Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2025 – 12:10 PM JST

PDB ID	:	8ZTZ / pdb_00008ztz
Title	:	Structure of ATP-dependent diazotase CmaA6
Authors	:	Katsuyama, Y.; Kawai, S.; Ohnishi, Y.
Deposited on	:	2024-06-07
Resolution	:	2.93 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:

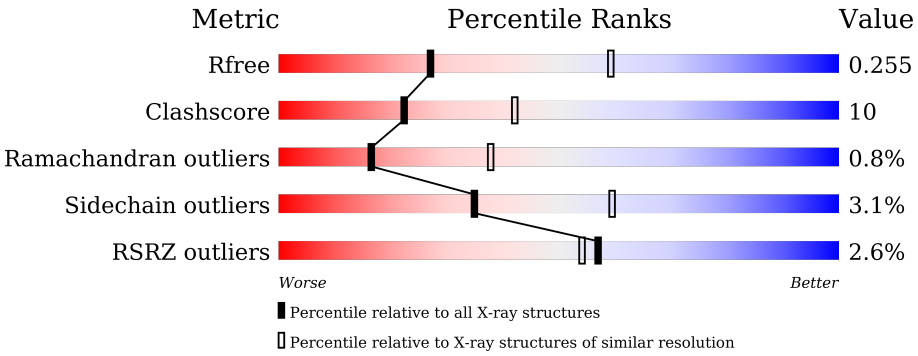
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.93 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}	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

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	569	73% 18% 8%
1	B	569	7% 64% 27% 8%
1	C	569	71% 19% 8%
1	D	569	73% 22%
1	E	569	97%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16715 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 AMP-binding enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	524	Total	C	N	O	S	0	0	0
			4003	2518	707	765	13			
1	A	521	Total	C	N	O	S	0	0	0
			3982	2507	704	758	13			
1	C	521	Total	C	N	O	S	0	0	0
			3982	2507	704	758	13			
1	D	553	Total	C	N	O	S	0	0	0
			4225	2651	754	806	14			
1	E	16	Total	C	N	O	S	0	0	0
			135	79	32	23	1			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP W5W4E6
B	2	ASN	-	expression tag	UNP W5W4E6
B	3	HIS	-	expression tag	UNP W5W4E6
B	4	LYS	-	expression tag	UNP W5W4E6
B	5	VAL	-	expression tag	UNP W5W4E6
B	6	HIS	-	expression tag	UNP W5W4E6
B	7	HIS	-	expression tag	UNP W5W4E6
B	8	HIS	-	expression tag	UNP W5W4E6
B	9	HIS	-	expression tag	UNP W5W4E6
B	10	HIS	-	expression tag	UNP W5W4E6
B	11	HIS	-	expression tag	UNP W5W4E6
B	12	ILE	-	expression tag	UNP W5W4E6
B	13	GLU	-	expression tag	UNP W5W4E6
B	14	GLY	-	expression tag	UNP W5W4E6
B	15	ARG	-	expression tag	UNP W5W4E6
B	16	HIS	-	expression tag	UNP W5W4E6
A	1	MET	-	initiating methionine	UNP W5W4E6
A	2	ASN	-	expression tag	UNP W5W4E6
A	3	HIS	-	expression tag	UNP W5W4E6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4	LYS	-	expression tag	UNP W5W4E6
A	5	VAL	-	expression tag	UNP W5W4E6
A	6	HIS	-	expression tag	UNP W5W4E6
A	7	HIS	-	expression tag	UNP W5W4E6
A	8	HIS	-	expression tag	UNP W5W4E6
A	9	HIS	-	expression tag	UNP W5W4E6
A	10	HIS	-	expression tag	UNP W5W4E6
A	11	HIS	-	expression tag	UNP W5W4E6
A	12	ILE	-	expression tag	UNP W5W4E6
A	13	GLU	-	expression tag	UNP W5W4E6
A	14	GLY	-	expression tag	UNP W5W4E6
A	15	ARG	-	expression tag	UNP W5W4E6
A	16	HIS	-	expression tag	UNP W5W4E6
C	1	MET	-	initiating methionine	UNP W5W4E6
C	2	ASN	-	expression tag	UNP W5W4E6
C	3	HIS	-	expression tag	UNP W5W4E6
C	4	LYS	-	expression tag	UNP W5W4E6
C	5	VAL	-	expression tag	UNP W5W4E6
C	6	HIS	-	expression tag	UNP W5W4E6
C	7	HIS	-	expression tag	UNP W5W4E6
C	8	HIS	-	expression tag	UNP W5W4E6
C	9	HIS	-	expression tag	UNP W5W4E6
C	10	HIS	-	expression tag	UNP W5W4E6
C	11	HIS	-	expression tag	UNP W5W4E6
C	12	ILE	-	expression tag	UNP W5W4E6
C	13	GLU	-	expression tag	UNP W5W4E6
C	14	GLY	-	expression tag	UNP W5W4E6
C	15	ARG	-	expression tag	UNP W5W4E6
C	16	HIS	-	expression tag	UNP W5W4E6
D	1	MET	-	initiating methionine	UNP W5W4E6
D	2	ASN	-	expression tag	UNP W5W4E6
D	3	HIS	-	expression tag	UNP W5W4E6
D	4	LYS	-	expression tag	UNP W5W4E6
D	5	VAL	-	expression tag	UNP W5W4E6
D	6	HIS	-	expression tag	UNP W5W4E6
D	7	HIS	-	expression tag	UNP W5W4E6
D	8	HIS	-	expression tag	UNP W5W4E6
D	9	HIS	-	expression tag	UNP W5W4E6
D	10	HIS	-	expression tag	UNP W5W4E6
D	11	HIS	-	expression tag	UNP W5W4E6
D	12	ILE	-	expression tag	UNP W5W4E6
D	13	GLU	-	expression tag	UNP W5W4E6

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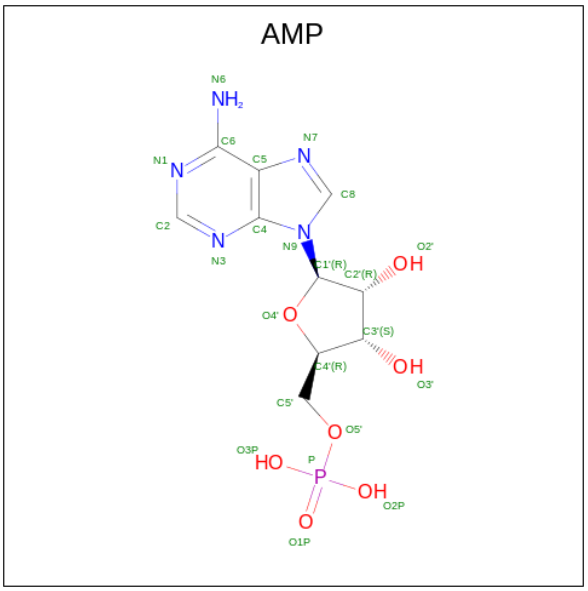
Chain	Residue	Modelled	Actual	Comment	Reference
D	14	GLY	-	expression tag	UNP W5W4E6
D	15	ARG	-	expression tag	UNP W5W4E6
D	16	HIS	-	expression tag	UNP W5W4E6
E	1	MET	-	initiating methionine	UNP W5W4E6
E	2	ASN	-	expression tag	UNP W5W4E6
E	3	HIS	-	expression tag	UNP W5W4E6
E	4	LYS	-	expression tag	UNP W5W4E6
E	5	VAL	-	expression tag	UNP W5W4E6
E	6	HIS	-	expression tag	UNP W5W4E6
E	7	HIS	-	expression tag	UNP W5W4E6
E	8	HIS	-	expression tag	UNP W5W4E6
E	9	HIS	-	expression tag	UNP W5W4E6
E	10	HIS	-	expression tag	UNP W5W4E6
E	11	HIS	-	expression tag	UNP W5W4E6
E	12	ILE	-	expression tag	UNP W5W4E6
E	13	GLU	-	expression tag	UNP W5W4E6
E	14	GLY	-	expression tag	UNP W5W4E6
E	15	ARG	-	expression tag	UNP W5W4E6
E	16	HIS	-	expression tag	UNP W5W4E6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	2	0
2	D	2	Total Mg 2 2	2	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	23	0
			23	10	5	7	1		

- Molecule 4 is water.

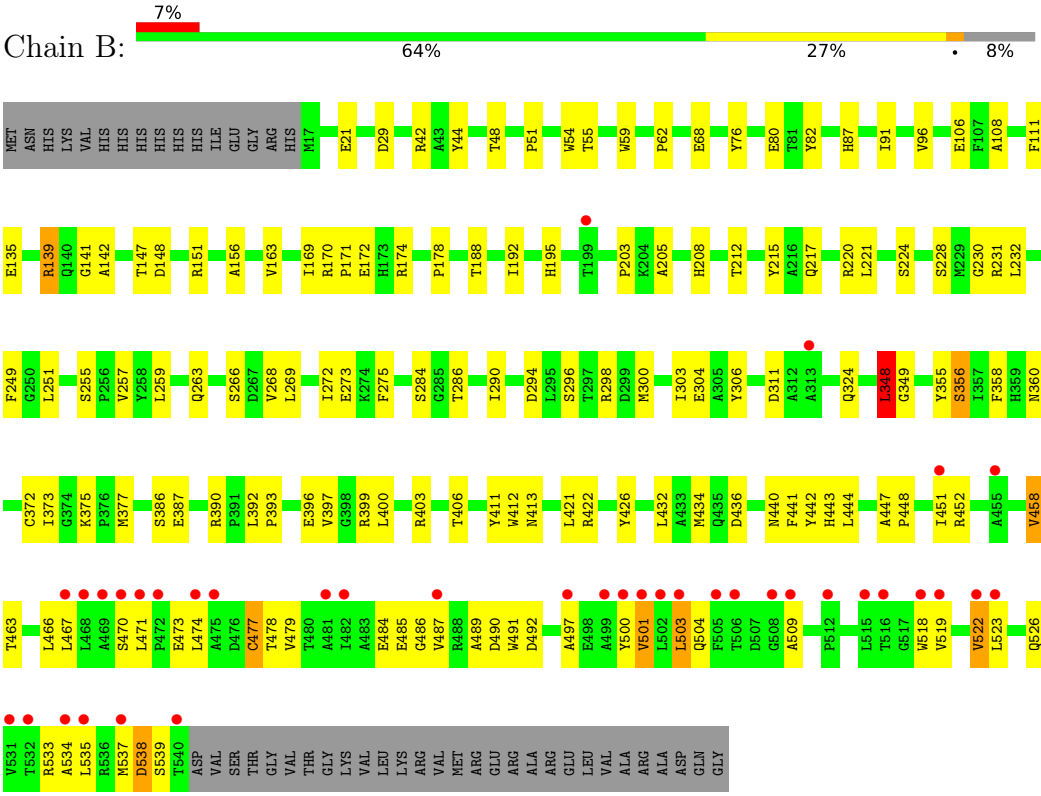
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	56	Total	O	0	0
			56	56		
4	A	134	Total	O	0	0
			134	134		
4	C	92	Total	O	0	0
			92	92		
4	D	78	Total	O	0	0
			78	78		
4	E	1	Total	O	0	0
			1	1		

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.

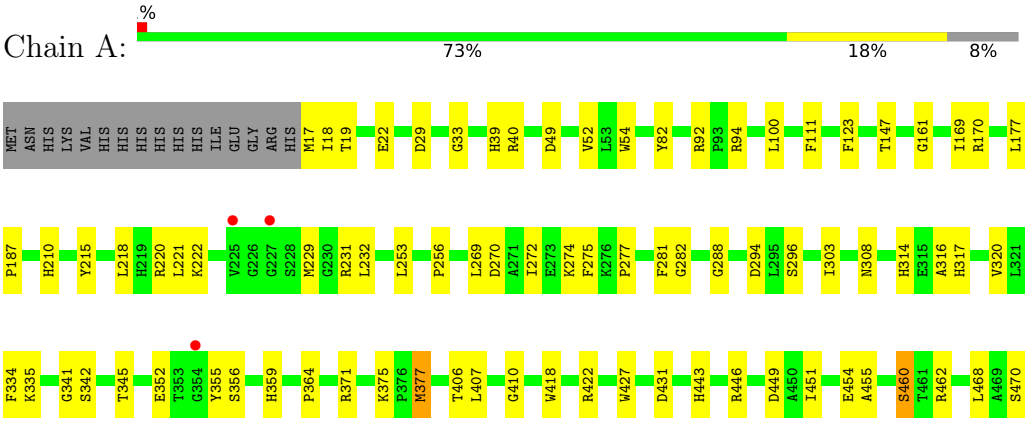
• Molecule 1: Putative AMP-binding enzyme

Chain B:



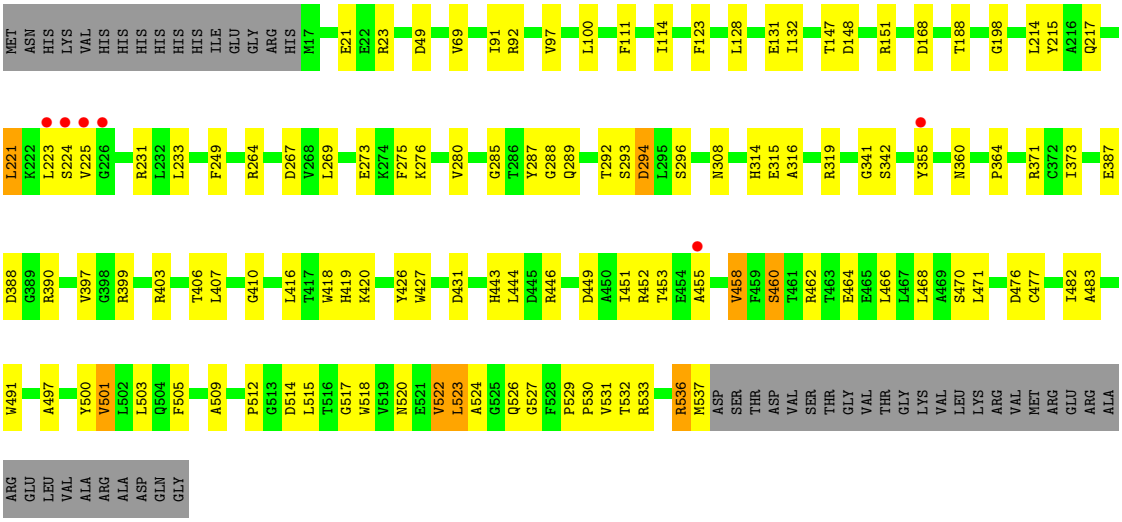
• Molecule 1: Putative AMP-binding enzyme

Chain A:



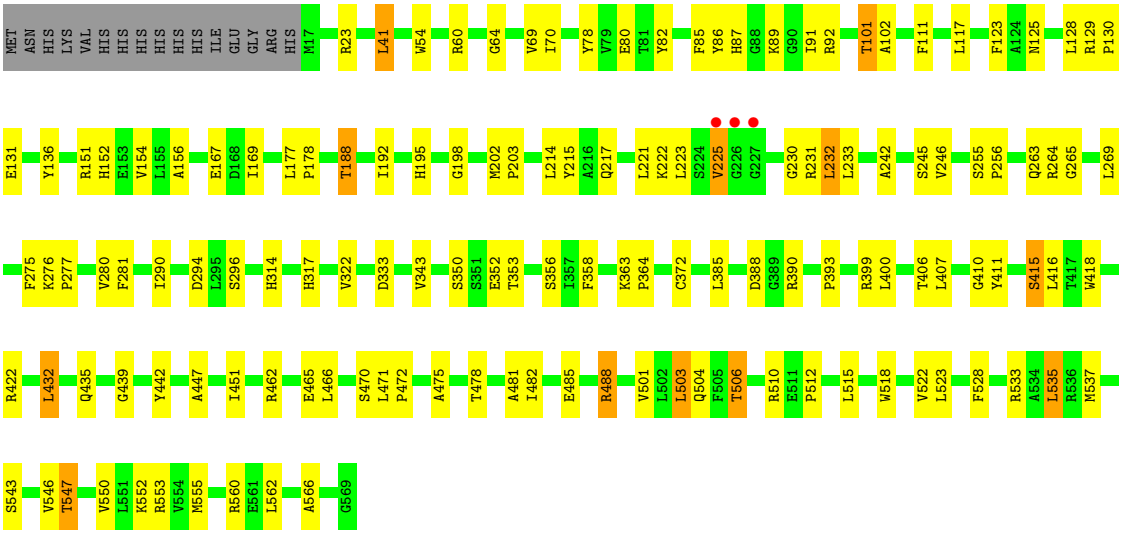
• Molecule 1: Putative AMP-binding enzyme

Chain C:



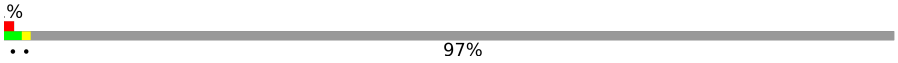
• Molecule 1: Putative AMP-binding enzyme

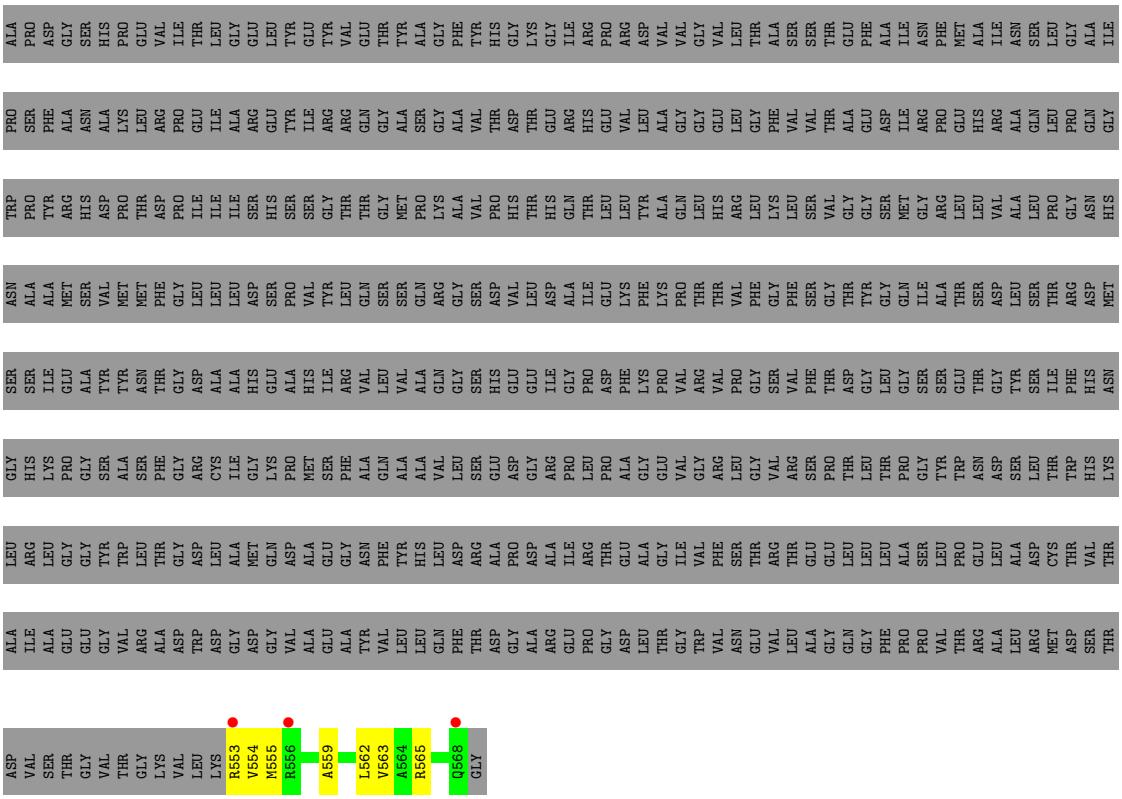
Chain D:



• Molecule 1: Putative AMP-binding enzyme

Chain E:




ALA PRO ASP GLY SER HIS PRO GLU VAL ILE THR LEU GLY GLU LEU TYR GLU TYR VAL GLU THR TYR ALA GLY PHE TYR HIS GLY LYS GLY ILE ARG PRO ARG ASP VAL VAL GLY VAL LEU THR ALA SER SER THR GLU PHE ALA ILE ASN PHE MET ALA ILE ASN SER LEU GLY ALA ILE
PRO SER PHE ALA ASN ALA LYS LEU ARG PRO GLU ILE ALA ARG GLU TYR ILE ARG ARG GLN GLY ALA SER GLY ALA VAL THR ASP THR GLU ARG HIS GLU VAL LEU ALA GLY GLY GLU LEU GLY PHE VAL VAL THR ALA GLU ASP ILE ARG PRO GLU HIS ARG ALA GLN LEU PRO GLN GLY
TRP PRO TYR ARG HIS ASP PRO THR ASP PRO ILE ILE ILE ILE SER HIS SER SER GLY THR THR GLY MET PRO LYS ALA VAL PRO HIS THR HIS GLN THR LEU LEU TYR ALA GLN LEU HIS ARG LEU LYS LEU SER VAL GLY GLY SER MET GLY ARG LEU LEU VAL ALA ALA LEU PRO GLY ASN HIS
ASN ALA ALA MET SER VAL MET MET PHE GLY LEU LEU LEU LEU ASP SER PRO VAL TYR LEU GLN SER SER GLN ARG GLY SER ASP VAL LEU ASP ALA ILE GLU THR THR LEU GLU LYS PHE LYS PRO THR THR VAL PHE GLY PHE SER GLY THR TYR GLY GLN ILE ALA THR SER ASP LEU SER THR ARG ASP MET
SER SER ILE GLU ALA TYR TYR ASN THR GLY ASP ALA HIS GLU ALA HIS ILE ARG VAL LEU VAL ALA ALA GLN GLY SER HIS GLU GLU ILE GLY PRO ASP PHE LYS PRO VAL ARG VAL PRO GLY SER VAL PHE THR ASP GLY LEU GLY SER SER GLU THR GLY GLY TYR SER ILE PHE HIS ASN
GLY HIS LYS PRO GLY SER ALA SER PHE GLY ARG CYS ILE GLY LYS PRO MET SER PHE ALA GLN ALA ALA ALA VAL LEU SER GLU ASP GLY ARG PRO LEU PRO ALA GLY GLU VAL GLY ARG LEU GLY VAL ARG SER PRO THR LEU THR PRO GLY TYR TRP ASN ASP SER LEU THR TRP HIS LYS
LEU ARG LEU GLY GLY TYR TRP LEU THR GLY ASP LEU ALA MET GLN ASP ALA GLU GLY ASN PHE TYR HIS LEU ASP ARG ALA PRO ASP ALA ILE ARG THR GLU ALA GLY ILE VAL PHE SER THR ARG THR GLU GLU LEU LEU LEU ALA SER LEU PRO GLU LEU ALA ASP CYS THR VAL THR
ALA ILE ALA GLU GLU GLY VAL ARG ALA ASP TRP ASP GLY ASP GLY VAL ALA GLU ALA TYR VAL LEU LEU GLN PHE THR ASP GLY ALA ARG GLU PRO GLY ASP LEU THR GLY TRP VAL ASN GLU VAL LEU ALA GLY GLN GLY PHE PRO PRO VAL THR ARG ALA LEU ALA ARG MET ASP SER THR
ASP VAL SER THR GLY VAL THR GLY LYS VAL LEU LYS R553 V554 M555 R556 A559 L562 V563 A564 R565 Q568 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.04Å 164.02Å 171.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.93 48.75 – 2.93	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.75-2.93) 100.0 (48.75-2.93)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.186 , 0.255 0.187 , 0.255	Depositor DCC
R_{free} test set	1936 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16715	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: MG, AMP

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	0.38	0/4082	0.56	2/5555 (0.0%)
1	B	0.35	0/4103	0.56	0/5584
1	C	0.39	0/4082	0.54	0/5555
1	D	0.36	0/4325	0.57	0/5880
1	E	0.46	0/134	0.56	0/176
All	All	0.37	0/16726	0.56	2/22750 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	VAL	CA-C-N	-5.56	113.72	122.73
1	A	52	VAL	C-N-CA	-5.56	113.72	122.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	369	PHE	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	3982	0	3866	67	1
1	B	4003	0	3882	107	0
1	C	3982	0	3866	77	1
1	D	4225	0	4120	90	0
1	E	135	0	141	4	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	D	23	0	12	0	0
4	A	134	0	0	5	0
4	B	56	0	0	1	0
4	C	92	0	0	2	0
4	D	78	0	0	2	0
4	E	1	0	0	0	0
All	All	16715	0	15887	335	1

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 10.

All (335) 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:D:471:LEU:HD21	1:D:522:VAL:HG21	1.45	0.99
1:B:434:MET:HE1	1:A:334:PHE:HB3	1.59	0.84
1:B:231:ARG:NH1	1:B:275:PHE:O	2.14	0.80
1:B:501:VAL:HG11	1:B:519:VAL:HG11	1.65	0.78
1:B:387:GLU:OE1	1:B:399:ARG:NH2	2.18	0.77
1:A:231:ARG:NH1	1:A:275:PHE:O	2.19	0.76
1:C:523:LEU:HD21	1:C:530:PRO:HA	1.69	0.75
1:B:397:VAL:HG22	1:B:434:MET:HE2	1.69	0.74
1:C:21:GLU:OE2	1:C:21:GLU:N	2.18	0.73
1:A:371:ARG:HD2	1:A:462:ARG:HD2	1.72	0.72
1:B:467:LEU:HD22	1:B:471:LEU:HD12	1.71	0.70
1:C:466:LEU:HD11	1:C:526:GLN:HG3	1.73	0.70
1:D:350:SER:HB3	1:D:353:THR:HG23	1.73	0.70
1:B:134:ARG:NH2	1:B:156:ALA:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:VAL:HB	1:B:529:PRO:HG2	1.73	0.70
1:C:388:ASP:OD2	1:C:390:ARG:NH1	2.25	0.70
1:D:202:MET:SD	1:D:203:PRO:HD2	2.31	0.69
1:D:533:ARG:HD3	1:D:566:ALA:HB1	1.73	0.69
1:B:348:LEU:HD23	1:B:349:GLY:H	1.58	0.68
1:B:360:ASN:ND2	1:B:372:CYS:O	2.23	0.68
1:D:543:SER:H	1:D:555:MET:CE	2.06	0.68
1:D:231:ARG:NH2	1:D:275:PHE:O	2.23	0.68
1:D:466:LEU:HD23	1:D:523:LEU:HD23	1.75	0.67
1:C:501:VAL:HG12	1:C:531:VAL:HG21	1.76	0.67
1:C:224:SER:HB2	1:D:393:PRO:HA	1.77	0.67
1:A:221:LEU:HD21	1:A:253:LEU:HD21	1.76	0.67
1:A:422:ARG:NH2	1:C:188:THR:OG1	2.27	0.67
1:C:468:LEU:HD21	1:C:476:ASP:HA	1.76	0.67
1:A:449:ASP:O	1:A:460:SER:OG	2.11	0.66
1:C:520:ASN:HA	1:C:523:LEU:HD22	1.77	0.66
1:D:129:ARG:NH2	1:D:131:GLU:OE2	2.20	0.66
1:D:128:LEU:HD23	1:D:546:VAL:HG11	1.77	0.66
1:C:198:GLY:HA2	1:E:555:MET:HE3	1.78	0.66
1:B:170:ARG:NE	1:B:172:GLU:OE2	2.23	0.65
1:A:215:TYR:HB3	1:A:406:THR:HG22	1.79	0.65
1:A:510:ARG:HD2	1:A:536:ARG:HH11	1.60	0.64
1:D:60:ARG:NH1	1:D:64:GLY:HA2	2.13	0.64
1:A:345:THR:HG21	1:A:359:HIS:HD2	1.62	0.63
1:D:23:ARG:HH22	1:D:225:VAL:HG22	1.63	0.63
1:D:451:ILE:HG12	1:D:481:ALA:HB2	1.81	0.63
1:C:23:ARG:HH22	1:C:225:VAL:HG22	1.62	0.63
1:B:503:LEU:HD21	1:B:534:ALA:HB1	1.81	0.62
1:C:288:GLY:O	1:C:292:THR:HG23	2.00	0.62
1:B:386:SER:HB3	1:B:392:LEU:HD21	1.82	0.62
1:C:451:ILE:HB	1:C:458:VAL:HG13	1.81	0.62
1:C:231:ARG:NH1	1:C:275:PHE:O	2.33	0.61
1:A:371:ARG:HD3	1:A:443:HIS:O	2.01	0.61
1:C:371:ARG:HD3	1:C:443:HIS:O	2.01	0.60
1:B:484:GLU:HB2	1:B:487:VAL:HB	1.84	0.60
1:A:431:ASP:OD1	1:A:446:ARG:NH1	2.35	0.60
1:C:397:VAL:O	4:C:601:HOH:O	2.15	0.60
1:B:111:PHE:CD2	1:B:244:MET:HE2	2.37	0.59
1:A:375:LYS:NZ	4:A:705:HOH:O	2.34	0.59
1:D:215:TYR:HB3	1:D:406:THR:HG22	1.84	0.59
1:E:562:LEU:HD22	1:E:565:ARG:HH21	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:GLY:HA3	1:D:333:ASP:HB3	1.84	0.59
1:D:475:ALA:HB2	1:D:506:THR:HG23	1.83	0.59
1:C:470:SER:OG	1:C:522:VAL:HG21	2.02	0.59
1:C:215:TYR:OH	4:C:602:HOH:O	2.17	0.59
1:B:284:SER:HB3	1:B:311:ASP:HB2	1.85	0.58
1:B:529:PRO:HB2	1:B:530:PRO:HD2	1.84	0.58
1:D:535:LEU:HD22	1:D:566:ALA:HA	1.86	0.58
1:E:559:ALA:O	1:E:563:VAL:HG23	2.02	0.58
1:D:232:LEU:HB3	1:D:281:PHE:HE1	1.69	0.58
1:B:300:MET:SD	1:B:324:GLN:HG2	2.44	0.57
1:B:269:LEU:HD23	1:B:272:ILE:HD12	1.86	0.57
1:A:314:HIS:HB2	1:A:317:HIS:ND1	2.19	0.57
1:A:329:GLU:OE2	4:A:701:HOH:O	2.17	0.57
1:D:177:LEU:HD12	1:D:178:PRO:HD2	1.86	0.57
1:B:444:LEU:O	1:B:462:ARG:NH1	2.36	0.57
1:C:315:GLU:OE2	1:C:319:ARG:NH2	2.28	0.57
1:C:341:GLY:HA3	1:C:364:PRO:HG2	1.85	0.57
1:B:55:THR:OG1	1:B:68:GLU:HA	2.05	0.56
1:D:152:HIS:CD2	1:D:156:ALA:HB2	2.40	0.56
1:B:484:GLU:O	1:B:486:GLY:N	2.32	0.56
1:D:70:ILE:HG23	1:D:78:TYR:HE2	1.70	0.56
1:B:355:TYR:HD1	1:B:356:SER:O	1.88	0.56
1:D:350:SER:OG	1:D:352:GLU:OE1	2.24	0.55
1:B:377:MET:HE2	1:B:377:MET:HA	1.88	0.55
1:A:536:ARG:HG2	1:A:537:MET:H	1.72	0.55
1:C:217:GLN:HG2	1:C:249:PHE:HB2	1.87	0.55
1:D:60:ARG:HH21	1:D:167:GLU:HA	1.72	0.55
1:C:23:ARG:NH2	1:C:225:VAL:HG22	2.21	0.55
1:B:29:ASP:OD2	1:B:44:TYR:OH	2.21	0.54
1:B:368:SER:O	1:B:368:SER:OG	2.24	0.54
1:A:29:ASP:OD2	1:A:40:ARG:HD3	2.07	0.54
1:C:483:ALA:HB2	1:C:497:ALA:HA	1.90	0.54
1:D:125:ASN:OD1	1:D:546:VAL:HB	2.07	0.54
1:B:459:PHE:O	1:B:463:THR:OG1	2.22	0.54
1:C:536:ARG:HD3	1:C:537:MET:H	1.72	0.53
1:B:358:PHE:HE2	1:B:441:PHE:CD2	2.27	0.53
1:D:533:ARG:CD	1:D:566:ALA:HB1	2.37	0.53
1:B:393:PRO:HD2	1:B:396:GLU:CD	2.34	0.53
1:A:345:THR:CG2	1:A:359:HIS:HD2	2.20	0.53
1:B:96:VAL:HB	1:B:142:ALA:HA	1.90	0.53
1:B:367:ALA:HA	1:B:369:PHE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:HG3	1:C:426:TYR:CD2	2.43	0.53
1:B:303:ILE:HG21	1:B:306:TYR:CZ	2.43	0.53
1:A:111:PHE:HB2	1:A:123:PHE:HZ	1.73	0.53
1:A:483:ALA:HB2	1:A:497:ALA:HB2	1.90	0.53
1:C:287:TYR:HD2	1:C:308:ASN:HD22	1.56	0.53
1:B:466:LEU:HD23	1:B:523:LEU:HD23	1.90	0.53
1:A:294:ASP:OD1	1:A:296:SER:OG	2.26	0.53
1:C:23:ARG:HH12	1:C:224:SER:HA	1.73	0.53
1:B:474:LEU:HD21	1:B:503:LEU:HB3	1.90	0.52
1:D:198:GLY:O	1:D:553:ARG:NH1	2.42	0.52
1:D:435:GLN:HE21	1:D:439:GLY:HA2	1.74	0.52
1:C:505:PHE:HB3	1:C:509:ALA:HB3	1.91	0.52
1:D:222:LYS:O	1:D:223:LEU:HD22	2.10	0.52
1:D:503:LEU:HD23	1:D:515:LEU:HD13	1.91	0.52
1:B:147:THR:HG22	1:B:148:ASP:O	2.10	0.52
1:B:21:GLU:CD	1:B:21:GLU:H	2.18	0.52
1:B:268:VAL:O	1:B:272:ILE:HG13	2.09	0.52
1:A:455:ALA:HB1	1:A:530:PRO:HD2	1.92	0.51
1:B:48:THR:HG23	4:B:613:HOH:O	2.09	0.51
1:B:479:VAL:HA	1:B:500:TYR:O	2.09	0.51
1:C:215:TYR:HB3	1:C:406:THR:HG22	1.92	0.51
1:B:367:ALA:HA	1:B:369:PHE:CE1	2.46	0.51
1:D:399:ARG:HD3	4:D:737:HOH:O	2.10	0.51
1:D:485:GLU:OE2	1:D:485:GLU:HA	2.10	0.51
1:C:449:ASP:HB3	1:C:460:SER:HB2	1.91	0.51
1:C:455:ALA:O	1:C:529:PRO:HB3	2.11	0.51
1:D:242:ALA:O	1:D:246:VAL:HG23	2.11	0.51
1:B:268:VAL:HB	1:B:290:ILE:HD11	1.92	0.51
1:C:500:TYR:CD2	1:C:533:ARG:HB3	2.46	0.51
1:C:471:LEU:HD13	1:C:518:TRP:CZ2	2.46	0.51
1:A:187:PRO:HD3	4:A:710:HOH:O	2.10	0.51
1:A:272:ILE:HD13	1:A:303:ILE:HD11	1.92	0.51
1:B:477:CYS:SG	1:B:478:THR:N	2.83	0.50
1:D:230:GLY:O	1:D:255:SER:HB2	2.12	0.50
1:D:294:ASP:OD1	1:D:296:SER:OG	2.25	0.50
1:C:444:LEU:O	1:C:462:ARG:NH1	2.40	0.50
1:D:80:GLU:HG2	1:D:177:LEU:HD22	1.94	0.50
1:B:135:GLU:O	1:B:139:ARG:HG3	2.12	0.50
1:B:269:LEU:HD11	1:B:290:ILE:HG23	1.93	0.50
1:B:537:MET:HG2	1:B:538:ASP:N	2.27	0.50
1:A:82:TYR:CE2	1:A:169:ILE:HD13	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:HG2	1:A:537:MET:N	2.26	0.50
1:D:422:ARG:NH1	4:D:707:HOH:O	2.45	0.50
1:B:247:MET:HE2	1:B:259:LEU:HD11	1.94	0.49
1:B:489:ALA:HB3	1:B:497:ALA:HB2	1.94	0.49
1:C:131:GLU:CD	1:C:131:GLU:H	2.20	0.49
1:A:100:LEU:HB3	1:A:147:THR:HG22	1.94	0.49
1:D:372:CYS:HB2	1:D:442:TYR:CE2	2.48	0.49
1:A:54:TRP:CZ3	1:A:256:PRO:HB3	2.47	0.49
1:C:514:ASP:OD1	1:C:517:GLY:N	2.42	0.49
1:D:543:SER:H	1:D:555:MET:HE3	1.77	0.49
1:B:141:GLY:HA3	1:D:416:LEU:HD22	1.95	0.48
1:C:23:ARG:NH1	1:C:224:SER:HA	2.28	0.48
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.65	0.48
1:A:220:ARG:HH21	1:A:377:MET:HE1	1.77	0.48
1:C:387:GLU:CD	1:C:399:ARG:HE	2.21	0.48
1:B:466:LEU:HD22	1:B:528:PHE:CD1	2.48	0.48
1:D:232:LEU:HB3	1:D:281:PHE:CE1	2.46	0.48
1:D:410:GLY:HA2	1:D:418:TRP:CD2	2.48	0.48
1:B:62:PRO:O	1:B:171:PRO:HD3	2.13	0.48
1:B:263:GLN:HB3	1:B:286:THR:OG1	2.14	0.48
1:A:33:GLY:HA3	1:A:210:HIS:CE1	2.49	0.48
1:D:136:TYR:CZ	1:D:195:HIS:HB3	2.48	0.48
1:B:538:ASP:CG	1:B:539:SER:H	2.22	0.48
1:C:468:LEU:HD11	1:C:477:CYS:H	1.79	0.48
1:D:352:GLU:OE2	1:D:411:TYR:OH	2.27	0.48
1:C:407:LEU:HD21	1:C:427:TRP:HB2	1.96	0.47
1:B:195:HIS:HB2	1:B:203:PRO:HB2	1.97	0.47
1:D:60:ARG:HH11	1:D:64:GLY:HA2	1.80	0.47
1:A:512:PRO:O	1:A:514:ASP:N	2.48	0.47
1:C:482:ILE:HB	1:C:500:TYR:CE1	2.48	0.47
1:C:536:ARG:CD	1:C:537:MET:H	2.27	0.47
1:B:147:THR:HG21	1:B:151:ARG:C	2.39	0.47
1:B:466:LEU:HD11	1:B:526:GLN:HG3	1.97	0.47
1:A:231:ARG:HB2	1:A:277:PRO:HA	1.96	0.47
1:C:111:PHE:HB2	1:C:123:PHE:HZ	1.79	0.47
1:C:503:LEU:O	1:C:536:ARG:HG2	2.14	0.47
1:D:470:SER:C	1:D:471:LEU:HD23	2.40	0.47
1:B:51:PRO:HB2	1:B:54:TRP:CH2	2.50	0.47
1:B:217:GLN:O	1:B:220:ARG:HG2	2.15	0.47
1:C:410:GLY:HA2	1:C:418:TRP:CD2	2.50	0.47
1:B:386:SER:OG	1:B:390:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HE	1:A:40:ARG:HA	1.80	0.46
1:B:247:MET:O	1:B:251:LEU:HD13	2.14	0.46
1:B:452:ARG:NH1	1:B:491:TRP:O	2.49	0.46
1:A:510:ARG:O	1:A:512:PRO:HD3	2.16	0.46
1:D:87:HIS:NE2	1:D:178:PRO:HB3	2.31	0.46
1:D:136:TYR:OH	1:D:195:HIS:HB3	2.14	0.46
1:D:269:LEU:HD11	1:D:290:ILE:HG23	1.97	0.46
1:B:205:ALA:HB3	1:B:412:TRP:HB3	1.98	0.46
1:C:264:ARG:HB2	1:C:267:ASP:OD2	2.15	0.46
1:C:431:ASP:OD1	1:C:446:ARG:HD2	2.14	0.46
1:D:353:THR:HA	1:D:407:LEU:HD12	1.97	0.46
1:A:352:GLU:O	1:A:407:LEU:HD12	2.15	0.46
1:C:314:HIS:HD2	1:C:316:ALA:HB3	1.81	0.46
1:D:432:LEU:HD22	1:D:447:ALA:HA	1.98	0.46
1:B:217:GLN:HG2	1:B:249:PHE:HB2	1.98	0.46
1:B:413:ASN:H	1:D:415:SER:HB2	1.81	0.46
1:B:436:ASP:OD2	1:B:442:TYR:OH	2.31	0.46
1:A:33:GLY:CA	1:A:210:HIS:CE1	3.00	0.45
1:A:355:TYR:HD2	1:A:356:SER:O	1.99	0.45
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.81	0.45
1:B:403:ARG:HG3	1:B:426:TYR:CD2	2.51	0.45
1:C:294:ASP:OD1	1:C:296:SER:OG	2.27	0.45
1:D:60:ARG:NH2	1:D:167:GLU:HA	2.30	0.45
1:B:188:THR:OG1	1:D:422:ARG:NH2	2.49	0.45
1:B:411:TYR:HE2	1:B:421:LEU:HD12	1.81	0.45
1:B:432:LEU:HD21	1:B:447:ALA:HA	1.98	0.45
1:B:474:LEU:HD21	1:B:503:LEU:HD12	1.98	0.45
1:D:314:HIS:HB2	1:D:317:HIS:ND1	2.30	0.45
1:A:473:GLU:OE2	4:A:702:HOH:O	2.21	0.45
1:D:111:PHE:HE1	1:D:192:ILE:HB	1.82	0.45
1:C:342:SER:O	1:C:364:PRO:HD3	2.17	0.45
1:B:348:LEU:CD2	1:B:349:GLY:H	2.29	0.45
1:B:108:ALA:HB2	1:B:247:MET:HE1	1.98	0.45
1:A:17:MET:SD	1:A:17:MET:N	2.89	0.45
1:D:533:ARG:HG2	1:D:535:LEU:HD21	1.98	0.44
1:B:82:TYR:CE2	1:B:169:ILE:HD13	2.51	0.44
1:A:316:ALA:O	1:A:320:VAL:HG23	2.17	0.44
1:D:111:PHE:HB2	1:D:123:PHE:HZ	1.82	0.44
1:D:470:SER:O	1:D:472:PRO:HD3	2.17	0.44
1:B:294:ASP:OD1	1:B:296:SER:OG	2.22	0.44
1:B:529:PRO:HB2	1:B:530:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLY:HA3	1:A:364:PRO:HG2	1.99	0.44
1:D:388:ASP:OD1	1:D:390:ARG:HG3	2.17	0.44
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.78	0.44
1:C:523:LEU:HD23	1:C:524:ALA:N	2.33	0.44
1:D:543:SER:H	1:D:555:MET:HE2	1.81	0.44
1:A:536:ARG:CG	1:A:537:MET:H	2.31	0.44
1:A:270:ASP:O	1:A:274:LYS:HG2	2.16	0.44
1:C:100:LEU:HB3	1:C:147:THR:HG22	2.00	0.44
1:C:451:ILE:HG22	1:C:453:THR:HG23	2.00	0.44
1:C:482:ILE:HB	1:C:500:TYR:HE1	1.83	0.44
1:A:94:ARG:HD2	1:C:419:HIS:HB3	1.99	0.43
1:C:514:ASP:O	1:C:515:LEU:HB2	2.18	0.43
1:B:375:LYS:HE3	1:B:440:ASN:OD1	2.18	0.43
1:C:111:PHE:HB2	1:C:123:PHE:CZ	2.53	0.43
1:C:148:ASP:OD1	1:C:151:ARG:HD2	2.17	0.43
1:D:363:LYS:HB2	1:D:364:PRO:HD2	2.00	0.43
1:D:512:PRO:HG2	1:D:518:TRP:CE2	2.53	0.43
1:C:91:ILE:O	1:C:92:ARG:HD3	2.19	0.43
1:D:230:GLY:O	1:D:256:PRO:HD2	2.17	0.43
1:D:510:ARG:HA	1:D:510:ARG:HD2	1.77	0.43
1:D:560:ARG:HG3	1:D:560:ARG:HH11	1.83	0.43
1:B:42:ARG:NH2	1:B:76:TYR:HB3	2.34	0.43
1:A:333:ASP:OD1	1:A:333:ASP:N	2.43	0.43
1:C:468:LEU:HD11	1:C:477:CYS:N	2.33	0.43
1:D:41:LEU:HD23	1:D:41:LEU:HA	1.83	0.43
1:B:263:GLN:HB3	1:B:286:THR:HG1	1.83	0.43
1:B:273:GLU:OE2	1:B:298:ARG:NH1	2.39	0.43
1:B:111:PHE:HB2	1:B:123:PHE:HZ	1.83	0.43
1:B:474:LEU:HD13	1:B:518:TRP:HH2	1.82	0.43
1:B:500:TYR:CE2	1:B:533:ARG:HB3	2.53	0.43
1:C:285:GLY:O	1:C:289:GLN:HG3	2.18	0.43
1:C:233:LEU:HD23	1:C:280:VAL:HG13	2.00	0.43
1:A:92:ARG:HD2	1:A:92:ARG:HA	1.78	0.43
1:B:87:HIS:CE1	1:B:178:PRO:HB3	2.53	0.43
1:D:263:GLN:HE22	1:D:547:THR:HA	1.84	0.43
1:D:488:ARG:HE	1:D:488:ARG:HA	1.83	0.43
1:D:231:ARG:HB2	1:D:277:PRO:HA	2.00	0.42
1:B:230:GLY:O	1:B:255:SER:HB3	2.19	0.42
1:B:451:ILE:HG23	1:B:497:ALA:HB3	2.01	0.42
1:C:214:LEU:HD12	1:C:214:LEU:HA	1.64	0.42
1:C:221:LEU:HD12	1:C:221:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ALA:HB1	1:C:530:PRO:HD2	2.00	0.42
1:D:85:PHE:O	1:D:89:LYS:HG2	2.19	0.42
1:A:477:CYS:HA	1:A:502:LEU:O	2.19	0.42
1:D:130:PRO:HB3	1:D:154:VAL:HG13	2.01	0.42
1:B:91:ILE:HD13	1:B:91:ILE:HA	1.87	0.42
1:A:514:ASP:O	1:A:516:THR:N	2.47	0.42
1:C:452:ARG:NH2	1:C:491:TRP:HA	2.34	0.42
1:C:471:LEU:HD11	1:C:522:VAL:HG11	2.02	0.42
1:B:473:GLU:O	1:B:474:LEU:HD12	2.20	0.42
1:C:97:VAL:HB	1:C:114:ILE:HD13	2.01	0.42
1:D:343:VAL:HG22	1:D:363:LYS:HB3	2.01	0.42
1:B:228:SER:OG	1:B:304:GLU:OE1	2.32	0.42
1:D:322:VAL:HB	1:D:364:PRO:HD3	2.01	0.42
1:B:387:GLU:OE1	1:B:387:GLU:HA	2.20	0.42
1:C:360:ASN:HD21	1:C:373:ILE:HA	1.85	0.42
1:D:87:HIS:O	1:D:92:ARG:NH2	2.53	0.42
1:B:447:ALA:N	1:B:448:PRO:HD2	2.34	0.42
1:B:156:ALA:HA	1:B:163:VAL:HG21	2.02	0.42
1:C:407:LEU:HA	1:C:407:LEU:HD12	1.72	0.42
1:D:54:TRP:CD1	1:D:69:VAL:HG22	2.55	0.42
1:B:534:ALA:C	1:B:535:LEU:HD12	2.44	0.42
1:D:151:ARG:HD2	1:D:151:ARG:N	2.34	0.42
1:A:288:GLY:HA2	1:A:317:HIS:CD2	2.54	0.41
1:D:86:TYR:O	1:D:91:ILE:HB	2.20	0.41
1:D:233:LEU:HB3	1:D:280:VAL:HG22	2.02	0.41
1:B:80:GLU:OE1	1:B:174:ARG:NH2	2.53	0.41
1:B:436:ASP:OD2	1:B:440:ASN:HB2	2.20	0.41
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.96	0.41
1:B:443:HIS:CD2	1:B:443:HIS:C	2.98	0.41
1:A:177:LEU:HD21	1:A:181:TRP:CE3	2.56	0.41
1:C:148:ASP:OD2	1:C:151:ARG:NH1	2.51	0.41
1:D:101:THR:OG1	1:D:102:ALA:N	2.54	0.41
1:D:358:PHE:CZ	1:D:400:LEU:HD11	2.56	0.41
1:B:59:TRP:HD1	1:B:106:GLU:HG3	1.85	0.41
1:B:471:LEU:HG	1:B:522:VAL:HG21	2.01	0.41
1:A:410:GLY:HA2	1:A:418:TRP:CD2	2.56	0.41
1:A:451:ILE:HD13	1:A:481:ALA:HB2	2.02	0.41
1:B:215:TYR:HB3	1:B:406:THR:HG22	2.03	0.41
1:A:218:LEU:O	1:A:222:LYS:HG3	2.20	0.41
1:D:214:LEU:HD22	1:D:217:GLN:HB2	2.02	0.41
1:B:422:ARG:NH2	1:D:188:THR:HB	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LEU:HD21	1:B:526:GLN:HB2	2.03	0.41
1:A:19:THR:N	1:A:22:GLU:OE1	2.37	0.41
1:A:407:LEU:HD21	1:A:427:TRP:HB2	2.03	0.41
1:D:478:THR:HG23	1:D:552:LYS:HE2	2.01	0.41
1:B:208:HIS:ND1	1:B:212:THR:OG1	2.40	0.41
1:B:232:LEU:HD12	1:B:257:VAL:HG22	2.03	0.41
1:B:358:PHE:CZ	1:B:400:LEU:HD11	2.55	0.41
1:B:466:LEU:HD13	1:B:528:PHE:CE1	2.56	0.41
1:A:161:GLY:N	4:A:714:HOH:O	2.50	0.41
1:A:186:ASP:CG	1:A:187:PRO:HD2	2.46	0.41
1:A:232:LEU:HD22	1:A:281:PHE:HE1	1.84	0.41
1:A:335:LYS:HE2	1:A:335:LYS:HB2	1.85	0.41
1:A:468:LEU:HA	1:A:468:LEU:HD23	1.89	0.41
1:A:371:ARG:HD2	1:A:462:ARG:CD	2.46	0.41
1:C:269:LEU:HD23	1:C:269:LEU:HA	1.88	0.41
1:B:397:VAL:HG13	1:B:444:LEU:HD12	2.03	0.40
1:A:470:SER:O	1:A:472:PRO:HD3	2.21	0.40
1:C:460:SER:O	1:C:464:GLU:HG3	2.20	0.40
1:D:504:GLN:HG3	1:D:537:MET:O	2.21	0.40
1:B:360:ASN:ND2	1:B:373:ILE:HA	2.36	0.40
1:A:322:VAL:HA	1:A:342:SER:OG	2.21	0.40
1:A:519:VAL:O	1:A:523:LEU:HG	2.21	0.40
1:D:276:LYS:HE3	1:D:276:LYS:HB2	1.88	0.40
1:D:462:ARG:HG2	1:D:528:PHE:CE2	2.55	0.40
1:D:482:ILE:HD11	1:D:562:LEU:HD12	2.02	0.40
1:C:273:GLU:O	1:C:276:LYS:HE3	2.21	0.40
1:C:360:ASN:ND2	1:C:373:ILE:HA	2.37	0.40
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.75	0.40
1:B:466:LEU:CD2	1:B:523:LEU:HA	2.51	0.40
1:A:39:HIS:CG	1:A:182:PRO:HG3	2.56	0.40
1:A:282:GLY:O	1:A:308:ASN:HA	2.21	0.40
1:C:416:LEU:O	1:C:420:LYS:HG3	2.21	0.40
1:D:82:TYR:CE2	1:D:169:ILE:HD13	2.56	0.40
1:E:555:MET:SD	1:E:555:MET:N	2.89	0.40

All (1) 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:A:170:ARG:NH2	1:C:168:ASP:OD1[4_545]	2.02	0.18

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	519/569 (91%)	494 (95%)	20 (4%)	5 (1%)	13	32
1	B	522/569 (92%)	464 (89%)	52 (10%)	6 (1%)	12	30
1	C	519/569 (91%)	487 (94%)	29 (6%)	3 (1%)	22	46
1	D	551/569 (97%)	515 (94%)	33 (6%)	3 (0%)	25	50
1	E	14/569 (2%)	14 (100%)	0	0	100	100
All	All	2125/2845 (75%)	1974 (93%)	134 (6%)	17 (1%)	16	38

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	348	LEU
1	B	538	ASP
1	A	229	MET
1	A	513	GLY
1	C	294	ASP
1	C	355	TYR
1	B	485	GLU
1	B	509	ALA
1	A	515	LEU
1	D	225	VAL
1	D	264	ARG
1	D	265	GLY
1	B	470	SER
1	A	377	MET
1	B	490	ASP
1	A	506	THR
1	C	512	PRO

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	414/455 (91%)	409 (99%)	5 (1%)	67 81
1	B	417/455 (92%)	404 (97%)	13 (3%)	35 59
1	C	414/455 (91%)	400 (97%)	14 (3%)	32 56
1	D	440/455 (97%)	422 (96%)	18 (4%)	26 50
1	E	13/455 (3%)	11 (85%)	2 (15%)	2 5
All	All	1698/2275 (75%)	1646 (97%)	52 (3%)	35 59

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	139	ARG
1	B	192	ILE
1	B	224	SER
1	B	266	SER
1	B	348	LEU
1	B	356	SER
1	B	458	VAL
1	B	477	CYS
1	B	492	ASP
1	B	501	VAL
1	B	503	LEU
1	B	504	GLN
1	B	522	VAL
1	A	18	ILE
1	A	49	ASP
1	A	454	GLU
1	A	460	SER
1	A	480	THR
1	C	49	ASP
1	C	69	VAL
1	C	128	LEU
1	C	132	ILE
1	C	221	LEU

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Mol	Chain	Res	Type
1	C	223	LEU
1	C	293	SER
1	C	458	VAL
1	C	460	SER
1	C	501	VAL
1	C	522	VAL
1	C	523	LEU
1	C	532	THR
1	C	536	ARG
1	D	41	LEU
1	D	101	THR
1	D	188	THR
1	D	221	LEU
1	D	232	LEU
1	D	245	SER
1	D	356	SER
1	D	385	LEU
1	D	415	SER
1	D	432	LEU
1	D	465	GLU
1	D	488	ARG
1	D	501	VAL
1	D	503	LEU
1	D	506	THR
1	D	535	LEU
1	D	547	THR
1	D	550	VAL
1	E	553	ARG
1	E	554	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	176	GLN
1	B	211	GLN
1	A	27	ASN
1	A	176	GLN
1	A	359	HIS
1	A	440	ASN
1	C	176	GLN
1	C	308	ASN
1	C	314	HIS

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Mol	Chain	Res	Type
1	C	359	HIS
1	C	360	ASN
1	C	440	ASN
1	D	27	ASN
1	D	289	GLN
1	D	308	ASN
1	D	381	GLN
1	D	435	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	AMP	D	601	2	22,25,25	0.79	1 (4%)	25,38,38	1.44	4 (16%)

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
3	AMP	D	601	2	-	4/6/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	AMP	C5-C4	2.26	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	601	AMP	C3'-C2'-C1'	3.24	105.85	100.98
3	D	601	AMP	N3-C2-N1	-2.84	124.24	128.68
3	D	601	AMP	C4-C5-N7	-2.54	106.75	109.40
3	D	601	AMP	O2P-P-O5'	-2.24	100.78	106.73

There are no chirality outliers.

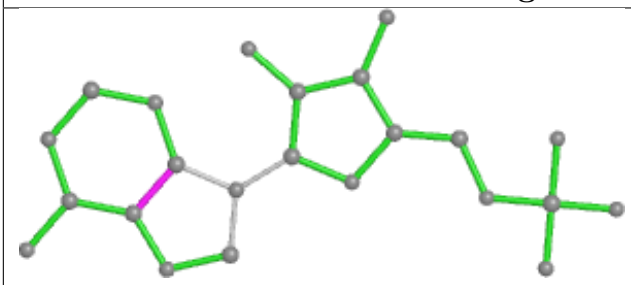
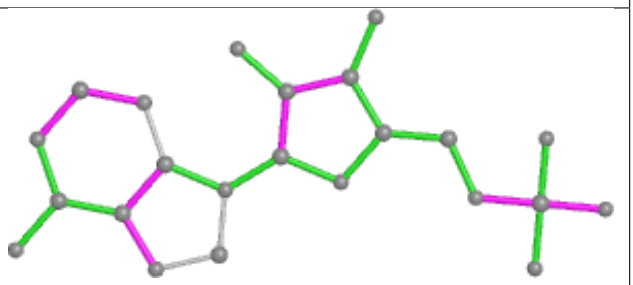
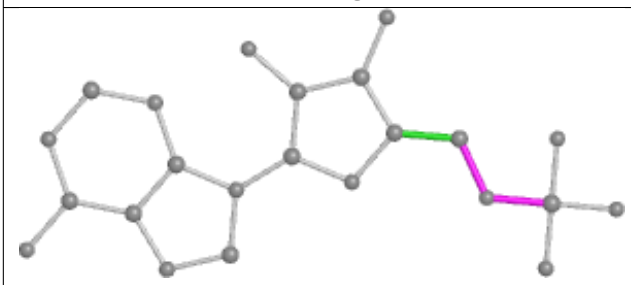
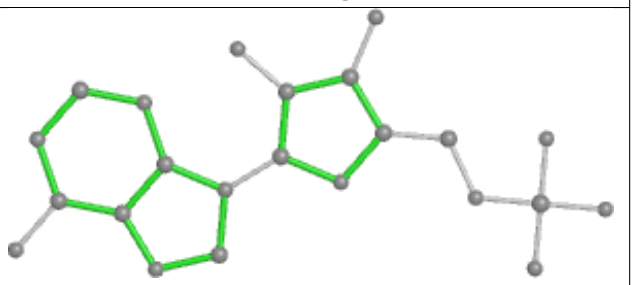
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	AMP	C5'-O5'-P-O1P
3	D	601	AMP	C5'-O5'-P-O2P
3	D	601	AMP	C5'-O5'-P-O3P
3	D	601	AMP	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AMP D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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^{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	521/569 (91%)	-0.75	3 (0%) 85 85	18, 36, 64, 93	0
1	B	524/569 (92%)	0.05	40 (7%) 21 22	27, 55, 129, 145	0
1	C	521/569 (91%)	-0.53	6 (1%) 76 74	17, 40, 91, 116	0
1	D	553/569 (97%)	-0.56	3 (0%) 87 86	25, 44, 65, 95	0
1	E	16/569 (2%)	1.17	3 (18%) 4 6	66, 79, 85, 91	0
All	All	2135/2845 (75%)	-0.43	55 (2%) 57 54	17, 44, 94, 145	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	VAL	4.5
1	B	469	ALA	4.5
1	B	482	ILE	4.0
1	B	503	LEU	4.0
1	B	515	LEU	4.0
1	B	475	ALA	3.6
1	B	468	LEU	3.4
1	B	487	VAL	3.3
1	B	451	ILE	3.3
1	B	499	ALA	3.2
1	B	474	LEU	3.2
1	D	226	GLY	3.1
1	B	512	PRO	3.0
1	B	535	LEU	3.0
1	B	522	VAL	3.0
1	B	534	ALA	3.0
1	B	501	VAL	3.0
1	C	225	VAL	2.8
1	B	481	ALA	2.8
1	B	506	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	531	VAL	2.8
1	B	467	LEU	2.7
1	B	540	THR	2.7
1	C	355	TYR	2.7
1	D	227	GLY	2.7
1	B	472	PRO	2.7
1	B	530	PRO	2.6
1	D	225	VAL	2.6
1	B	455	ALA	2.6
1	B	497	ALA	2.6
1	C	455	ALA	2.6
1	B	523	LEU	2.6
1	B	505	PHE	2.5
1	B	518	TRP	2.5
1	A	225	VAL	2.5
1	E	556	ARG	2.5
1	B	532	THR	2.4
1	B	508	GLY	2.3
1	C	224	SER	2.3
1	B	516	THR	2.3
1	B	460	SER	2.3
1	A	354	GLY	2.2
1	A	227	GLY	2.2
1	C	226	GLY	2.2
1	B	509	ALA	2.2
1	B	500	TYR	2.2
1	B	537	MET	2.2
1	E	568	GLN	2.1
1	B	313	ALA	2.1
1	B	502	LEU	2.1
1	B	470	SER	2.1
1	B	471	LEU	2.1
1	E	553	ARG	2.1
1	B	199	THR	2.0
1	C	223	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 monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.