Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:20 PM GMT

PDB ID	:	4C5U
Title	:	Structural Investigations into the Stereochemistry and Activity of a Phenylalanine-2,3-Aminomutase from Taxus chinensis
Authors	:	Wybenga, G.G.; Szymanski, W.; Wu, B.; Feringa, B.L.; Janssen, D.B.; Dijkstra, B.W.
Deposited on	:	2013-09-16
Resolution	:	2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

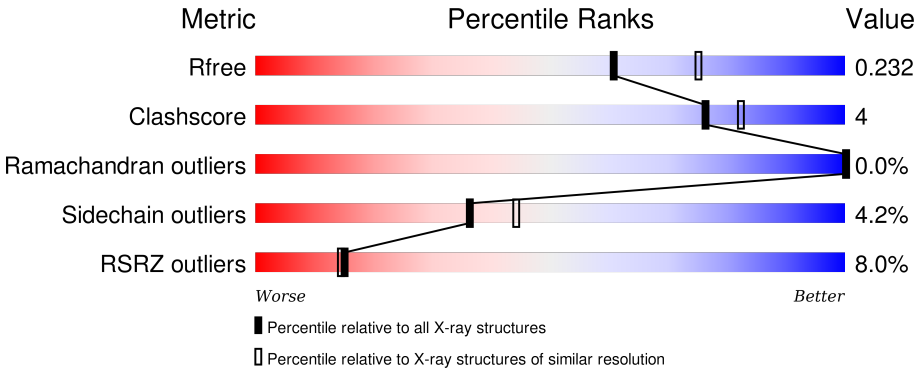
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	707	7% 77% 13% • 9%
1	B	707	6% 80% 9% • 10%
1	C	707	8% 78% 12% • 10%
1	D	707	7% 78% 11% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19779 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 PHENYLALANINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			4962	3147	855	937	23			
1	B	636	Total	C	N	O	S	0	0	0
			4922	3120	847	932	23			
1	C	639	Total	C	N	O	S	0	0	0
			4941	3133	853	932	23			
1	D	636	Total	C	N	O	S	0	0	0
			4917	3121	848	925	23			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q68G84
A	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
A	-17	SER	-	EXPRESSION TAG	UNP Q68G84
A	-16	SER	-	EXPRESSION TAG	UNP Q68G84
A	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-9	SER	-	EXPRESSION TAG	UNP Q68G84
A	-8	SER	-	EXPRESSION TAG	UNP Q68G84
A	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
A	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
A	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
A	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
A	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
A	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
A	-1	SER	-	EXPRESSION TAG	UNP Q68G84
A	0	HIS	-	EXPRESSION TAG	UNP Q68G84
A	322	ALA	TYR	ENGINEERED MUTATION	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP Q68G84
B	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
B	-17	SER	-	EXPRESSION TAG	UNP Q68G84
B	-16	SER	-	EXPRESSION TAG	UNP Q68G84
B	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-9	SER	-	EXPRESSION TAG	UNP Q68G84
B	-8	SER	-	EXPRESSION TAG	UNP Q68G84
B	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
B	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
B	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
B	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
B	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
B	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
B	-1	SER	-	EXPRESSION TAG	UNP Q68G84
B	0	HIS	-	EXPRESSION TAG	UNP Q68G84
B	322	ALA	TYR	ENGINEERED MUTATION	UNP Q68G84
C	-19	MET	-	EXPRESSION TAG	UNP Q68G84
C	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-17	SER	-	EXPRESSION TAG	UNP Q68G84
C	-16	SER	-	EXPRESSION TAG	UNP Q68G84
C	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-9	SER	-	EXPRESSION TAG	UNP Q68G84
C	-8	SER	-	EXPRESSION TAG	UNP Q68G84
C	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
C	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
C	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
C	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
C	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-1	SER	-	EXPRESSION TAG	UNP Q68G84
C	0	HIS	-	EXPRESSION TAG	UNP Q68G84
C	322	ALA	TYR	ENGINEERED MUTATION	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	EXPRESSION TAG	UNP Q68G84
D	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-17	SER	-	EXPRESSION TAG	UNP Q68G84
D	-16	SER	-	EXPRESSION TAG	UNP Q68G84
D	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-9	SER	-	EXPRESSION TAG	UNP Q68G84
D	-8	SER	-	EXPRESSION TAG	UNP Q68G84
D	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
D	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
D	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
D	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
D	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-1	SER	-	EXPRESSION TAG	UNP Q68G84
D	0	HIS	-	EXPRESSION TAG	UNP Q68G84
D	322	ALA	TYR	ENGINEERED MUTATION	UNP Q68G84

- Molecule 2 is water.

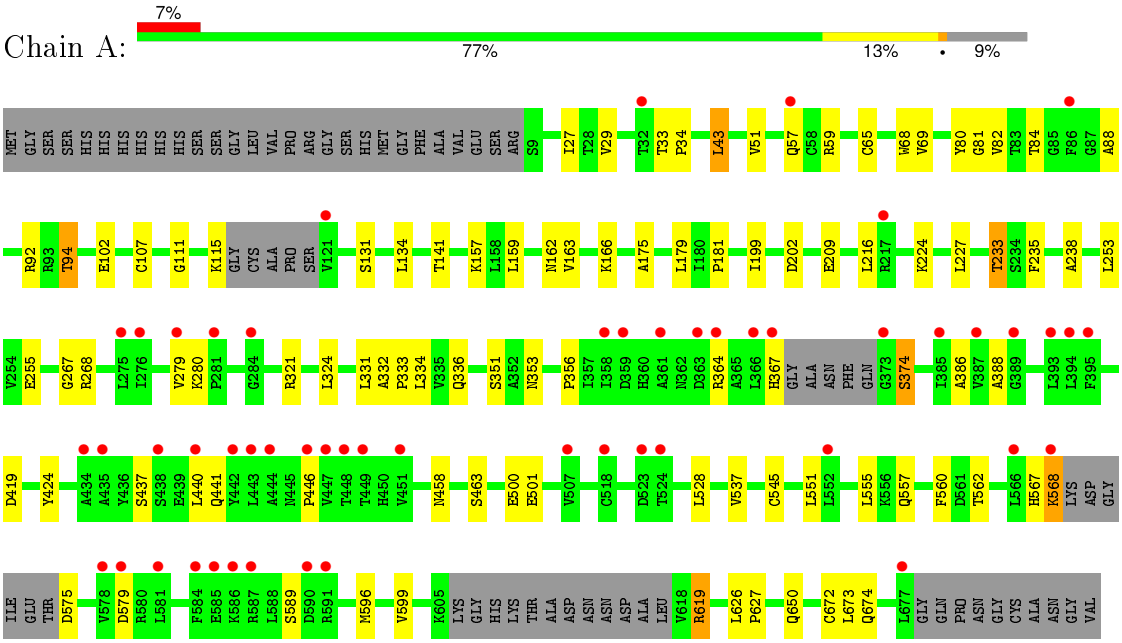
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	6	Total O 6 6	0	0
2	C	10	Total O 10 10	0	0
2	D	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

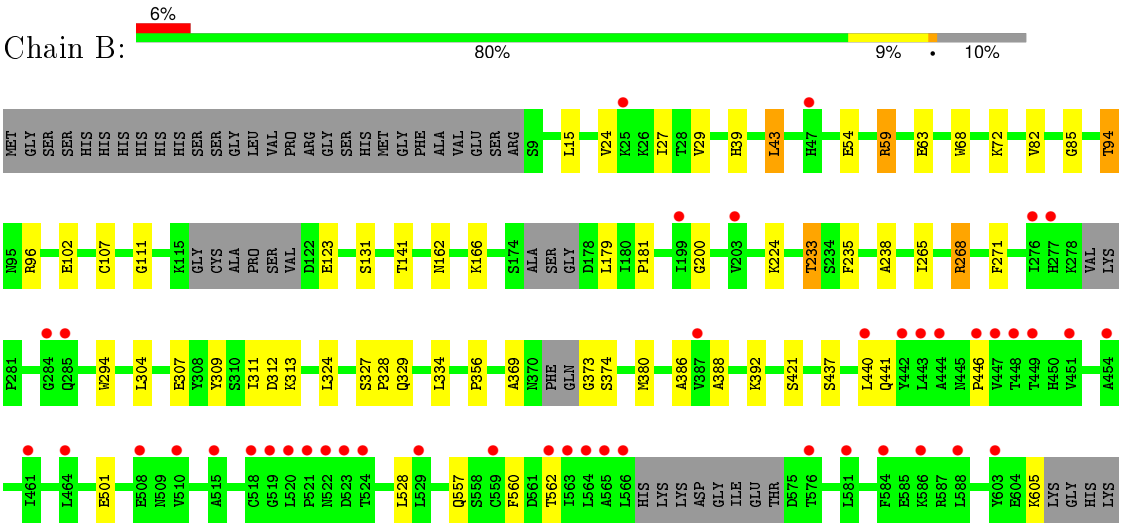
- Molecule 1: PHENYLALANINE AMMONIA-LYASE

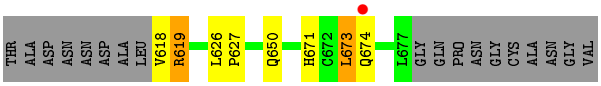
Chain A:



- Molecule 1: PHENYLALANINE AMMONIA-LYASE

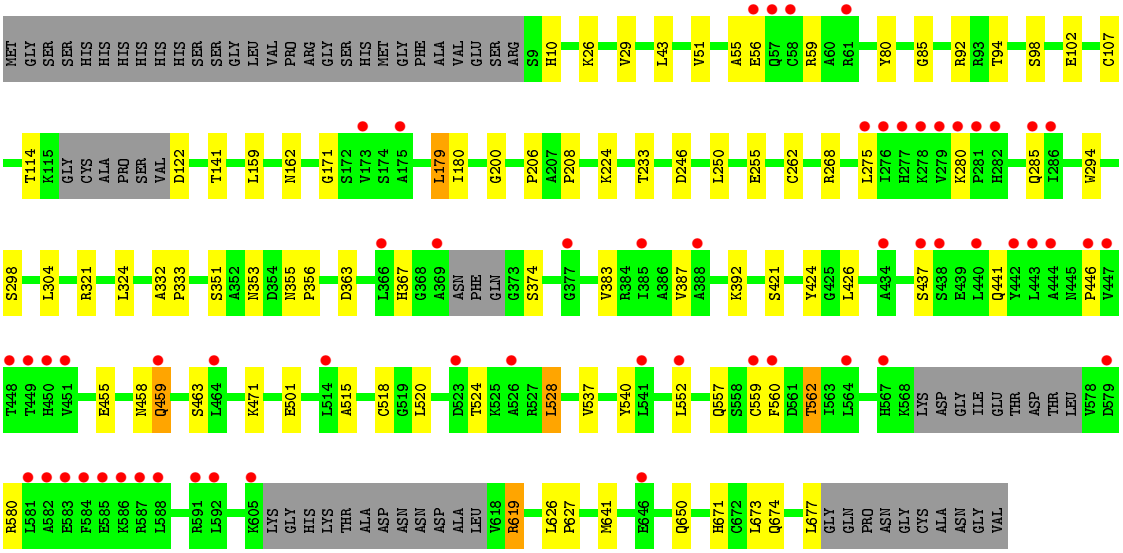
Chain B:





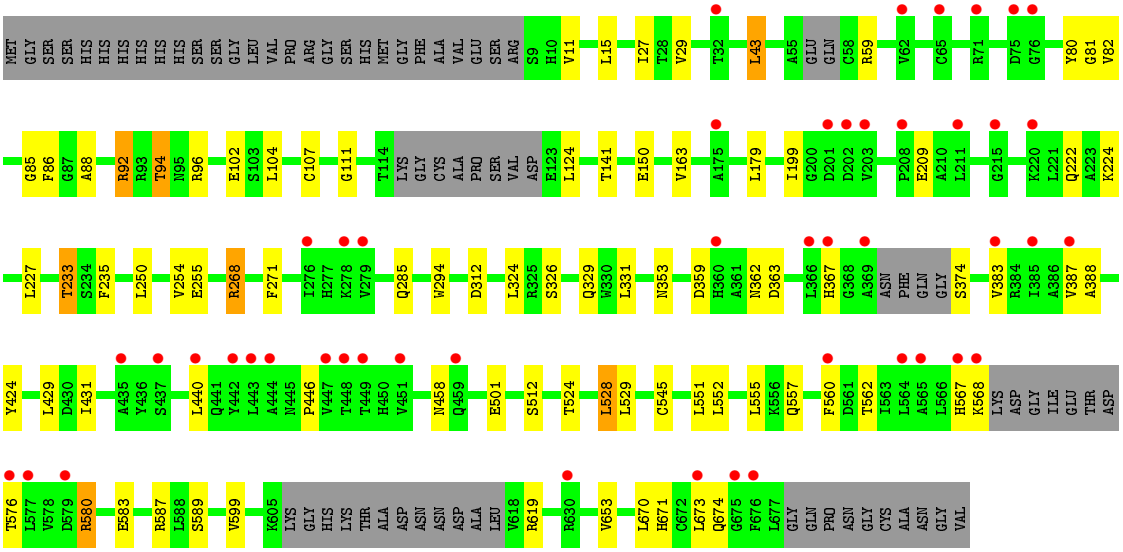
• Molecule 1: PHENYLALANINE AMMONIA-LYASE

Chain C:



• Molecule 1: PHENYLALANINE AMMONIA-LYASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.48Å 147.27Å 99.77Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	48.38 – 2.19 48.38 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.38-2.19) 98.1 (48.38-2.19)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.189 , 0.224 0.194 , 0.232	Depositor DCC
R_{free} test set	7176 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.3	EDS
Estimated twinning fraction	0.865 for H, K, L 0.135 for L, -K, H 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.865 for H, K, L 0.135 for L, -K, H	Depositor
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	1 of 141777 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19779	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.57	1/5045 (0.0%)	0.69	1/6843 (0.0%)
1	B	0.54	2/5002 (0.0%)	0.65	1/6782 (0.0%)
1	C	0.55	1/5024 (0.0%)	0.67	1/6813 (0.0%)
1	D	0.55	1/4999 (0.0%)	0.68	0/6780
All	All	0.56	5/20070 (0.0%)	0.67	3/27218 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	294	TRP	CD2-CE2	5.71	1.48	1.41
1	B	68	TRP	CD2-CE2	5.47	1.48	1.41
1	B	294	TRP	CD2-CE2	5.26	1.47	1.41
1	A	68	TRP	CD2-CE2	5.07	1.47	1.41
1	D	294	TRP	CD2-CE2	5.06	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	619	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	619	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	321	ARG	NE-CZ-NH2	-5.37	117.62	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4962	0	5044	50	0
1	B	4922	0	4993	40	0
1	C	4941	0	5021	45	0
1	D	4917	0	5004	40	0
2	A	15	0	0	0	0
2	B	6	0	0	0	0
2	C	10	0	0	0	0
2	D	6	0	0	0	0
All	All	19779	0	20062	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (151) 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:29:VAL:HG12	1:A:141:THR:HG21	1.58	0.85
1:D:580:ARG:HH11	1:D:580:ARG:CG	2.01	0.74
1:A:80:TYR:HB3	1:A:367:HIS:HD2	1.52	0.73
1:B:671:HIS:O	1:B:674:GLN:HG2	1.89	0.72
1:D:29:VAL:HG12	1:D:141:THR:HG21	1.71	0.71
1:B:446:PRO:HD3	1:D:446:PRO:HD3	1.72	0.71
1:A:557:GLN:NE2	1:D:557:GLN:OE1	2.21	0.71
1:C:501:GLU:OE1	1:C:619:ARG:HD2	1.91	0.70
1:B:557:GLN:NE2	1:C:557:GLN:OE1	2.23	0.69
1:A:650:GLN:HG3	1:B:111:GLY:O	1.93	0.68
1:A:80:TYR:HB3	1:A:367:HIS:CD2	2.30	0.66
1:C:224:LYS:HE2	1:C:356:PRO:HD2	1.78	0.65
1:A:43:LEU:HD22	1:A:134:LEU:HD22	1.79	0.64
1:B:224:LYS:HE2	1:B:356:PRO:HD2	1.80	0.63
1:C:515:ALA:HA	1:C:520:LEU:HD12	1.82	0.61
1:D:163:VAL:HG22	1:D:199:ILE:HG12	1.83	0.61
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.82	0.60
1:C:304:LEU:HD11	1:C:619:ARG:HD3	1.84	0.60
1:B:233:THR:HG21	1:B:373:GLY:N	2.15	0.60
1:C:437:SER:O	1:C:441:GLN:HG2	2.02	0.59
1:B:123:GLU:OE1	1:B:166:LYS:HE3	2.05	0.57
1:D:580:ARG:HH11	1:D:580:ARG:HG3	1.68	0.57
1:C:524:THR:HG22	1:C:528:LEU:HD22	1.87	0.56
1:C:29:VAL:HG12	1:C:141:THR:HG21	1.86	0.56
1:C:455:GLU:HB3	1:C:459:GLN:HG3	1.88	0.55
1:C:171:GLY:O	1:C:180:ILE:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HD2	1:A:216:LEU:HD21	1.88	0.55
1:A:374:SER:HA	1:A:463:SER:HB3	1.89	0.54
1:D:82:VAL:HG22	1:D:224:LYS:HB2	1.87	0.54
1:A:501:GLU:OE1	1:A:619:ARG:HD2	2.06	0.54
1:A:446:PRO:HD3	1:C:446:PRO:HD3	1.90	0.54
1:D:671:HIS:O	1:D:674:GLN:HG2	2.08	0.54
1:D:501:GLU:OE1	1:D:619:ARG:HD2	2.08	0.53
1:A:255:GLU:HG2	1:A:331:LEU:HD13	1.91	0.52
1:A:351:SER:HB2	1:C:280:LYS:HA	1.91	0.52
1:A:88:ALA:HB2	1:A:458:ASN:HB2	1.90	0.52
1:A:424:TYR:OH	1:B:85:GLY:HA2	2.10	0.52
1:A:81:GLY:HA3	1:A:227:LEU:HD22	1.92	0.52
1:A:551:LEU:O	1:A:555:LEU:HG	2.10	0.52
1:D:233:THR:HG23	1:D:233:THR:O	2.10	0.51
1:A:321:ARG:HG2	1:C:458:ASN:HA	1.93	0.50
1:C:179:LEU:HD23	1:D:431:ILE:HD13	1.94	0.50
1:A:29:VAL:CG1	1:A:141:THR:HG21	2.36	0.50
1:B:334:LEU:HD22	1:B:386:ALA:HA	1.93	0.50
1:B:327:SER:OG	1:B:328:PRO:HD3	2.12	0.50
1:D:94:THR:HB	1:D:96:ARG:H	1.77	0.50
1:B:265:ILE:HG21	1:B:324:LEU:HD12	1.94	0.49
1:B:388:ALA:HA	1:B:440:LEU:HG	1.94	0.49
1:C:114:THR:OG1	1:C:122:ASP:HB2	2.12	0.49
1:C:80:TYR:HB3	1:C:367:HIS:CD2	2.48	0.49
1:B:15:LEU:HD21	1:B:673:LEU:HD23	1.95	0.49
1:C:285:GLN:HB2	1:C:332:ALA:HB2	1.95	0.49
1:A:332:ALA:HB3	1:A:333:PRO:CD	2.42	0.49
1:C:374:SER:HA	1:C:463:SER:HB2	1.95	0.49
1:B:437:SER:O	1:B:441:GLN:HG2	2.13	0.48
1:D:88:ALA:HB2	1:D:458:ASN:HB2	1.94	0.48
1:C:10:HIS:NE2	1:C:255:GLU:OE1	2.47	0.48
1:A:545:CYS:SG	1:A:589:SER:HA	2.54	0.48
1:C:671:HIS:O	1:C:674:GLN:HG2	2.14	0.48
1:A:334:LEU:HD22	1:A:386:ALA:HA	1.95	0.48
1:C:332:ALA:HB3	1:C:333:PRO:HD3	1.94	0.48
1:B:27:ILE:CD1	1:B:43:LEU:HB2	2.43	0.48
1:B:329:GLN:O	1:D:374:SER:OG	2.27	0.48
1:D:27:ILE:CD1	1:D:43:LEU:HB2	2.44	0.47
1:A:437:SER:O	1:A:441:GLN:HG2	2.13	0.47
1:A:267:GLY:HA3	1:A:324:LEU:HD11	1.96	0.47
1:C:424:TYR:OH	1:D:85:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:PHE:HB2	1:D:560:PHE:HB2	1.96	0.47
1:A:579:ASP:OD1	1:D:567:HIS:NE2	2.42	0.47
1:D:429:LEU:HD21	1:D:653:VAL:HG21	1.96	0.47
1:B:501:GLU:OE1	1:B:619:ARG:HD2	2.14	0.47
1:B:131:SER:HB2	1:B:238:ALA:HB1	1.97	0.47
1:A:388:ALA:HA	1:A:440:LEU:HG	1.97	0.47
1:C:383:VAL:O	1:C:387:VAL:HG23	2.14	0.46
1:A:567:HIS:O	1:A:568:LYS:HD3	2.15	0.46
1:B:24:VAL:HG21	1:B:39:HIS:HD2	1.80	0.46
1:A:94:THR:HG23	1:B:421:SER:OG	2.16	0.46
1:D:81:GLY:HA3	1:D:227:LEU:HD22	1.98	0.46
1:B:59:ARG:HD2	1:B:63:GLU:OE1	2.16	0.46
1:D:86:PHE:CD2	1:D:104:LEU:HD13	2.51	0.46
1:A:419:ASP:OD2	1:B:96:ARG:NH1	2.47	0.46
1:C:304:LEU:CD1	1:C:619:ARG:HD3	2.45	0.46
1:A:596:MET:O	1:A:599:VAL:HG12	2.16	0.46
1:A:27:ILE:CD1	1:A:43:LEU:HB2	2.47	0.45
1:A:181:PRO:HB2	1:A:235:PHE:CD2	2.51	0.45
1:C:518:CYS:O	1:C:580:ARG:HD3	2.16	0.45
1:D:268:ARG:O	1:D:271:PHE:HD1	1.99	0.45
1:B:181:PRO:HB2	1:B:235:PHE:CD2	2.51	0.45
1:B:369:ALA:CB	1:D:326:SER:HB3	2.46	0.45
1:C:559:CYS:O	1:C:562:THR:HG22	2.16	0.45
1:D:359:ASP:OD2	1:D:362:ASN:HB2	2.17	0.45
1:A:500:GLU:HG3	1:A:537:VAL:HG12	1.97	0.45
1:C:246:ASP:O	1:C:250:LEU:HG	2.16	0.45
1:A:80:TYR:CB	1:A:367:HIS:CD2	3.00	0.45
1:D:285:GLN:CD	1:D:329:GLN:HG3	2.38	0.45
1:A:374:SER:HA	1:A:463:SER:CB	2.47	0.44
1:B:560:PHE:CE1	1:C:559:CYS:HB3	2.52	0.44
1:A:224:LYS:O	1:A:224:LYS:HG2	2.18	0.44
1:D:383:VAL:O	1:D:387:VAL:HG23	2.17	0.44
1:A:163:VAL:HG22	1:A:199:ILE:HG23	1.99	0.44
1:C:332:ALA:HB3	1:C:333:PRO:CD	2.47	0.44
1:C:51:VAL:HG21	1:C:159:LEU:HD13	2.00	0.44
1:D:11:VAL:O	1:D:15:LEU:HG	2.18	0.44
1:B:560:PHE:HB2	1:C:560:PHE:HB2	2.00	0.44
1:C:537:VAL:HA	1:C:540:TYR:CE2	2.53	0.43
1:C:421:SER:HB3	1:D:92:ARG:NH1	2.33	0.43
1:B:27:ILE:HD12	1:B:43:LEU:HB2	2.01	0.43
1:A:111:GLY:O	1:B:650:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:PRO:HB2	1:C:208:PRO:HD2	1.99	0.43
1:B:268:ARG:O	1:B:271:PHE:HD1	2.01	0.43
1:D:524:THR:HG22	1:D:528:LEU:HD22	2.01	0.43
1:B:309:TYR:O	1:B:313:LYS:HG3	2.19	0.43
1:C:426:LEU:HD11	1:C:641:MET:SD	2.58	0.43
1:D:512:SER:HB2	1:D:529:LEU:HD21	2.00	0.43
1:A:131:SER:CB	1:A:238:ALA:HB1	2.49	0.43
1:D:388:ALA:HA	1:D:440:LEU:HG	2.01	0.43
1:A:82:VAL:HG22	1:A:224:LYS:HB2	2.01	0.43
1:D:545:CYS:SG	1:D:589:SER:HA	2.58	0.43
1:A:80:TYR:CB	1:A:367:HIS:HD2	2.27	0.42
1:B:626:LEU:HB3	1:B:627:PRO:HD3	2.01	0.42
1:C:355:ASN:OD1	1:C:356:PRO:HA	2.19	0.42
1:C:55:ALA:O	1:C:59:ARG:HB3	2.20	0.42
1:A:233:THR:O	1:A:233:THR:HG23	2.20	0.42
1:B:307:GLU:O	1:B:311:ILE:HG12	2.19	0.42
1:A:279:VAL:O	1:C:351:SER:HB2	2.18	0.42
1:B:54:GLU:OE1	1:B:54:GLU:HA	2.20	0.41
1:B:82:VAL:HG22	1:B:224:LYS:HB2	2.01	0.41
1:A:332:ALA:O	1:A:336:GLN:HG3	2.20	0.41
1:D:255:GLU:HG2	1:D:331:LEU:HD13	2.03	0.41
1:C:85:GLY:HA2	1:D:424:TYR:OH	2.20	0.41
1:C:262:CYS:HB2	1:C:324:LEU:HD21	2.02	0.41
1:D:124:LEU:HD13	1:D:235:PHE:CE1	2.54	0.41
1:D:250:LEU:O	1:D:254:VAL:HG23	2.21	0.41
1:D:583:GLU:O	1:D:587:ARG:HG3	2.20	0.41
1:A:626:LEU:HB3	1:A:627:PRO:HD3	2.01	0.41
1:A:51:VAL:HG21	1:A:159:LEU:HD13	2.02	0.41
1:A:280:LYS:HA	1:C:351:SER:HB2	2.03	0.41
1:C:626:LEU:N	1:C:627:PRO:HD2	2.36	0.41
1:B:72:LYS:HD3	1:B:72:LYS:HA	1.91	0.41
1:B:94:THR:HG22	1:B:96:ARG:H	1.85	0.41
1:C:471:LYS:HA	1:C:471:LYS:HD3	1.90	0.41
1:D:80:TYR:HB3	1:D:367:HIS:CD2	2.56	0.41
1:B:162:ASN:ND2	1:B:200:GLY:HA2	2.36	0.41
1:A:33:THR:HA	1:A:34:PRO:HD3	1.87	0.41
1:D:551:LEU:O	1:D:555:LEU:HG	2.21	0.40
1:C:650:GLN:HG3	1:D:111:GLY:O	2.22	0.40
1:B:304:LEU:HD11	1:B:619:ARG:HD3	2.04	0.40
1:A:65:CYS:O	1:A:69:VAL:HG23	2.20	0.40
1:C:162:ASN:ND2	1:C:200:GLY:HA2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:HE2	1:A:356:PRO:HD2	2.04	0.40
1:B:380:MET:CE	1:B:380:MET:HA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	631/707 (89%)	616 (98%)	14 (2%)	1 (0%)	52 59
1	B	622/707 (88%)	603 (97%)	19 (3%)	0	100 100
1	C	629/707 (89%)	609 (97%)	20 (3%)	0	100 100
1	D	624/707 (88%)	610 (98%)	14 (2%)	0	100 100
All	All	2506/2828 (89%)	2438 (97%)	67 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ALA

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	543/592 (92%)	516 (95%)	27 (5%)	30 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	538/592 (91%)	522 (97%)	16 (3%)	48 60
1	C	539/592 (91%)	516 (96%)	23 (4%)	35 43
1	D	537/592 (91%)	512 (95%)	25 (5%)	32 39
All	All	2157/2368 (91%)	2066 (96%)	91 (4%)	36 44

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	57	GLN
1	A	59	ARG
1	A	84	THR
1	A	92	ARG
1	A	94	THR
1	A	102	GLU
1	A	107	CYS
1	A	115	LYS
1	A	162	ASN
1	A	166	LYS
1	A	179	LEU
1	A	202	ASP
1	A	209	GLU
1	A	233	THR
1	A	253	LEU
1	A	268	ARG
1	A	353	ASN
1	A	364	ARG
1	A	374	SER
1	A	528	LEU
1	A	562	THR
1	A	568	LYS
1	A	575	ASP
1	A	672	CYS
1	A	673	LEU
1	A	674	GLN
1	B	43	LEU
1	B	59	ARG
1	B	94	THR
1	B	102	GLU
1	B	107	CYS
1	B	179	LEU

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Mol	Chain	Res	Type
1	B	233	THR
1	B	268	ARG
1	B	312	ASP
1	B	374	SER
1	B	392	LYS
1	B	528	LEU
1	B	562	THR
1	B	605	LYS
1	B	618	VAL
1	B	673	LEU
1	C	26	LYS
1	C	43	LEU
1	C	56	GLU
1	C	92	ARG
1	C	94	THR
1	C	98	SER
1	C	102	GLU
1	C	107	CYS
1	C	179	LEU
1	C	233	THR
1	C	268	ARG
1	C	275	LEU
1	C	298	SER
1	C	353	ASN
1	C	363	ASP
1	C	392	LYS
1	C	459	GLN
1	C	528	LEU
1	C	552	LEU
1	C	562	THR
1	C	619	ARG
1	C	673	LEU
1	C	677	LEU
1	D	43	LEU
1	D	59	ARG
1	D	92	ARG
1	D	94	THR
1	D	102	GLU
1	D	107	CYS
1	D	150	GLU
1	D	179	LEU
1	D	209	GLU

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Mol	Chain	Res	Type
1	D	222	GLN
1	D	233	THR
1	D	268	ARG
1	D	312	ASP
1	D	324	LEU
1	D	353	ASN
1	D	363	ASP
1	D	528	LEU
1	D	552	LEU
1	D	562	THR
1	D	568	LYS
1	D	576	THR
1	D	580	ARG
1	D	599	VAL
1	D	670	LEU
1	D	673	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	D	674	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	641/707 (90%)	0.54	53 (8%)	14	13	20, 37, 61, 92	0
1	B	636/707 (89%)	0.51	45 (7%)	19	18	20, 40, 66, 81	0
1	C	639/707 (90%)	0.55	58 (9%)	11	11	19, 39, 72, 93	0
1	D	636/707 (89%)	0.56	47 (7%)	17	17	20, 39, 64, 85	0
All	All	2552/2828 (90%)	0.54	203 (7%)	15	14	19, 39, 66, 93	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ILE	7.3
1	C	279	VAL	7.3
1	C	275	LEU	6.6
1	B	276	ILE	5.5
1	C	369	ALA	5.5
1	C	278	LYS	4.9
1	C	281	PRO	4.7
1	C	277	HIS	4.3
1	A	86	PHE	4.2
1	D	279	VAL	4.0
1	A	276	ILE	4.0
1	B	564	LEU	4.0
1	C	579	ASP	3.9
1	A	275	LEU	3.8
1	C	443	LEU	3.8
1	D	568	LYS	3.8
1	B	522	ASN	3.7
1	C	451	VAL	3.7
1	A	32	THR	3.7
1	C	57	GLN	3.7
1	A	363	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	444	ALA	3.5
1	D	577	LEU	3.5
1	A	590	ASP	3.5
1	B	584	PHE	3.3
1	B	284	GLY	3.3
1	B	565	ALA	3.3
1	C	280	LYS	3.3
1	C	583	GLU	3.3
1	D	360	HIS	3.3
1	D	440	LEU	3.3
1	A	57	GLN	3.2
1	B	562	THR	3.2
1	C	440	LEU	3.2
1	C	282	HIS	3.2
1	D	369	ALA	3.2
1	C	447	VAL	3.1
1	D	366	LEU	3.1
1	C	56	GLU	3.1
1	B	510	VAL	3.1
1	C	591	ARG	3.1
1	B	443	LEU	3.1
1	B	449	THR	3.1
1	A	587	ARG	3.1
1	D	443	LEU	3.0
1	B	451	VAL	3.0
1	C	588	LEU	3.0
1	B	529	LEU	3.0
1	A	443	LEU	3.0
1	D	442	TYR	3.0
1	A	359	ASP	3.0
1	A	358	ILE	3.0
1	C	514	LEU	2.9
1	A	373	GLY	2.9
1	D	75	ASP	2.9
1	A	364	ARG	2.9
1	A	385	ILE	2.9
1	C	585	GLU	2.9
1	C	285	GLN	2.9
1	D	62	VAL	2.9
1	D	444	ALA	2.9
1	B	523	ASP	2.9
1	C	175	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	175	ALA	2.8
1	C	567	HIS	2.8
1	D	71	ARG	2.8
1	C	442	TYR	2.8
1	A	584	PHE	2.8
1	D	215	GLY	2.8
1	B	444	ALA	2.8
1	B	447	VAL	2.8
1	C	61	ARG	2.8
1	C	587	ARG	2.8
1	C	559	CYS	2.7
1	B	588	LEU	2.7
1	A	581	LEU	2.7
1	C	385	ILE	2.7
1	D	447	VAL	2.7
1	B	586	LYS	2.7
1	D	387	VAL	2.7
1	A	591	ARG	2.7
1	A	552	LEU	2.7
1	A	279	VAL	2.7
1	D	576	THR	2.7
1	B	442	TYR	2.7
1	C	438	SER	2.7
1	D	675	GLY	2.7
1	B	508	GLU	2.6
1	D	208	PRO	2.6
1	A	395	PHE	2.6
1	D	567	HIS	2.6
1	B	461	ILE	2.6
1	D	448	THR	2.6
1	B	674	GLN	2.6
1	D	673	LEU	2.6
1	D	202	ASP	2.6
1	A	394	LEU	2.6
1	D	367	HIS	2.6
1	B	524	THR	2.6
1	B	566	LEU	2.6
1	D	451	VAL	2.6
1	A	448	THR	2.5
1	C	526	ALA	2.5
1	B	199	ILE	2.5
1	C	444	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	58	CYS	2.5
1	C	581	LEU	2.5
1	C	446	PRO	2.5
1	A	367	HIS	2.5
1	D	449	THR	2.5
1	C	388	ALA	2.5
1	A	121	VAL	2.5
1	B	576	THR	2.5
1	C	449	THR	2.5
1	C	646	GLU	2.5
1	B	518	CYS	2.5
1	D	65	CYS	2.5
1	D	383	VAL	2.5
1	C	564	LEU	2.5
1	B	446	PRO	2.5
1	B	563	ILE	2.5
1	A	524	THR	2.5
1	A	579	ASP	2.4
1	B	448	THR	2.4
1	B	454	ALA	2.4
1	C	584	PHE	2.4
1	C	586	LYS	2.4
1	C	450	HIS	2.4
1	B	521	PRO	2.4
1	C	560	PHE	2.4
1	D	676	PHE	2.4
1	A	442	TYR	2.4
1	B	464	LEU	2.4
1	D	76	GLY	2.4
1	D	211	LEU	2.4
1	A	578	VAL	2.3
1	A	389	GLY	2.3
1	A	449	THR	2.3
1	B	440	LEU	2.3
1	B	559	CYS	2.3
1	A	507	VAL	2.3
1	A	586	LYS	2.3
1	C	286	ILE	2.3
1	D	276	ILE	2.3
1	D	437	SER	2.3
1	B	285	GLN	2.3
1	D	630	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	464	LEU	2.3
1	B	203	VAL	2.3
1	C	434	ALA	2.3
1	B	47	HIS	2.3
1	C	605	LYS	2.3
1	A	284	GLY	2.2
1	D	203	VAL	2.2
1	A	366	LEU	2.2
1	A	440	LEU	2.2
1	B	581	LEU	2.2
1	A	446	PRO	2.2
1	A	393	LEU	2.2
1	C	592	LEU	2.2
1	C	448	THR	2.2
1	A	387	VAL	2.2
1	A	523	ASP	2.2
1	C	582	ALA	2.2
1	A	566	LEU	2.2
1	B	277	HIS	2.2
1	D	579	ASP	2.2
1	A	451	VAL	2.2
1	C	541	LEU	2.1
1	A	217	ARG	2.1
1	D	201	ASP	2.1
1	D	459	GLN	2.1
1	D	565	ALA	2.1
1	B	387	VAL	2.1
1	D	32	THR	2.1
1	C	523	ASP	2.1
1	B	520	LEU	2.1
1	C	366	LEU	2.1
1	C	377	GLY	2.1
1	C	173	VAL	2.1
1	D	220	LYS	2.1
1	D	278	LYS	2.1
1	D	385	ILE	2.1
1	C	552	LEU	2.1
1	A	281	PRO	2.1
1	A	435	ALA	2.1
1	D	435	ALA	2.1
1	A	568	LYS	2.0
1	D	564	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	519	GLY	2.0
1	A	434	ALA	2.0
1	C	437	SER	2.0
1	A	585	GLU	2.0
1	D	560	PHE	2.0
1	A	447	VAL	2.0
1	B	603	TYR	2.0
1	A	438	SER	2.0
1	A	677	LEU	2.0
1	A	361	ALA	2.0
1	B	515	ALA	2.0
1	B	25	LYS	2.0
1	C	459	GLN	2.0
1	A	518	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.