53	0
3	CA	C	501	1/1	0.96	0.06	51,51,51,51	0
3	CA	B	502	1/1	0.98	0.04	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.