Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:19 AM GMT

PDB ID	:	3HZR
Title	:	Tryptophanyl-tRNA synthetase homolog from Entamoeba histolytica
Authors	:	Arakaki, T.; Merritt, E.A.
Deposited on	:	2009-06-24
Resolution	:	3.00 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:

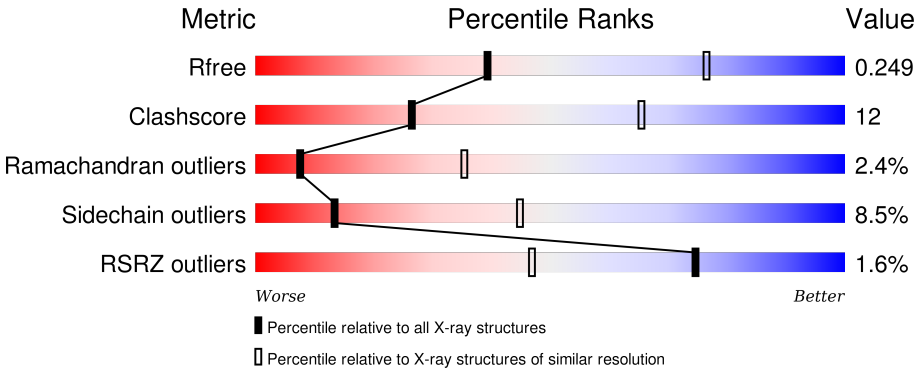
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	386	2% 71% 20% 5%
1	B	386	1% 73% 18% 6%
1	C	386	1% 70% 21% 6%
1	D	386	72% 19% 5%
1	E	386	6% 73% 18% 5%

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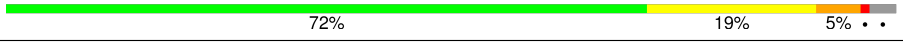
Mol	Chain	Length	Quality of chain
1	F	386	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17738 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2958	1905	479	565	9			
1	B	374	Total	C	N	O	S	0	0	0
			2954	1903	479	563	9			
1	C	374	Total	C	N	O	S	0	0	0
			2957	1906	479	563	9			
1	D	374	Total	C	N	O	S	0	0	0
			2958	1905	479	565	9			
1	E	374	Total	C	N	O	S	0	0	0
			2954	1903	479	563	9			
1	F	374	Total	C	N	O	S	0	0	0
			2957	1906	479	563	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	PDB 3HZR
A	-7	ALA	-	EXPRESSION TAG	PDB 3HZR
A	-6	HIS	-	EXPRESSION TAG	PDB 3HZR
A	-5	HIS	-	EXPRESSION TAG	PDB 3HZR
A	-4	HIS	-	EXPRESSION TAG	PDB 3HZR
A	-3	HIS	-	EXPRESSION TAG	PDB 3HZR
A	-2	HIS	-	EXPRESSION TAG	PDB 3HZR
A	-1	HIS	-	EXPRESSION TAG	PDB 3HZR
B	-8	MET	-	EXPRESSION TAG	PDB 3HZR
B	-7	ALA	-	EXPRESSION TAG	PDB 3HZR
B	-6	HIS	-	EXPRESSION TAG	PDB 3HZR
B	-5	HIS	-	EXPRESSION TAG	PDB 3HZR
B	-4	HIS	-	EXPRESSION TAG	PDB 3HZR
B	-3	HIS	-	EXPRESSION TAG	PDB 3HZR
B	-2	HIS	-	EXPRESSION TAG	PDB 3HZR
B	-1	HIS	-	EXPRESSION TAG	PDB 3HZR
C	-8	MET	-	EXPRESSION TAG	PDB 3HZR

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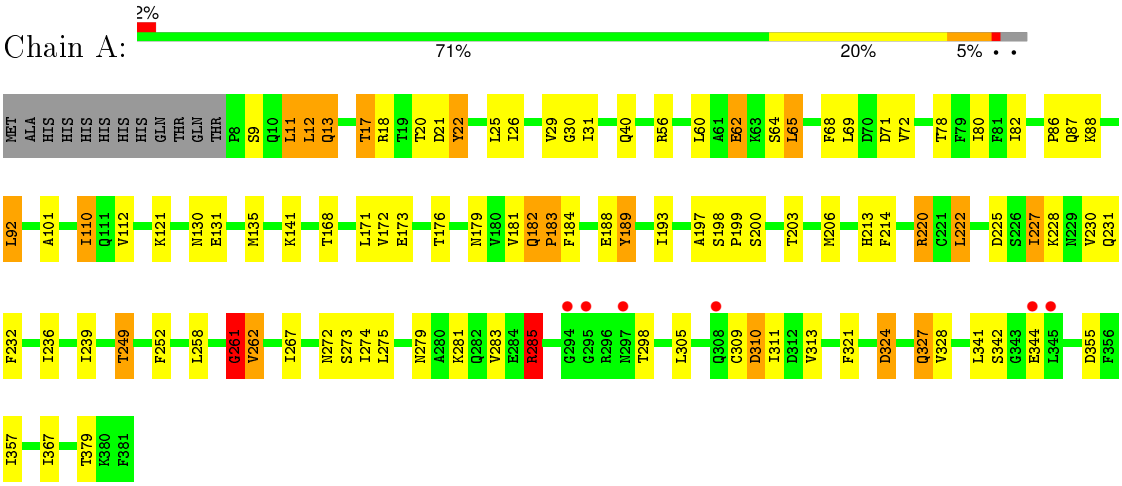
Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	EXPRESSION TAG	PDB 3HZR
C	-6	HIS	-	EXPRESSION TAG	PDB 3HZR
C	-5	HIS	-	EXPRESSION TAG	PDB 3HZR
C	-4	HIS	-	EXPRESSION TAG	PDB 3HZR
C	-3	HIS	-	EXPRESSION TAG	PDB 3HZR
C	-2	HIS	-	EXPRESSION TAG	PDB 3HZR
C	-1	HIS	-	EXPRESSION TAG	PDB 3HZR
D	-8	MET	-	EXPRESSION TAG	PDB 3HZR
D	-7	ALA	-	EXPRESSION TAG	PDB 3HZR
D	-6	HIS	-	EXPRESSION TAG	PDB 3HZR
D	-5	HIS	-	EXPRESSION TAG	PDB 3HZR
D	-4	HIS	-	EXPRESSION TAG	PDB 3HZR
D	-3	HIS	-	EXPRESSION TAG	PDB 3HZR
D	-2	HIS	-	EXPRESSION TAG	PDB 3HZR
D	-1	HIS	-	EXPRESSION TAG	PDB 3HZR
E	-8	MET	-	EXPRESSION TAG	PDB 3HZR
E	-7	ALA	-	EXPRESSION TAG	PDB 3HZR
E	-6	HIS	-	EXPRESSION TAG	PDB 3HZR
E	-5	HIS	-	EXPRESSION TAG	PDB 3HZR
E	-4	HIS	-	EXPRESSION TAG	PDB 3HZR
E	-3	HIS	-	EXPRESSION TAG	PDB 3HZR
E	-2	HIS	-	EXPRESSION TAG	PDB 3HZR
E	-1	HIS	-	EXPRESSION TAG	PDB 3HZR
F	-8	MET	-	EXPRESSION TAG	PDB 3HZR
F	-7	ALA	-	EXPRESSION TAG	PDB 3HZR
F	-6	HIS	-	EXPRESSION TAG	PDB 3HZR
F	-5	HIS	-	EXPRESSION TAG	PDB 3HZR
F	-4	HIS	-	EXPRESSION TAG	PDB 3HZR
F	-3	HIS	-	EXPRESSION TAG	PDB 3HZR
F	-2	HIS	-	EXPRESSION TAG	PDB 3HZR
F	-1	HIS	-	EXPRESSION TAG	PDB 3HZR

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.

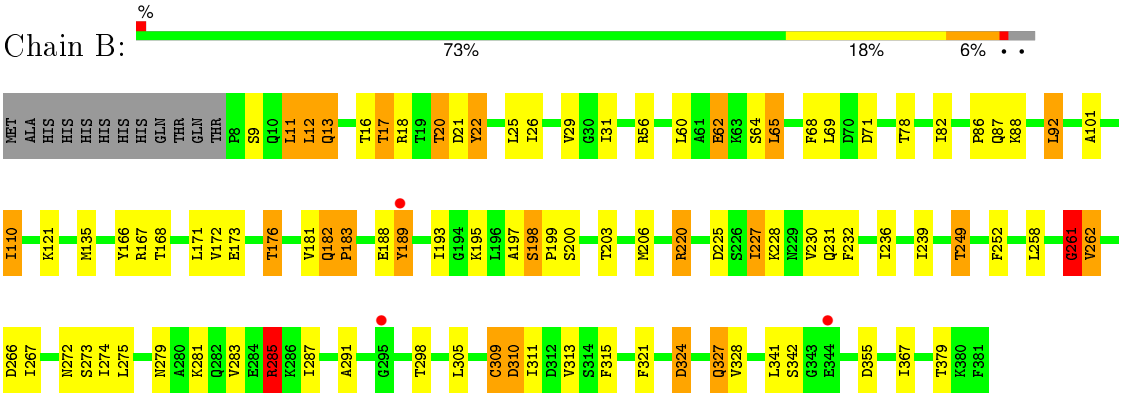
- Molecule 1: Tryptophanyl-tRNA synthetase

Chain A:



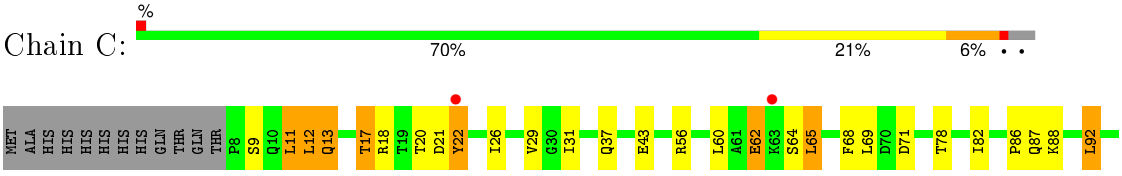
- Molecule 1: Tryptophanyl-tRNA synthetase

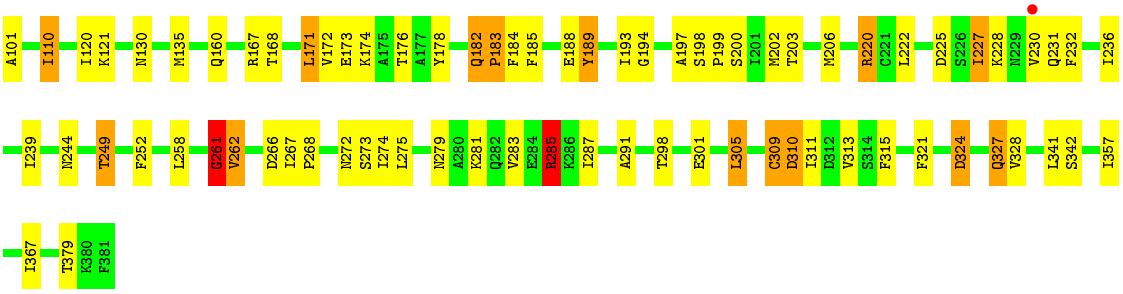
Chain B:



- Molecule 1: Tryptophanyl-tRNA synthetase

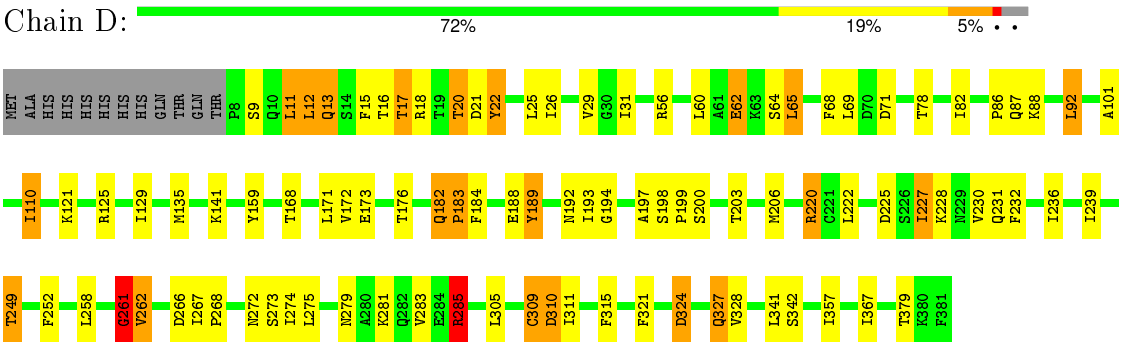
Chain C:





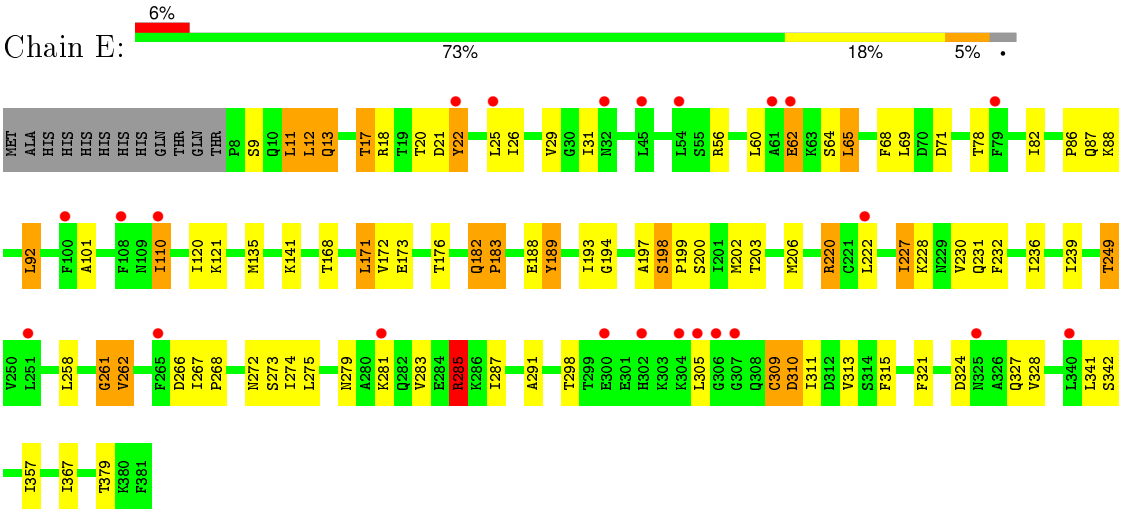
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain D:



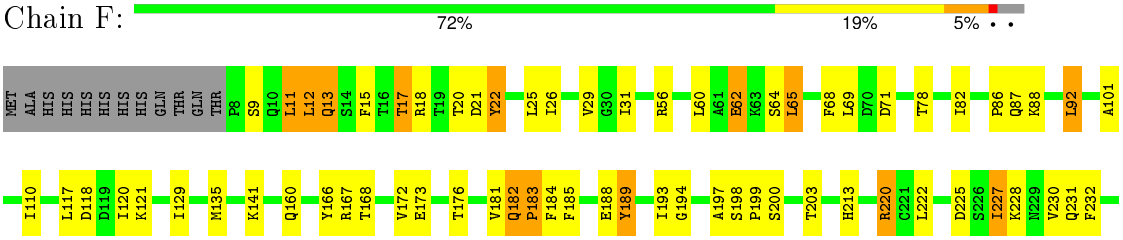
• Molecule 1: Tryptophanyl-tRNA synthetase

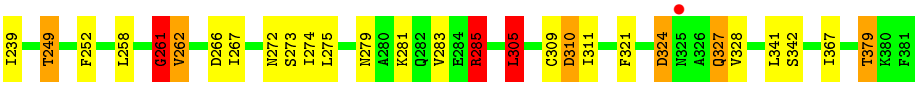
Chain E:



• Molecule 1: Tryptophanyl-tRNA synthetase

Chain F:




I239
T249
F252
L258
G261
V262
D266
I267
N272
S273
I274
L275
N279
A280
K281
Q282
V283
E284
R285
L305
C309
D310
I311
F321
D324
N325
A326
Q327
V328
I341
S342
I367
T379
K380
F381

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.20Å 158.88Å 100.28Å 90.00° 107.33° 90.00°	Depositor
Resolution (Å)	47.89 – 3.00 47.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.89-3.00) 97.6 (47.86-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.228 , 0.250 0.226 , 0.249	Depositor DCC
R_{free} test set	2753 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	80.9	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 54371 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17738	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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	0.61	0/3019	0.70	2/4084 (0.0%)
1	B	0.61	0/3015	0.70	2/4079 (0.0%)
1	C	0.56	1/3018 (0.0%)	0.68	2/4083 (0.0%)
1	D	0.60	0/3019	0.69	2/4084 (0.0%)
1	E	0.50	0/3015	0.65	1/4079 (0.0%)
1	F	0.59	1/3018 (0.0%)	0.70	2/4083 (0.0%)
All	All	0.58	2/18104 (0.0%)	0.69	11/24492 (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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	160	GLN	CG-CD	5.97	1.64	1.51
1	C	160	GLN	CG-CD	5.30	1.63	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	285	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	F	285	ARG	NE-CZ-NH1	7.97	124.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	285	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	285	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	D	285	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	E	285	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	F	261	GLY	N-CA-C	-5.64	99.00	113.10
1	D	261	GLY	N-CA-C	-5.46	99.46	113.10
1	C	261	GLY	N-CA-C	-5.40	99.60	113.10
1	A	261	GLY	N-CA-C	-5.22	100.04	113.10
1	B	261	GLY	N-CA-C	-5.06	100.44	113.10

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide
1	A	309	CYS	Peptide
1	B	261	GLY	Peptide
1	B	309	CYS	Peptide
1	C	261	GLY	Peptide
1	C	309	CYS	Peptide
1	D	261	GLY	Peptide
1	D	309	CYS	Peptide
1	E	261	GLY	Peptide
1	E	309	CYS	Peptide
1	F	261	GLY	Peptide
1	F	309	CYS	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	2958	0	2910	76	4
1	B	2954	0	2906	70	2
1	C	2957	0	2915	88	3
1	D	2958	0	2910	83	1
1	E	2954	0	2906	73	0
1	F	2957	0	2915	75	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17738	0	17462	429	6

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 12.

All (429) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:HG11	1:B:230:VAL:HG11	1.24	1.16
1:F:29:VAL:HG11	1:F:230:VAL:HG11	1.34	1.08
1:E:29:VAL:HG11	1:E:230:VAL:HG11	1.32	1.07
1:C:29:VAL:HG11	1:C:230:VAL:HG11	1.34	1.05
1:A:29:VAL:HG11	1:A:230:VAL:HG11	1.33	1.03
1:D:29:VAL:HG11	1:D:230:VAL:HG11	1.38	1.00
1:C:197:ALA:HA	1:D:193:ILE:HG23	1.47	0.96
1:B:29:VAL:CG1	1:B:230:VAL:HG11	2.05	0.87
1:E:197:ALA:HA	1:F:193:ILE:HG23	1.56	0.86
1:A:87:GLN:C	1:A:135:MET:HE2	1.97	0.85
1:C:87:GLN:C	1:C:135:MET:HE2	2.01	0.81
1:E:197:ALA:HA	1:F:193:ILE:CG2	2.10	0.80
1:A:199:PRO:O	1:A:203:THR:HG23	1.80	0.80
1:A:29:VAL:CG1	1:A:230:VAL:HG11	2.13	0.79
1:D:199:PRO:O	1:D:203:THR:HG23	1.83	0.78
1:B:87:GLN:C	1:B:135:MET:HE2	2.04	0.77
1:B:29:VAL:HG11	1:B:230:VAL:CG1	2.11	0.76
1:E:29:VAL:CG1	1:E:230:VAL:HG11	2.13	0.76
1:C:29:VAL:CG1	1:C:230:VAL:HG11	2.15	0.76
1:C:197:ALA:HA	1:D:193:ILE:CG2	2.15	0.76
1:B:88:LYS:N	1:B:135:MET:CE	2.50	0.75
1:C:11:LEU:HD12	1:C:12:LEU:N	2.03	0.74
1:D:227:ILE:O	1:D:230:VAL:HG23	1.87	0.74
1:B:11:LEU:HD12	1:B:12:LEU:N	2.03	0.73
1:A:197:ALA:HA	1:B:193:ILE:HG23	1.69	0.73
1:F:29:VAL:CG1	1:F:230:VAL:HG11	2.16	0.72
1:E:171:LEU:HD13	1:F:129:ILE:HD11	1.71	0.72
1:A:227:ILE:O	1:A:230:VAL:HG23	1.88	0.72
1:A:88:LYS:N	1:A:135:MET:CE	2.52	0.72
1:F:367:ILE:O	1:F:367:ILE:HG22	1.87	0.72
1:E:87:GLN:C	1:E:135:MET:HE2	2.08	0.72
1:F:29:VAL:HG11	1:F:230:VAL:CG1	2.17	0.72
1:F:11:LEU:HD12	1:F:12:LEU:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:LYS:N	1:C:135:MET:CE	2.53	0.71
1:B:172:VAL:O	1:B:176:THR:HG23	1.90	0.71
1:F:172:VAL:O	1:F:176:THR:HG23	1.90	0.71
1:E:193:ILE:HG23	1:F:197:ALA:HA	1.71	0.71
1:E:29:VAL:HG11	1:E:230:VAL:CG1	2.18	0.71
1:F:227:ILE:O	1:F:230:VAL:HG23	1.90	0.70
1:D:11:LEU:HD12	1:D:12:LEU:N	2.07	0.70
1:A:29:VAL:HG11	1:A:230:VAL:CG1	2.19	0.70
1:B:367:ILE:HG22	1:B:367:ILE:O	1.90	0.70
1:B:199:PRO:O	1:B:203:THR:HG23	1.92	0.69
1:A:11:LEU:HD12	1:A:12:LEU:N	2.07	0.69
1:E:199:PRO:O	1:E:203:THR:HG23	1.93	0.69
1:E:11:LEU:HD12	1:E:12:LEU:N	2.08	0.69
1:E:18:ARG:NH2	1:E:310:ASP:OD2	2.26	0.69
1:E:227:ILE:O	1:E:230:VAL:HG23	1.92	0.68
1:F:87:GLN:C	1:F:135:MET:HE2	2.13	0.68
1:F:18:ARG:NH2	1:F:310:ASP:OD2	2.26	0.68
1:B:227:ILE:O	1:B:230:VAL:HG23	1.94	0.68
1:A:193:ILE:HG23	1:B:197:ALA:HA	1.75	0.68
1:A:18:ARG:NH2	1:A:310:ASP:OD2	2.27	0.68
1:E:88:LYS:N	1:E:135:MET:CE	2.57	0.68
1:F:199:PRO:O	1:F:203:THR:HG23	1.93	0.68
1:B:11:LEU:O	1:B:13:GLN:N	2.26	0.67
1:D:18:ARG:NH2	1:D:310:ASP:OD2	2.27	0.67
1:C:227:ILE:O	1:C:230:VAL:HG23	1.94	0.67
1:D:88:LYS:N	1:D:135:MET:CE	2.57	0.66
1:D:11:LEU:O	1:D:13:GLN:N	2.27	0.66
1:A:11:LEU:O	1:A:13:GLN:N	2.26	0.66
1:C:18:ARG:NH2	1:C:310:ASP:OD2	2.28	0.66
1:C:193:ILE:HG23	1:D:197:ALA:HA	1.77	0.66
1:D:29:VAL:CG1	1:D:230:VAL:HG11	2.19	0.66
1:B:18:ARG:NH2	1:B:310:ASP:OD2	2.29	0.66
1:A:214:PHE:C	1:C:130:ASN:ND2	2.49	0.66
1:C:267:ILE:O	1:C:272:ASN:ND2	2.30	0.65
1:C:21:ASP:O	1:C:22:TYR:HB2	1.97	0.64
1:B:65:LEU:HD22	1:B:69:LEU:CD1	2.27	0.64
1:D:172:VAL:O	1:D:176:THR:HG23	1.95	0.64
1:E:193:ILE:CG2	1:F:197:ALA:HA	2.26	0.64
1:C:199:PRO:O	1:C:203:THR:HG23	1.98	0.64
1:C:29:VAL:HG11	1:C:230:VAL:CG1	2.20	0.64
1:C:65:LEU:HD22	1:C:69:LEU:CD1	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:SER:HB2	1:C:249:THR:HG22	1.79	0.64
1:F:65:LEU:HD22	1:F:69:LEU:CD1	2.28	0.64
1:E:367:ILE:HG22	1:E:367:ILE:O	1.97	0.64
1:D:367:ILE:O	1:D:367:ILE:HG22	1.95	0.63
1:D:29:VAL:HG11	1:D:230:VAL:CG1	2.22	0.63
1:A:267:ILE:O	1:A:272:ASN:ND2	2.32	0.63
1:A:21:ASP:O	1:A:22:TYR:HB2	1.97	0.63
1:F:11:LEU:O	1:F:13:GLN:N	2.32	0.63
1:F:88:LYS:N	1:F:135:MET:CE	2.62	0.63
1:D:87:GLN:C	1:D:135:MET:HE2	2.19	0.63
1:E:65:LEU:HD22	1:E:69:LEU:CD1	2.29	0.62
1:A:367:ILE:HG22	1:A:367:ILE:O	1.98	0.62
1:A:88:LYS:N	1:A:135:MET:HE2	2.12	0.62
1:E:267:ILE:O	1:E:272:ASN:ND2	2.32	0.62
1:D:176:THR:HG22	1:D:239:ILE:CD1	2.29	0.62
1:C:172:VAL:O	1:C:176:THR:HG23	1.99	0.62
1:A:193:ILE:CG2	1:B:197:ALA:HA	2.30	0.62
1:B:88:LYS:N	1:B:135:MET:HE2	2.15	0.61
1:E:172:VAL:O	1:E:176:THR:HG23	1.99	0.61
1:A:176:THR:HG22	1:A:239:ILE:CD1	2.30	0.61
1:E:64:SER:HB2	1:E:249:THR:HG22	1.82	0.61
1:C:87:GLN:HG2	1:C:121:LYS:NZ	2.16	0.61
1:E:11:LEU:O	1:E:13:GLN:N	2.31	0.61
1:C:174:LYS:HE3	1:D:125:ARG:HA	1.82	0.61
1:E:26:ILE:HG23	1:E:31:ILE:O	2.01	0.61
1:F:21:ASP:O	1:F:22:TYR:HB2	2.01	0.60
1:D:267:ILE:O	1:D:272:ASN:ND2	2.35	0.60
1:F:88:LYS:N	1:F:135:MET:HE2	2.17	0.60
1:A:65:LEU:HD22	1:A:69:LEU:CD1	2.31	0.60
1:E:21:ASP:O	1:E:22:TYR:HB2	2.01	0.60
1:E:88:LYS:N	1:E:135:MET:HE2	2.17	0.60
1:F:64:SER:HB2	1:F:249:THR:HG22	1.84	0.59
1:A:197:ALA:HA	1:B:193:ILE:CG2	2.32	0.59
1:D:65:LEU:HD22	1:D:69:LEU:CD1	2.32	0.59
1:C:173:GLU:HB3	1:D:194:GLY:HA3	1.83	0.59
1:D:87:GLN:HG2	1:D:121:LYS:HZ3	1.68	0.59
1:B:21:ASP:O	1:B:22:TYR:HB2	2.03	0.59
1:C:88:LYS:N	1:C:135:MET:HE2	2.15	0.59
1:B:87:GLN:C	1:B:135:MET:CE	2.70	0.59
1:C:367:ILE:O	1:C:367:ILE:HG22	2.03	0.59
1:F:176:THR:HG22	1:F:239:ILE:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:GLN:HG2	1:F:121:LYS:HZ3	1.68	0.58
1:A:172:VAL:O	1:A:176:THR:HG23	2.02	0.58
1:E:71:ASP:OD1	1:E:220:ARG:HG3	2.03	0.58
1:D:21:ASP:O	1:D:22:TYR:HB2	2.03	0.58
1:C:176:THR:HG22	1:C:239:ILE:CD1	2.34	0.58
1:B:267:ILE:O	1:B:272:ASN:ND2	2.36	0.58
1:B:64:SER:HB2	1:B:249:THR:HG22	1.85	0.58
1:D:64:SER:HB2	1:D:249:THR:HG22	1.86	0.58
1:C:26:ILE:HG23	1:C:31:ILE:O	2.04	0.58
1:D:11:LEU:C	1:D:13:GLN:H	2.07	0.57
1:A:26:ILE:HG23	1:A:31:ILE:O	2.03	0.57
1:C:71:ASP:OD1	1:C:220:ARG:HG3	2.04	0.57
1:F:267:ILE:O	1:F:272:ASN:ND2	2.37	0.57
1:D:258:LEU:HD22	1:D:272:ASN:HB3	1.87	0.57
1:C:11:LEU:O	1:C:13:GLN:N	2.35	0.56
1:F:11:LEU:C	1:F:13:GLN:H	2.08	0.56
1:A:11:LEU:C	1:A:13:GLN:H	2.08	0.56
1:E:11:LEU:C	1:E:13:GLN:H	2.09	0.55
1:E:87:GLN:HG2	1:E:121:LYS:NZ	2.21	0.55
1:E:176:THR:HG22	1:E:239:ILE:CD1	2.37	0.55
1:A:71:ASP:OD1	1:A:220:ARG:HG3	2.06	0.55
1:A:87:GLN:HG2	1:A:121:LYS:HZ3	1.72	0.55
1:F:87:GLN:HG2	1:F:121:LYS:NZ	2.21	0.55
1:F:62:GLU:HG3	1:F:65:LEU:HB2	1.89	0.55
1:B:11:LEU:C	1:B:13:GLN:H	2.07	0.55
1:C:301:GLU:O	1:C:305:LEU:HB2	2.07	0.55
1:B:285:ARG:HH11	1:B:285:ARG:CG	2.19	0.55
1:B:92:LEU:HD22	1:B:321:PHE:CZ	2.42	0.55
1:D:173:GLU:HG2	1:D:200:SER:OG	2.07	0.55
1:D:88:LYS:N	1:D:135:MET:HE2	2.21	0.54
1:B:87:GLN:HG2	1:B:121:LYS:NZ	2.23	0.54
1:A:285:ARG:CG	1:A:285:ARG:HH11	2.21	0.54
1:D:274:ILE:HD13	1:D:283:VAL:HG13	1.90	0.54
1:D:71:ASP:OD1	1:D:220:ARG:HG3	2.07	0.54
1:A:78:THR:OG1	1:A:110:ILE:HD11	2.08	0.54
1:B:26:ILE:HG23	1:B:31:ILE:O	2.07	0.54
1:A:279:ASN:ND2	1:A:281:LYS:HE3	2.22	0.54
1:D:62:GLU:HG3	1:D:65:LEU:HB2	1.89	0.53
1:C:87:GLN:C	1:C:135:MET:CE	2.72	0.53
1:C:11:LEU:C	1:C:13:GLN:H	2.11	0.53
1:B:62:GLU:HG3	1:B:65:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ASP:OD1	1:B:220:ARG:HG3	2.09	0.53
1:C:92:LEU:HD22	1:C:321:PHE:CZ	2.44	0.53
1:F:25:LEU:HD12	1:F:29:VAL:HG23	1.91	0.53
1:A:62:GLU:HG3	1:A:65:LEU:HB2	1.91	0.53
1:F:9:SER:H	1:F:231:GLN:HE22	1.57	0.53
1:E:92:LEU:HD22	1:E:321:PHE:CZ	2.44	0.53
1:C:285:ARG:CG	1:C:285:ARG:HH11	2.22	0.53
1:E:285:ARG:HH11	1:E:285:ARG:CG	2.22	0.53
1:F:258:LEU:HD22	1:F:272:ASN:HB3	1.90	0.52
1:B:87:GLN:HG2	1:B:121:LYS:HZ3	1.74	0.52
1:D:87:GLN:HG2	1:D:121:LYS:NZ	2.23	0.52
1:C:261:GLY:HA2	1:C:262:VAL:HG23	1.91	0.52
1:A:92:LEU:HD22	1:A:321:PHE:CZ	2.44	0.52
1:F:26:ILE:HG23	1:F:31:ILE:O	2.09	0.52
1:E:274:ILE:HD13	1:E:283:VAL:HG13	1.91	0.52
1:D:176:THR:HG22	1:D:239:ILE:HD11	1.92	0.52
1:E:86:PRO:O	1:E:121:LYS:HD3	2.09	0.52
1:B:29:VAL:CG1	1:B:230:VAL:CG1	2.81	0.52
1:B:195:LYS:O	1:B:198:SER:OG	2.24	0.52
1:F:78:THR:HG22	1:F:220:ARG:HB2	1.91	0.52
1:B:87:GLN:HA	1:B:135:MET:HE1	1.92	0.52
1:E:78:THR:HG22	1:E:220:ARG:HB2	1.92	0.52
1:A:64:SER:HB2	1:A:249:THR:HG22	1.92	0.52
1:D:92:LEU:HD22	1:D:321:PHE:CZ	2.45	0.52
1:C:174:LYS:CE	1:D:125:ARG:HA	2.40	0.52
1:A:206:MET:SD	1:A:236:ILE:HD13	2.49	0.51
1:A:261:GLY:HA2	1:A:262:VAL:HG23	1.91	0.51
1:E:261:GLY:HA2	1:E:262:VAL:HG23	1.90	0.51
1:A:68:PHE:HB2	1:A:249:THR:HG21	1.91	0.51
1:E:62:GLU:HG3	1:E:65:LEU:HB2	1.92	0.51
1:F:68:PHE:HB2	1:F:249:THR:HG21	1.92	0.51
1:C:193:ILE:CG2	1:D:197:ALA:HA	2.39	0.51
1:B:258:LEU:HD22	1:B:272:ASN:HB3	1.91	0.51
1:D:68:PHE:HB2	1:D:249:THR:HG21	1.93	0.51
1:A:78:THR:HG22	1:A:220:ARG:HB2	1.93	0.51
1:B:285:ARG:HG2	1:B:285:ARG:HH11	1.75	0.51
1:D:87:GLN:HA	1:D:135:MET:HE1	1.92	0.51
1:E:197:ALA:HA	1:F:193:ILE:HG21	1.92	0.51
1:C:274:ILE:HD13	1:C:283:VAL:HG13	1.92	0.51
1:C:62:GLU:HG3	1:C:65:LEU:HB2	1.93	0.51
1:A:258:LEU:HD22	1:A:272:ASN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLY:HA2	1:B:262:VAL:HG23	1.91	0.51
1:E:82:ILE:HD11	1:E:101:ALA:HB2	1.93	0.51
1:F:285:ARG:CG	1:F:285:ARG:HH11	2.23	0.50
1:A:176:THR:HG22	1:A:239:ILE:HD11	1.92	0.50
1:B:279:ASN:ND2	1:B:281:LYS:HE3	2.25	0.50
1:F:188:GLU:O	1:F:189:TYR:CD2	2.65	0.50
1:A:87:GLN:HG2	1:A:121:LYS:NZ	2.27	0.50
1:F:71:ASP:OD1	1:F:220:ARG:HG3	2.11	0.50
1:D:285:ARG:CG	1:D:285:ARG:HH11	2.23	0.50
1:B:176:THR:HG22	1:B:239:ILE:CD1	2.42	0.50
1:D:26:ILE:HG23	1:D:31:ILE:O	2.12	0.50
1:B:78:THR:HG22	1:B:220:ARG:HB2	1.94	0.50
1:C:258:LEU:HD22	1:C:272:ASN:HB3	1.93	0.49
1:A:285:ARG:HH11	1:A:285:ARG:HG2	1.77	0.49
1:A:130:ASN:ND2	1:F:213:HIS:O	2.41	0.49
1:F:274:ILE:HD13	1:F:283:VAL:HG13	1.94	0.49
1:C:188:GLU:O	1:C:189:TYR:CD2	2.65	0.49
1:B:206:MET:SD	1:B:236:ILE:HD13	2.53	0.49
1:C:197:ALA:HB2	1:D:197:ALA:HB2	1.94	0.49
1:E:87:GLN:C	1:E:135:MET:CE	2.81	0.49
1:E:197:ALA:CA	1:F:193:ILE:HG23	2.37	0.49
1:E:279:ASN:ND2	1:E:281:LYS:HE3	2.28	0.49
1:F:92:LEU:HD22	1:F:321:PHE:CZ	2.48	0.49
1:F:261:GLY:HA2	1:F:262:VAL:HG23	1.95	0.49
1:B:9:SER:H	1:B:231:GLN:HE22	1.59	0.49
1:C:167:ARG:HA	1:D:159:TYR:CE2	2.48	0.49
1:C:285:ARG:HH11	1:C:285:ARG:HG2	1.77	0.48
1:C:173:GLU:HG2	1:C:200:SER:OG	2.13	0.48
1:C:176:THR:HG22	1:C:239:ILE:HD11	1.95	0.48
1:D:182:GLN:N	1:D:183:PRO:CD	2.76	0.48
1:C:173:GLU:O	1:D:192:ASN:HB2	2.12	0.48
1:B:65:LEU:HD22	1:B:69:LEU:HD11	1.94	0.48
1:E:285:ARG:HG2	1:E:285:ARG:HH11	1.77	0.48
1:C:262:VAL:HG23	1:C:313:VAL:HG22	1.94	0.48
1:D:188:GLU:O	1:D:189:TYR:CD2	2.66	0.48
1:C:68:PHE:HB2	1:C:249:THR:HG21	1.95	0.48
1:E:78:THR:OG1	1:E:110:ILE:HD11	2.13	0.48
1:F:17:THR:O	1:F:18:ARG:HB3	2.14	0.48
1:F:173:GLU:HG2	1:F:200:SER:OG	2.14	0.48
1:B:68:PHE:HB2	1:B:249:THR:HG21	1.96	0.48
1:D:78:THR:HG22	1:D:220:ARG:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD22	1:A:321:PHE:CE1	2.48	0.48
1:F:324:ASP:OD1	1:F:327:GLN:HG2	2.13	0.48
1:D:87:GLN:C	1:D:135:MET:CE	2.82	0.48
1:D:17:THR:O	1:D:18:ARG:HB3	2.13	0.47
1:E:92:LEU:HD22	1:E:321:PHE:CE1	2.50	0.47
1:E:206:MET:SD	1:E:236:ILE:HD13	2.54	0.47
1:C:206:MET:SD	1:C:236:ILE:HD13	2.54	0.47
1:F:182:GLN:N	1:F:183:PRO:CD	2.77	0.47
1:F:176:THR:HG22	1:F:239:ILE:HD11	1.96	0.47
1:C:78:THR:HG22	1:C:220:ARG:HB2	1.94	0.47
1:D:13:GLN:CG	1:D:13:GLN:O	2.61	0.47
1:E:203:THR:HG22	1:E:232:PHE:CZ	2.50	0.47
1:E:172:VAL:HG11	1:E:203:THR:OG1	2.14	0.47
1:B:262:VAL:HG23	1:B:313:VAL:HG22	1.96	0.47
1:D:25:LEU:HD12	1:D:29:VAL:HG23	1.96	0.47
1:B:82:ILE:HD11	1:B:101:ALA:HB2	1.96	0.47
1:E:87:GLN:HG2	1:E:121:LYS:HZ3	1.80	0.47
1:E:68:PHE:HB2	1:E:249:THR:HG21	1.95	0.47
1:C:92:LEU:HD22	1:C:321:PHE:CE1	2.49	0.47
1:D:261:GLY:HA2	1:D:262:VAL:HG23	1.96	0.47
1:D:324:ASP:OD1	1:D:327:GLN:HG2	2.15	0.47
1:C:279:ASN:ND2	1:C:281:LYS:HE3	2.29	0.47
1:C:65:LEU:HD22	1:C:69:LEU:HD11	1.95	0.47
1:A:9:SER:H	1:A:231:GLN:HE22	1.61	0.47
1:E:173:GLU:HG2	1:E:200:SER:OG	2.14	0.47
1:C:86:PRO:O	1:C:121:LYS:HD3	2.15	0.47
1:C:87:GLN:HG2	1:C:121:LYS:HZ3	1.80	0.47
1:B:182:GLN:N	1:B:183:PRO:CD	2.78	0.47
1:A:172:VAL:HG11	1:A:203:THR:OG1	2.15	0.46
1:B:203:THR:HG22	1:B:232:PHE:CZ	2.49	0.46
1:C:9:SER:H	1:C:231:GLN:HE22	1.62	0.46
1:A:86:PRO:O	1:A:121:LYS:HD3	2.15	0.46
1:A:225:ASP:O	1:A:252:PHE:HA	2.15	0.46
1:B:78:THR:OG1	1:B:110:ILE:HD11	2.14	0.46
1:D:285:ARG:HG2	1:D:285:ARG:HH11	1.81	0.46
1:A:56:ARG:CZ	1:A:328:VAL:HG21	2.46	0.46
1:B:287:ILE:O	1:B:291:ALA:HB3	2.16	0.46
1:F:285:ARG:HG2	1:F:285:ARG:HH11	1.81	0.46
1:E:287:ILE:O	1:E:291:ALA:HB3	2.16	0.46
1:B:56:ARG:CZ	1:B:328:VAL:HG21	2.46	0.46
1:F:193:ILE:HG22	1:F:194:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD22	1:B:321:PHE:CE1	2.51	0.46
1:A:17:THR:O	1:A:18:ARG:HB3	2.16	0.46
1:A:188:GLU:O	1:A:189:TYR:CD2	2.69	0.46
1:B:25:LEU:HD12	1:B:29:VAL:HG23	1.98	0.46
1:E:65:LEU:HD22	1:E:69:LEU:HD11	1.97	0.46
1:A:214:PHE:CA	1:C:130:ASN:ND2	2.79	0.46
1:C:193:ILE:HG22	1:C:194:GLY:N	2.31	0.45
1:E:171:LEU:CD1	1:F:129:ILE:HD11	2.44	0.45
1:A:182:GLN:N	1:A:183:PRO:CD	2.79	0.45
1:F:379:THR:O	1:F:379:THR:HG23	2.16	0.45
1:A:324:ASP:OD1	1:A:327:GLN:HG2	2.16	0.45
1:D:184:PHE:CZ	1:D:232:PHE:HB2	2.51	0.45
1:E:188:GLU:O	1:E:189:TYR:CD2	2.68	0.45
1:D:206:MET:SD	1:D:236:ILE:HD13	2.55	0.45
1:C:13:GLN:CG	1:C:13:GLN:O	2.64	0.45
1:C:78:THR:OG1	1:C:110:ILE:HD11	2.16	0.45
1:E:29:VAL:CG1	1:E:230:VAL:CG1	2.88	0.45
1:A:29:VAL:CG1	1:A:230:VAL:CG1	2.89	0.45
1:C:203:THR:HG22	1:C:232:PHE:CZ	2.51	0.45
1:C:173:GLU:HB3	1:D:194:GLY:CA	2.47	0.45
1:B:188:GLU:O	1:B:189:TYR:CD2	2.70	0.45
1:C:171:LEU:HD13	1:D:129:ILE:HD11	1.98	0.45
1:B:17:THR:O	1:B:18:ARG:HB3	2.17	0.45
1:A:30:GLY:O	1:A:31:ILE:HG23	2.17	0.45
1:D:203:THR:HG22	1:D:232:PHE:CZ	2.52	0.45
1:E:171:LEU:HD13	1:F:129:ILE:CD1	2.45	0.45
1:E:13:GLN:O	1:E:13:GLN:CG	2.64	0.45
1:C:172:VAL:HG11	1:C:203:THR:OG1	2.17	0.45
1:F:184:PHE:CZ	1:F:232:PHE:HB2	2.52	0.45
1:A:13:GLN:O	1:A:13:GLN:CG	2.65	0.45
1:E:258:LEU:HD22	1:E:272:ASN:HB3	1.98	0.45
1:C:178:TYR:CD2	1:D:189:TYR:HB2	2.52	0.45
1:D:9:SER:H	1:D:231:GLN:HE22	1.64	0.45
1:E:9:SER:H	1:E:231:GLN:HE22	1.65	0.45
1:B:367:ILE:O	1:B:367:ILE:CG2	2.63	0.45
1:C:56:ARG:CZ	1:C:328:VAL:HG21	2.47	0.45
1:C:17:THR:O	1:C:18:ARG:HB3	2.17	0.44
1:D:220:ARG:HG3	1:D:220:ARG:HH11	1.81	0.44
1:C:283:VAL:HG21	1:C:357:ILE:HG13	1.99	0.44
1:F:86:PRO:O	1:F:121:LYS:HD3	2.17	0.44
1:C:120:ILE:HD13	1:C:202:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLU:HG2	1:B:200:SER:OG	2.17	0.44
1:E:56:ARG:CZ	1:E:328:VAL:HG21	2.47	0.44
1:B:13:GLN:O	1:B:13:GLN:CG	2.64	0.44
1:F:29:VAL:CG1	1:F:230:VAL:CG1	2.90	0.44
1:F:65:LEU:HD22	1:F:69:LEU:HD11	1.99	0.44
1:E:262:VAL:HG23	1:E:313:VAL:HG22	1.99	0.44
1:B:181:VAL:HG11	1:B:199:PRO:HG2	2.00	0.44
1:D:65:LEU:HD22	1:D:69:LEU:HD11	1.98	0.44
1:D:92:LEU:HD22	1:D:321:PHE:CE1	2.52	0.44
1:B:324:ASP:OD1	1:B:327:GLN:HG2	2.18	0.44
1:E:176:THR:HG22	1:E:239:ILE:HD11	1.98	0.44
1:E:193:ILE:HG22	1:E:194:GLY:N	2.31	0.44
1:F:62:GLU:CG	1:F:65:LEU:HB2	2.47	0.44
1:D:62:GLU:CG	1:D:65:LEU:HB2	2.48	0.44
1:C:182:GLN:N	1:C:183:PRO:CD	2.81	0.44
1:F:56:ARG:CZ	1:F:328:VAL:HG21	2.48	0.44
1:A:82:ILE:HD11	1:A:101:ALA:HB2	2.00	0.43
1:A:25:LEU:HD12	1:A:29:VAL:HG23	1.98	0.43
1:F:203:THR:HG22	1:F:232:PHE:CZ	2.52	0.43
1:C:268:PRO:HA	1:C:272:ASN:HD22	1.82	0.43
1:D:225:ASP:O	1:D:252:PHE:HA	2.19	0.43
1:C:287:ILE:O	1:C:291:ALA:HB3	2.18	0.43
1:D:88:LYS:HB2	1:D:135:MET:HE3	2.00	0.43
1:D:78:THR:OG1	1:D:110:ILE:HD11	2.18	0.43
1:E:220:ARG:HH11	1:E:220:ARG:HG3	1.84	0.43
1:B:274:ILE:HD13	1:B:283:VAL:HG13	1.99	0.43
1:A:222:LEU:C	1:A:222:LEU:HD12	2.39	0.43
1:B:166:TYR:O	1:B:167:ARG:C	2.56	0.43
1:A:181:VAL:HG11	1:A:199:PRO:HG2	2.00	0.43
1:B:86:PRO:O	1:B:121:LYS:HD3	2.18	0.43
1:F:13:GLN:CG	1:F:13:GLN:O	2.66	0.43
1:B:172:VAL:HG11	1:B:203:THR:OG1	2.19	0.43
1:E:198:SER:O	1:E:199:PRO:C	2.57	0.43
1:F:82:ILE:HD11	1:F:101:ALA:HB2	2.00	0.43
1:D:279:ASN:ND2	1:D:281:LYS:HE3	2.33	0.43
1:E:120:ILE:HD13	1:E:202:MET:CE	2.48	0.43
1:C:197:ALA:CA	1:D:193:ILE:HG23	2.33	0.43
1:D:309:CYS:HB3	1:D:315:PHE:CD2	2.54	0.43
1:C:324:ASP:OD1	1:C:327:GLN:HG2	2.19	0.43
1:E:17:THR:O	1:E:18:ARG:HB3	2.18	0.42
1:A:62:GLU:CG	1:A:65:LEU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:HD11	1:D:101:ALA:HB2	2.01	0.42
1:F:92:LEU:HD22	1:F:321:PHE:CE1	2.54	0.42
1:C:178:TYR:HD2	1:D:189:TYR:HB2	1.84	0.42
1:A:131:GLU:O	1:A:135:MET:HG3	2.20	0.42
1:C:87:GLN:HG2	1:C:121:LYS:HZ1	1.82	0.42
1:A:11:LEU:HD23	1:A:13:GLN:NE2	2.34	0.42
1:A:68:PHE:O	1:A:72:VAL:HG23	2.19	0.42
1:A:173:GLU:HG2	1:A:200:SER:OG	2.19	0.42
1:A:203:THR:HG22	1:A:232:PHE:CZ	2.55	0.42
1:F:181:VAL:HG11	1:F:199:PRO:HG2	2.00	0.42
1:E:182:GLN:N	1:E:183:PRO:CD	2.82	0.42
1:C:87:GLN:HA	1:C:135:MET:HE1	2.02	0.42
1:F:166:TYR:O	1:F:167:ARG:C	2.59	0.42
1:A:65:LEU:HD22	1:A:69:LEU:HD11	1.99	0.42
1:A:283:VAL:HG21	1:A:357:ILE:HG13	2.01	0.42
1:D:125:ARG:HH22	1:D:192:ASN:HB3	1.85	0.42
1:F:267:ILE:O	1:F:267:ILE:HG23	2.20	0.42
1:E:171:LEU:CD1	1:F:129:ILE:CD1	2.98	0.41
1:B:198:SER:O	1:B:199:PRO:C	2.58	0.41
1:D:268:PRO:HA	1:D:272:ASN:HD22	1.85	0.41
1:F:305:LEU:HD22	1:F:305:LEU:HA	1.91	0.41
1:A:213:HIS:O	1:C:130:ASN:ND2	2.53	0.41
1:E:283:VAL:HG21	1:E:357:ILE:HG13	2.03	0.41
1:C:225:ASP:O	1:C:252:PHE:HA	2.19	0.41
1:D:193:ILE:HG22	1:D:194:GLY:N	2.35	0.41
1:A:184:PHE:CZ	1:A:232:PHE:HB2	2.56	0.41
1:E:141:LYS:HA	1:E:367:ILE:HG21	2.01	0.41
1:E:62:GLU:CG	1:E:65:LEU:HB2	2.51	0.41
1:C:220:ARG:HH11	1:C:220:ARG:HG3	1.84	0.41
1:B:324:ASP:O	1:B:328:VAL:HG23	2.19	0.41
1:E:309:CYS:HB3	1:E:315:PHE:CD2	2.55	0.41
1:B:62:GLU:CG	1:B:65:LEU:HB2	2.51	0.41
1:D:367:ILE:HD12	1:D:367:ILE:N	2.34	0.41
1:C:261:GLY:CA	1:C:262:VAL:HB	2.51	0.41
1:E:268:PRO:HA	1:E:272:ASN:HD22	1.86	0.41
1:C:267:ILE:HG23	1:C:267:ILE:O	2.21	0.41
1:F:118:ASP:OD1	1:F:118:ASP:N	2.53	0.41
1:A:80:ILE:HB	1:A:112:VAL:HG22	2.03	0.41
1:C:309:CYS:HB3	1:C:315:PHE:CD2	2.55	0.41
1:F:172:VAL:HG11	1:F:203:THR:OG1	2.19	0.41
1:C:64:SER:HB2	1:C:249:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:HD11	1:C:101:ALA:HB2	2.03	0.41
1:E:25:LEU:HD12	1:E:29:VAL:HG23	2.02	0.41
1:F:141:LYS:HA	1:F:367:ILE:HG21	2.02	0.41
1:C:184:PHE:CZ	1:C:232:PHE:HB2	2.56	0.41
1:D:56:ARG:CZ	1:D:328:VAL:HG21	2.50	0.41
1:F:117:LEU:HD13	1:F:120:ILE:HD12	2.03	0.41
1:F:225:ASP:O	1:F:252:PHE:HA	2.21	0.41
1:A:193:ILE:HG21	1:A:193:ILE:HD13	1.68	0.41
1:D:258:LEU:HD22	1:D:272:ASN:CB	2.49	0.41
1:C:167:ARG:CZ	1:D:159:TYR:HB3	2.51	0.41
1:B:225:ASP:O	1:B:252:PHE:HA	2.20	0.40
1:F:279:ASN:ND2	1:F:281:LYS:HE3	2.36	0.40
1:D:86:PRO:O	1:D:121:LYS:HD3	2.20	0.40
1:A:141:LYS:HA	1:A:367:ILE:HG21	2.03	0.40
1:F:261:GLY:CA	1:F:262:VAL:HB	2.51	0.40
1:A:274:ILE:HD13	1:A:283:VAL:HG13	2.02	0.40
1:B:16:THR:OG1	1:B:20:THR:HA	2.22	0.40
1:D:141:LYS:HA	1:D:367:ILE:HG21	2.03	0.40
1:D:283:VAL:HG21	1:D:357:ILE:HG13	2.02	0.40
1:D:16:THR:OG1	1:D:20:THR:HA	2.21	0.40
1:C:29:VAL:CG1	1:C:230:VAL:CG1	2.92	0.40
1:A:214:PHE:HA	1:C:130:ASN:HD22	1.86	0.40
1:A:179:ASN:HB3	1:B:189:TYR:CD1	2.57	0.40
1:F:117:LEU:HD22	1:F:120:ILE:HD12	2.03	0.40
1:D:172:VAL:HG11	1:D:203:THR:OG1	2.21	0.40
1:A:262:VAL:HG23	1:A:313:VAL:HG22	2.03	0.40
1:B:309:CYS:HB3	1:B:315:PHE:CD2	2.56	0.40

All (6) 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:344:GLU:OE2	1:C:244:ASN:ND2[2_546]	1.90	0.30
1:B:189:TYR:CB	1:C:37:GLN:NE2[1_655]	1.97	0.23
1:A:189:TYR:OH	1:C:43:GLU:OE1[1_655]	2.00	0.20
1:B:355:ASP:OD2	1:F:88:LYS:NZ[2_555]	2.09	0.11
1:A:40:GLN:NE2	1:F:18:ARG:NE[1_556]	2.14	0.06
1:A:355:ASP:OD2	1:D:88:LYS:NZ[2_546]	2.17	0.03

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	372/386 (96%)	345 (93%)	19 (5%)	8 (2%)	8	38
1	B	372/386 (96%)	347 (93%)	16 (4%)	9 (2%)	7	35
1	C	372/386 (96%)	346 (93%)	17 (5%)	9 (2%)	7	35
1	D	372/386 (96%)	347 (93%)	16 (4%)	9 (2%)	7	35
1	E	372/386 (96%)	347 (93%)	16 (4%)	9 (2%)	7	35
1	F	372/386 (96%)	346 (93%)	17 (5%)	9 (2%)	7	35
All	All	2232/2316 (96%)	2078 (93%)	101 (4%)	53 (2%)	7	35

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	22	TYR
1	A	182	GLN
1	A	228	LYS
1	A	310	ASP
1	B	12	LEU
1	B	182	GLN
1	B	228	LYS
1	B	310	ASP
1	C	182	GLN
1	C	228	LYS
1	C	262	VAL
1	C	305	LEU
1	C	310	ASP
1	D	12	LEU
1	D	182	GLN
1	D	262	VAL
1	D	310	ASP
1	E	182	GLN
1	E	228	LYS

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Mol	Chain	Res	Type
1	E	310	ASP
1	F	12	LEU
1	F	182	GLN
1	F	262	VAL
1	F	310	ASP
1	A	262	VAL
1	A	305	LEU
1	B	22	TYR
1	B	262	VAL
1	B	305	LEU
1	C	12	LEU
1	C	22	TYR
1	D	22	TYR
1	D	183	PRO
1	D	228	LYS
1	D	266	ASP
1	D	305	LEU
1	E	12	LEU
1	E	22	TYR
1	E	262	VAL
1	E	305	LEU
1	F	22	TYR
1	F	183	PRO
1	F	228	LYS
1	F	305	LEU
1	A	183	PRO
1	B	183	PRO
1	B	266	ASP
1	C	183	PRO
1	E	183	PRO
1	F	266	ASP
1	E	266	ASP
1	C	266	ASP

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	323/348 (93%)	296 (92%)	27 (8%)	14	45
1	B	322/348 (92%)	295 (92%)	27 (8%)	14	45
1	C	323/348 (93%)	295 (91%)	28 (9%)	13	43
1	D	323/348 (93%)	296 (92%)	27 (8%)	14	45
1	E	322/348 (92%)	295 (92%)	27 (8%)	14	45
1	F	323/348 (93%)	295 (91%)	28 (9%)	13	43
All	All	1936/2088 (93%)	1772 (92%)	164 (8%)	13	45

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	13	GLN
1	A	17	THR
1	A	20	THR
1	A	60	LEU
1	A	62	GLU
1	A	65	LEU
1	A	92	LEU
1	A	110	ILE
1	A	168	THR
1	A	171	LEU
1	A	189	TYR
1	A	198	SER
1	A	220	ARG
1	A	222	LEU
1	A	227	ILE
1	A	249	THR
1	A	273	SER
1	A	275	LEU
1	A	285	ARG
1	A	298	THR
1	A	311	ILE
1	A	324	ASP
1	A	327	GLN
1	A	341	LEU
1	A	342	SER
1	A	379	THR
1	B	11	LEU
1	B	13	GLN
1	B	17	THR

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Mol	Chain	Res	Type
1	B	20	THR
1	B	60	LEU
1	B	62	GLU
1	B	65	LEU
1	B	92	LEU
1	B	110	ILE
1	B	168	THR
1	B	171	LEU
1	B	176	THR
1	B	189	TYR
1	B	198	SER
1	B	220	ARG
1	B	227	ILE
1	B	249	THR
1	B	273	SER
1	B	275	LEU
1	B	285	ARG
1	B	298	THR
1	B	311	ILE
1	B	324	ASP
1	B	327	GLN
1	B	341	LEU
1	B	342	SER
1	B	379	THR
1	C	11	LEU
1	C	13	GLN
1	C	17	THR
1	C	20	THR
1	C	60	LEU
1	C	62	GLU
1	C	65	LEU
1	C	92	LEU
1	C	110	ILE
1	C	168	THR
1	C	171	LEU
1	C	185	PHE
1	C	189	TYR
1	C	198	SER
1	C	220	ARG
1	C	222	LEU
1	C	227	ILE
1	C	249	THR

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Mol	Chain	Res	Type
1	C	273	SER
1	C	275	LEU
1	C	285	ARG
1	C	298	THR
1	C	311	ILE
1	C	324	ASP
1	C	327	GLN
1	C	341	LEU
1	C	342	SER
1	C	379	THR
1	D	11	LEU
1	D	13	GLN
1	D	15	PHE
1	D	17	THR
1	D	20	THR
1	D	60	LEU
1	D	62	GLU
1	D	65	LEU
1	D	92	LEU
1	D	110	ILE
1	D	168	THR
1	D	171	LEU
1	D	189	TYR
1	D	198	SER
1	D	220	ARG
1	D	222	LEU
1	D	227	ILE
1	D	249	THR
1	D	273	SER
1	D	275	LEU
1	D	285	ARG
1	D	311	ILE
1	D	324	ASP
1	D	327	GLN
1	D	341	LEU
1	D	342	SER
1	D	379	THR
1	E	11	LEU
1	E	13	GLN
1	E	17	THR
1	E	20	THR
1	E	60	LEU

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Mol	Chain	Res	Type
1	E	62	GLU
1	E	65	LEU
1	E	92	LEU
1	E	110	ILE
1	E	168	THR
1	E	171	LEU
1	E	189	TYR
1	E	198	SER
1	E	220	ARG
1	E	222	LEU
1	E	227	ILE
1	E	249	THR
1	E	273	SER
1	E	275	LEU
1	E	285	ARG
1	E	298	THR
1	E	311	ILE
1	E	324	ASP
1	E	327	GLN
1	E	341	LEU
1	E	342	SER
1	E	379	THR
1	F	11	LEU
1	F	13	GLN
1	F	15	PHE
1	F	17	THR
1	F	20	THR
1	F	60	LEU
1	F	62	GLU
1	F	65	LEU
1	F	92	LEU
1	F	110	ILE
1	F	168	THR
1	F	185	PHE
1	F	189	TYR
1	F	198	SER
1	F	220	ARG
1	F	222	LEU
1	F	227	ILE
1	F	249	THR
1	F	273	SER
1	F	275	LEU

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Mol	Chain	Res	Type
1	F	285	ARG
1	F	305	LEU
1	F	311	ILE
1	F	324	ASP
1	F	327	GLN
1	F	341	LEU
1	F	342	SER
1	F	379	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	ASN
1	A	279	ASN
1	B	272	ASN
1	B	279	ASN
1	C	130	ASN
1	C	272	ASN
1	C	279	ASN
1	D	272	ASN
1	D	279	ASN
1	E	272	ASN
1	E	279	ASN
1	F	272	ASN
1	F	279	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	374/386 (96%)	-0.08	6 (1%) 74 47	20, 20, 20, 50	0
1	B	374/386 (96%)	-0.10	3 (0%) 87 67	20, 20, 20, 50	0
1	C	374/386 (96%)	-0.09	3 (0%) 87 67	20, 20, 20, 50	0
1	D	374/386 (96%)	-0.23	0 100 100	20, 20, 20, 50	0
1	E	374/386 (96%)	0.29	23 (6%) 25 9	20, 20, 20, 50	0
1	F	374/386 (96%)	-0.21	1 (0%) 94 84	20, 20, 20, 50	0
All	All	2244/2316 (96%)	-0.07	36 (1%) 74 47	20, 20, 20, 50	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	61	ALA	4.6
1	E	54	LEU	4.2
1	E	22	TYR	3.7
1	A	308	GLN	3.6
1	E	45	LEU	3.4
1	E	307	GLY	3.1
1	B	295	GLY	3.0
1	E	265	PHE	2.9
1	E	110	ILE	2.8
1	A	345	LEU	2.8
1	B	344	GLU	2.8
1	A	344	GLU	2.8
1	A	295	GLY	2.8
1	E	302	HIS	2.7
1	E	281	LYS	2.7
1	E	304	LYS	2.7
1	C	63	LYS	2.7
1	E	100	PHE	2.6
1	E	251	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	325	ASN	2.5
1	C	22	TYR	2.5
1	E	340	LEU	2.4
1	E	306	GLY	2.3
1	E	325	ASN	2.3
1	A	297	ASN	2.3
1	E	25	LEU	2.2
1	E	62	GLU	2.2
1	E	32	ASN	2.2
1	C	230	VAL	2.2
1	E	300	GLU	2.2
1	E	305	LEU	2.2
1	E	79	PHE	2.1
1	A	294	GLY	2.1
1	E	108	PHE	2.1
1	B	189	TYR	2.1
1	E	222	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.