



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2021 – 12:10 PM JST

PDB ID : 7DMO
Title : Crystal structures of two pericyclases catalyzing [4+2] cycloadditions
Authors : Wang, Z.D.; Chi, C.B.; Ma, M.
Deposited on : 2020-12-04
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

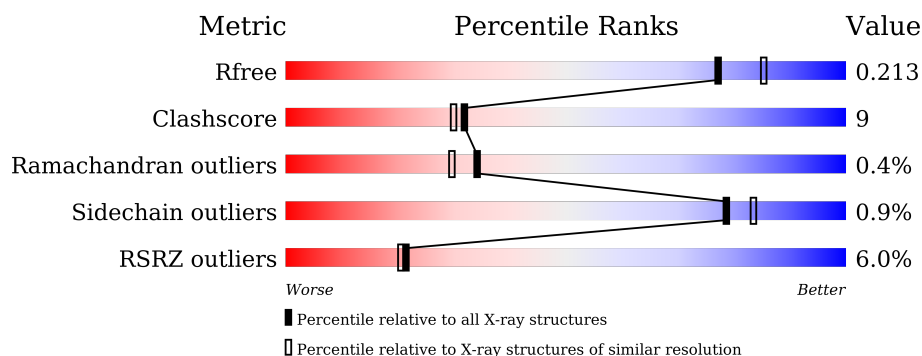
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 $\leq 5\%$. 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	389	<div> <div>7%</div> <div>87%</div> <div>7%</div> <div>• •</div> </div>
1	B	389	<div> <div>4%</div> <div>83%</div> <div>12%</div> <div>• •</div> </div>
1	C	389	<div> <div>7%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
1	D	389	<div> <div>6%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	E	389	<div> <div>5%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>
1	F	389	<div> <div>6%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18922 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 Diels-Alderase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2835	1798	475	554	8			
1	B	375	Total	C	N	O	S	0	0	0
			2843	1802	476	557	8			
1	C	375	Total	C	N	O	S	0	0	0
			2844	1804	477	555	8			
1	D	374	Total	C	N	O	S	0	0	0
			2835	1798	475	554	8			
1	E	375	Total	C	N	O	S	0	0	0
			2844	1804	477	555	8			
1	F	374	Total	C	N	O	S	0	0	0
			2838	1801	476	553	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A2Z5XAU0
A	2	SER	-	expression tag	UNP A0A2Z5XAU0
A	3	HIS	-	expression tag	UNP A0A2Z5XAU0
B	1	GLY	-	expression tag	UNP A0A2Z5XAU0
B	2	SER	-	expression tag	UNP A0A2Z5XAU0
B	3	HIS	-	expression tag	UNP A0A2Z5XAU0
C	1	GLY	-	expression tag	UNP A0A2Z5XAU0
C	2	SER	-	expression tag	UNP A0A2Z5XAU0
C	3	HIS	-	expression tag	UNP A0A2Z5XAU0
D	1	GLY	-	expression tag	UNP A0A2Z5XAU0
D	2	SER	-	expression tag	UNP A0A2Z5XAU0
D	3	HIS	-	expression tag	UNP A0A2Z5XAU0
E	1	GLY	-	expression tag	UNP A0A2Z5XAU0
E	2	SER	-	expression tag	UNP A0A2Z5XAU0
E	3	HIS	-	expression tag	UNP A0A2Z5XAU0
F	1	GLY	-	expression tag	UNP A0A2Z5XAU0
F	2	SER	-	expression tag	UNP A0A2Z5XAU0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	3	HIS	-	expression tag	UNP A0A2Z5XAU0

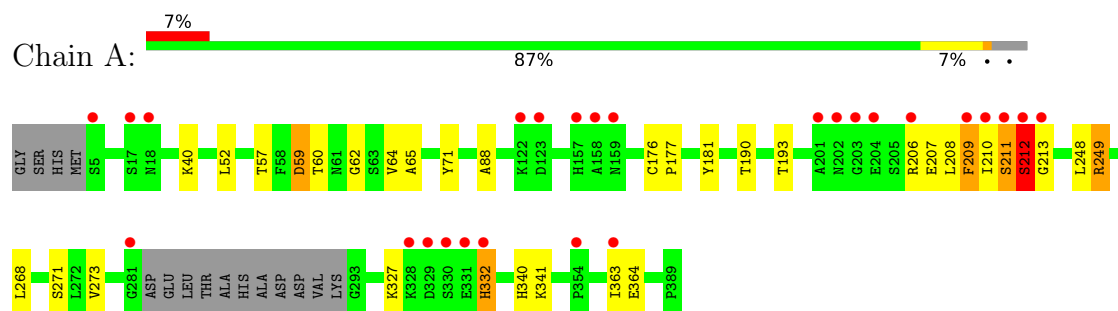
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	304	Total 304	O 304	0	0
2	B	308	Total 308	O 308	0	0
2	C	325	Total 325	O 325	0	0
2	D	317	Total 317	O 317	0	0
2	E	324	Total 324	O 324	0	0
2	F	305	Total 305	O 305	0	0

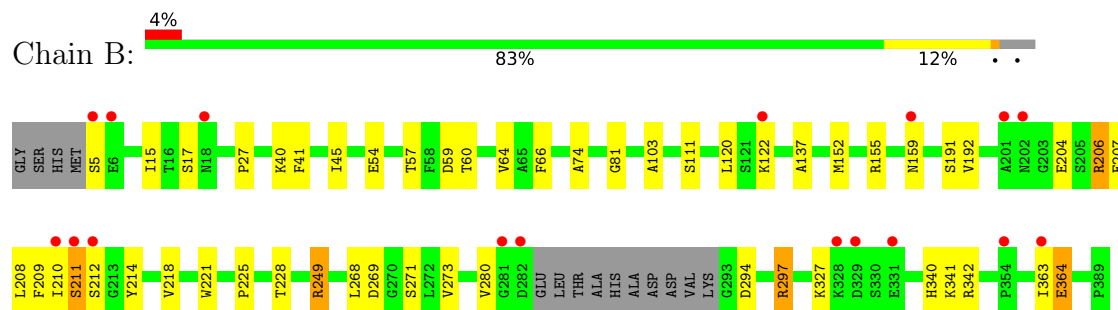
3 Residue-property plots [i](#)

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

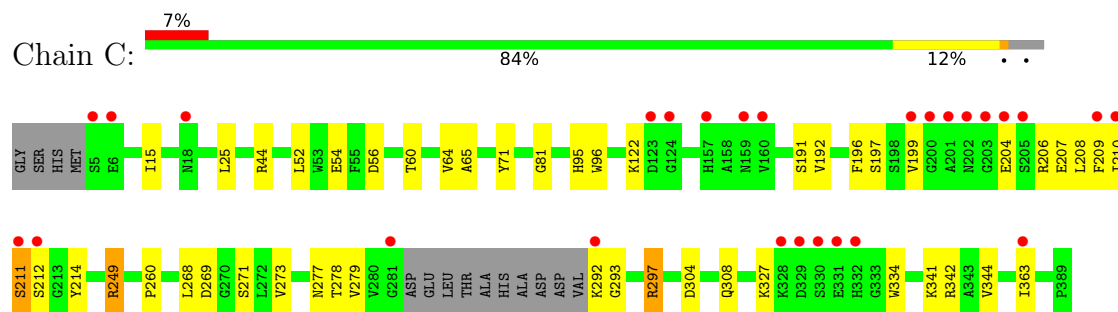
• Molecule 1: Diels-Alderase



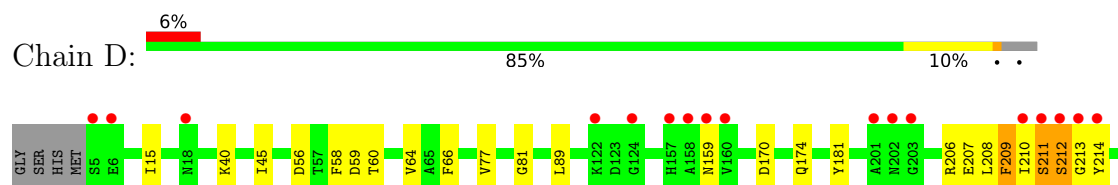
• Molecule 1: Diels-Alderase

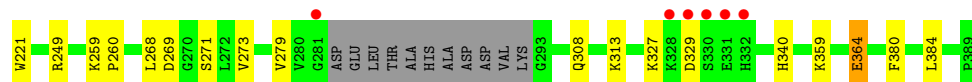


• Molecule 1: Diels-Alderase

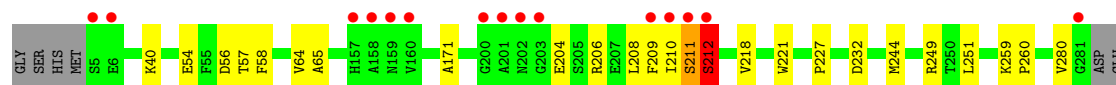
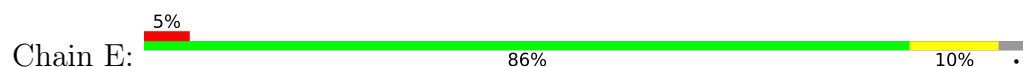


• Molecule 1: Diels-Alderase

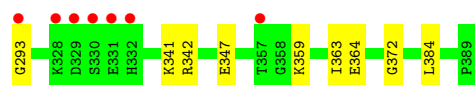
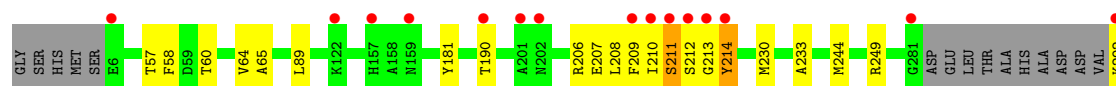
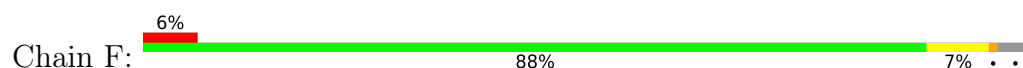




● Molecule 1: Diels-Alderase



● Molecule 1: Diels-Alderase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.20Å 150.53Å 100.05Å 90.00° 96.94° 90.00°	Depositor
Resolution (Å)	13.43 – 2.00 13.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (13.43-2.00) 93.5 (13.43-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 1.99Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.173 , 0.210 0.181 , 0.213	Depositor DCC
R_{free} test set	1853 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18922	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2655e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.52	1/2916 (0.0%)	0.68	0/3972
1	B	0.53	0/2924	0.69	2/3983 (0.1%)
1	C	0.53	0/2925	0.68	2/3983 (0.1%)
1	D	0.57	2/2916 (0.1%)	0.69	1/3972 (0.0%)
1	E	0.55	1/2925 (0.0%)	0.69	0/3983
1	F	0.54	2/2919 (0.1%)	0.67	0/3975
All	All	0.54	6/17525 (0.0%)	0.68	5/23868 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	364	GLU	CD-OE2	-5.58	1.19	1.25
1	F	207	GLU	CG-CD	-5.35	1.44	1.51
1	E	364	GLU	CD-OE2	-5.18	1.20	1.25
1	A	209	PHE	CB-CG	-5.13	1.42	1.51
1	D	209	PHE	CB-CG	-5.09	1.42	1.51
1	D	209	PHE	CD1-CE1	-5.08	1.29	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	297	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	D	181	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	B	120	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	297	ARG	NE-CZ-NH2	-5.01	117.80	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	2835	0	2683	58	0
1	B	2843	0	2687	52	0
1	C	2844	0	2696	77	0
1	D	2835	0	2683	70	0
1	E	2844	0	2696	40	0
1	F	2838	0	2691	73	0
2	A	304	0	0	0	0
2	B	308	0	0	0	0
2	C	325	0	0	0	0
2	D	317	0	0	0	0
2	E	324	0	0	0	0
2	F	305	0	0	0	0
All	All	18922	0	16136	294	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 9.

All (294) 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:F:57:THR:CG2	1:F:190:THR:HG21	1.57	1.33
1:D:210:ILE:O	1:D:212:SER:N	1.61	1.33
1:A:271:SER:HB2	1:C:210:ILE:CD1	1.57	1.31
1:A:271:SER:CB	1:C:210:ILE:HD12	1.60	1.28
1:C:271:SER:HB2	1:F:210:ILE:CD1	1.63	1.28
1:C:271:SER:CB	1:F:210:ILE:HD12	1.61	1.28
1:C:268:LEU:O	1:F:210:ILE:HG13	1.22	1.27
1:F:64:VAL:HB	1:F:209:PHE:CE1	1.69	1.26
1:A:268:LEU:O	1:C:210:ILE:HG13	1.26	1.24
1:C:64:VAL:HG22	1:C:209:PHE:CZ	1.77	1.18
1:A:64:VAL:CG1	1:A:209:PHE:HE1	1.58	1.17
1:A:208:LEU:HD13	1:F:372:GLY:HA2	1.24	1.15
1:D:340:HIS:ND1	1:D:364:GLU:OE1	1.81	1.13
1:F:64:VAL:CB	1:F:209:PHE:HE1	1.62	1.10
1:B:268:LEU:O	1:D:210:ILE:HD13	1.49	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:THR:HG22	1:F:190:THR:HG21	1.26	1.09
1:F:190:THR:HB	1:F:213:GLY:O	1.54	1.07
1:C:210:ILE:O	1:C:212:SER:N	1.86	1.06
1:F:60:THR:HG21	1:F:212:SER:OG	1.54	1.05
1:B:271:SER:HB2	1:D:210:ILE:HG12	1.31	1.04
1:A:64:VAL:HG12	1:A:209:PHE:CE1	1.92	1.04
1:A:208:LEU:HD13	1:F:372:GLY:CA	1.88	1.04
1:B:271:SER:CB	1:D:210:ILE:HG12	1.88	1.03
1:A:64:VAL:CG1	1:A:209:PHE:CE1	2.45	0.98
1:C:268:LEU:O	1:F:210:ILE:CG1	2.11	0.98
1:B:340:HIS:ND1	1:B:364:GLU:OE1	1.97	0.97
1:F:57:THR:CG2	1:F:190:THR:CG2	2.42	0.97
1:A:327:LYS:HD2	1:C:206:ARG:HD3	1.46	0.96
1:E:64:VAL:HG13	1:E:209:PHE:HE1	1.30	0.96
1:F:60:THR:CG2	1:F:212:SER:OG	2.17	0.93
1:A:268:LEU:O	1:C:210:ILE:CG1	2.17	0.92
1:A:332:HIS:CE1	1:C:206:ARG:HB2	2.04	0.92
1:F:64:VAL:HB	1:F:209:PHE:HE1	0.77	0.92
1:A:273:VAL:HG12	1:C:208:LEU:HD22	1.52	0.91
1:F:210:ILE:O	1:F:212:SER:N	2.02	0.91
1:C:308:GLN:OE1	1:D:308:GLN:NE2	2.04	0.90
1:A:64:VAL:HG12	1:A:209:PHE:HE1	1.28	0.88
1:A:332:HIS:HE1	1:C:206:ARG:HB2	1.39	0.88
1:D:60:THR:N	1:D:212:SER:O	2.07	0.87
1:C:210:ILE:C	1:C:212:SER:H	1.77	0.87
1:F:64:VAL:CB	1:F:209:PHE:CE1	2.47	0.86
1:D:271:SER:HB2	1:E:210:ILE:HD12	1.57	0.84
1:F:57:THR:HG21	1:F:190:THR:HG21	1.57	0.83
1:A:271:SER:OG	1:C:210:ILE:HG23	1.79	0.82
1:B:271:SER:HB2	1:D:210:ILE:CG1	2.10	0.82
1:D:271:SER:CB	1:E:210:ILE:HD12	2.09	0.82
1:A:327:LYS:HD2	1:C:206:ARG:CD	2.11	0.81
1:F:210:ILE:C	1:F:212:SER:H	1.85	0.81
1:F:230:MET:CE	1:F:233:ALA:HB2	2.11	0.80
1:C:64:VAL:HG22	1:C:209:PHE:CE1	2.16	0.80
1:C:192:VAL:HB	1:C:209:PHE:HD2	1.44	0.79
1:F:57:THR:HG22	1:F:190:THR:CG2	2.07	0.79
1:C:249:ARG:HD2	1:C:249:ARG:C	2.03	0.79
1:F:190:THR:CB	1:F:213:GLY:O	2.31	0.79
1:D:64:VAL:HB	1:D:209:PHE:HE1	1.46	0.79
1:A:190:THR:O	1:A:211:SER:HA	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:C	1:D:212:SER:H	1.84	0.78
1:B:268:LEU:O	1:D:210:ILE:CD1	2.29	0.78
1:B:210:ILE:O	1:B:212:SER:N	2.17	0.78
1:C:273:VAL:HG12	1:F:208:LEU:HD22	1.67	0.77
1:B:273:VAL:HG12	1:D:208:LEU:HD22	1.65	0.77
1:E:64:VAL:HG13	1:E:209:PHE:CE1	2.18	0.77
1:D:271:SER:OG	1:E:210:ILE:HG23	1.84	0.77
1:F:57:THR:HG21	1:F:190:THR:CG2	2.10	0.76
1:F:57:THR:CB	1:F:190:THR:HG21	2.16	0.75
1:D:359:LYS:HE2	1:D:384:LEU:HD12	1.69	0.74
1:D:268:LEU:O	1:E:210:ILE:HG13	1.88	0.74
1:A:268:LEU:C	1:C:210:ILE:HG13	2.06	0.73
1:C:65:ALA:HB2	1:C:363:ILE:HD11	1.70	0.73
1:A:64:VAL:CB	1:A:209:PHE:HE1	2.00	0.73
1:F:64:VAL:C	1:F:209:PHE:HZ	1.91	0.72
1:B:269:ASP:OD2	1:D:212:SER:HB3	1.90	0.72
1:B:271:SER:OG	1:D:210:ILE:HG12	1.90	0.71
1:C:64:VAL:HG13	1:C:209:PHE:CE1	2.24	0.71
1:B:269:ASP:OD2	1:D:212:SER:CB	2.38	0.71
1:A:52:LEU:HD13	1:A:71:TYR:CE2	2.26	0.70
1:D:271:SER:HB2	1:E:210:ILE:CD1	2.20	0.70
1:A:340:HIS:ND1	1:A:364:GLU:OE1	2.24	0.70
1:C:96:TRP:CD1	1:C:199:VAL:HG22	2.27	0.70
1:D:268:LEU:HD23	1:E:210:ILE:HG12	1.72	0.69
1:F:64:VAL:CG1	1:F:209:PHE:CE1	2.75	0.69
1:E:259:LYS:HD2	1:E:260:PRO:HD2	1.74	0.69
1:F:64:VAL:C	1:F:209:PHE:CZ	2.66	0.69
1:A:340:HIS:HA	1:A:364:GLU:OE1	1.92	0.68
1:A:249:ARG:HD2	1:A:249:ARG:C	2.14	0.68
1:B:327:LYS:HD2	1:D:206:ARG:HH11	1.59	0.68
1:F:65:ALA:N	1:F:209:PHE:HZ	1.91	0.68
1:A:60:THR:CG2	1:A:212:SER:OG	2.43	0.67
1:A:190:THR:N	1:A:213:GLY:O	2.26	0.67
1:F:65:ALA:HB2	1:F:363:ILE:HD11	1.76	0.67
1:F:210:ILE:HG22	1:F:211:SER:N	2.10	0.67
1:C:273:VAL:CG1	1:F:208:LEU:HD22	2.25	0.66
1:B:280:VAL:HG11	1:B:297:ARG:NH2	2.10	0.66
1:D:210:ILE:C	1:D:212:SER:N	2.44	0.66
1:D:273:VAL:HG12	1:E:208:LEU:HD22	1.76	0.66
1:A:273:VAL:CG1	1:C:208:LEU:HD22	2.25	0.66
1:F:230:MET:HE3	1:F:233:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:VAL:HB	1:C:209:PHE:CD2	2.28	0.66
1:A:60:THR:HG21	1:A:212:SER:OG	1.95	0.65
1:C:249:ARG:O	1:C:249:ARG:NH2	2.28	0.65
1:F:359:LYS:HE2	1:F:384:LEU:HD12	1.79	0.65
1:A:208:LEU:CD1	1:F:372:GLY:HA2	2.15	0.65
1:C:64:VAL:HG22	1:C:209:PHE:HZ	1.58	0.64
1:C:271:SER:HB2	1:F:210:ILE:HD12	0.75	0.64
1:D:59:ASP:HA	1:D:212:SER:O	1.97	0.64
1:B:206:ARG:HH11	1:E:371:LYS:HG2	1.63	0.63
1:E:65:ALA:HB2	1:E:363:ILE:HD11	1.79	0.63
1:E:294:ASP:OD2	1:E:327:LYS:HD2	1.99	0.63
1:E:64:VAL:HG22	1:E:209:PHE:CE1	2.34	0.63
1:C:260:PRO:HG2	1:C:279:VAL:HG21	1.80	0.63
1:B:341:LYS:HB3	1:B:363:ILE:O	1.99	0.63
1:C:341:LYS:HB3	1:C:363:ILE:O	1.99	0.62
1:F:60:THR:CG2	1:F:212:SER:O	2.47	0.62
1:E:64:VAL:CG1	1:E:209:PHE:HE1	2.10	0.62
1:D:268:LEU:O	1:E:210:ILE:HG21	1.99	0.61
1:A:52:LEU:HD13	1:A:71:TYR:CZ	2.36	0.61
1:C:342:ARG:HB2	1:C:363:ILE:HB	1.82	0.61
1:C:268:LEU:C	1:F:210:ILE:HG13	2.15	0.61
1:A:190:THR:OG1	1:A:213:GLY:HA3	2.01	0.61
1:F:60:THR:HG21	1:F:212:SER:HG	1.65	0.61
1:C:268:LEU:HD23	1:F:210:ILE:HG12	1.84	0.60
1:B:363:ILE:O	1:B:363:ILE:HG22	2.01	0.60
1:D:359:LYS:HE2	1:D:384:LEU:CD1	2.32	0.59
1:A:64:VAL:HG12	1:A:209:PHE:CZ	2.34	0.59
1:F:58:PHE:O	1:F:213:GLY:HA2	2.03	0.59
1:F:210:ILE:C	1:F:212:SER:N	2.53	0.59
1:B:268:LEU:HB3	1:D:210:ILE:CD1	2.33	0.59
1:C:271:SER:OG	1:F:210:ILE:HG23	2.03	0.58
1:C:278:THR:OG1	1:C:292:LYS:HE3	2.02	0.58
1:A:59:ASP:OD1	1:A:62:GLY:N	2.37	0.58
1:D:327:LYS:O	1:D:329:ASP:N	2.36	0.58
1:E:171:ALA:HB1	1:E:292:LYS:HE3	1.86	0.58
1:D:327:LYS:HD2	1:E:206:ARG:HD3	1.85	0.57
1:D:64:VAL:HG13	1:D:89:LEU:O	2.05	0.57
1:F:60:THR:HG23	1:F:212:SER:O	2.03	0.57
1:E:341:LYS:HB3	1:E:363:ILE:O	2.05	0.57
1:F:210:ILE:HG22	1:F:211:SER:H	1.70	0.57
1:C:96:TRP:HD1	1:C:199:VAL:HG22	1.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:CB	1:B:122:LYS:HE3	2.36	0.56
1:E:359:LYS:HE2	1:E:384:LEU:HD12	1.88	0.56
1:A:341:LYS:HB3	1:A:363:ILE:O	2.05	0.56
1:A:64:VAL:HB	1:A:209:PHE:CE1	2.41	0.55
1:C:25:LEU:HD11	1:C:44:ARG:HG3	1.87	0.55
1:A:64:VAL:HG11	1:A:209:PHE:HE1	1.65	0.55
1:B:327:LYS:HD2	1:D:206:ARG:NH1	2.20	0.55
1:C:197:SER:O	1:C:204:GLU:HB3	2.05	0.55
1:B:191:SER:HB3	1:B:211:SER:HA	1.88	0.55
1:B:54:GLU:HB3	1:B:218:VAL:HB	1.89	0.54
1:C:249:ARG:HD2	1:C:249:ARG:O	2.07	0.54
1:F:249:ARG:HD2	1:F:249:ARG:C	2.28	0.54
1:E:57:THR:HG1	1:E:209:PHE:HE2	1.51	0.54
1:A:64:VAL:CB	1:A:209:PHE:CE1	2.87	0.54
1:A:64:VAL:HB	1:A:209:PHE:HE1	1.72	0.54
1:E:54:GLU:HB3	1:E:218:VAL:HB	1.88	0.54
1:B:66:PHE:HB2	1:B:207:GLU:OE1	2.07	0.53
1:F:60:THR:HG23	1:F:212:SER:OG	2.06	0.53
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.73	0.53
1:D:64:VAL:CB	1:D:209:PHE:HE1	2.20	0.53
1:B:342:ARG:HB2	1:B:363:ILE:HB	1.90	0.53
1:F:210:ILE:CG2	1:F:211:SER:H	2.22	0.53
1:A:268:LEU:HG	1:C:210:ILE:HG12	1.91	0.52
1:B:249:ARG:C	1:B:249:ARG:HD2	2.29	0.52
1:F:210:ILE:CG2	1:F:211:SER:N	2.72	0.52
1:F:190:THR:OG1	1:F:214:TYR:O	2.24	0.52
1:A:208:LEU:HD22	1:F:372:GLY:HA3	1.91	0.52
1:B:5:SER:HB2	1:B:111:SER:HB3	1.90	0.52
1:B:45:ILE:HD11	1:B:74:ALA:HA	1.91	0.52
1:E:249:ARG:C	1:E:249:ARG:HD2	2.29	0.52
1:B:269:ASP:OD2	1:D:212:SER:HB2	2.09	0.52
1:D:159:ASN:OD1	1:E:211:SER:HB2	2.10	0.52
1:A:271:SER:HG	1:C:210:ILE:HG23	1.72	0.51
1:C:277:ASN:H	1:C:292:LYS:NZ	2.08	0.51
1:F:341:LYS:HB3	1:F:363:ILE:O	2.10	0.51
1:C:210:ILE:C	1:C:212:SER:N	2.46	0.50
1:B:60:THR:HG22	1:B:214:TYR:CE2	2.47	0.50
1:C:277:ASN:H	1:C:292:LYS:HZ3	1.60	0.50
1:A:64:VAL:HG13	1:A:207:GLU:OE2	2.11	0.50
1:B:59:ASP:OD2	1:B:64:VAL:HG22	2.11	0.50
1:B:210:ILE:C	1:B:212:SER:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:SER:O	1:D:213:GLY:N	2.39	0.50
1:E:342:ARG:HB2	1:E:363:ILE:HB	1.94	0.50
1:C:54:GLU:OE2	1:C:56:ASP:OD2	2.29	0.50
1:A:193:THR:HA	1:A:208:LEU:HD23	1.94	0.50
1:B:225:PRO:HG2	1:B:228:THR:HG23	1.94	0.50
1:D:359:LYS:CE	1:D:384:LEU:HD12	2.40	0.49
1:B:294:ASP:OD1	1:B:327:LYS:HD3	2.12	0.49
1:D:249:ARG:HD2	1:D:249:ARG:C	2.33	0.49
1:B:269:ASP:O	1:D:210:ILE:HG22	2.11	0.49
1:A:64:VAL:HG11	1:A:209:PHE:CE1	2.42	0.49
1:C:304:ASP:OD2	1:D:313:LYS:NZ	2.42	0.49
1:A:57:THR:OG1	1:A:209:PHE:CE2	2.64	0.49
1:F:57:THR:HB	1:F:190:THR:HG21	1.91	0.49
1:C:192:VAL:CB	1:C:209:PHE:HD2	2.22	0.49
1:C:327:LYS:HE2	1:F:206:ARG:HD3	1.95	0.49
1:F:292:LYS:HG3	1:F:293:GLY:H	1.77	0.49
1:D:59:ASP:CA	1:D:212:SER:O	2.61	0.48
1:D:260:PRO:HG2	1:D:279:VAL:HG21	1.95	0.48
1:C:292:LYS:HD2	1:C:293:GLY:H	1.79	0.48
1:F:64:VAL:HG12	1:F:209:PHE:CZ	2.48	0.48
1:C:268:LEU:O	1:F:210:ILE:HG21	2.14	0.48
1:E:232:ASP:HB3	1:E:251:LEU:HB2	1.94	0.48
1:B:271:SER:HB2	1:D:210:ILE:CD1	2.44	0.48
1:F:347:GLU:HB2	1:F:359:LYS:HG3	1.96	0.48
1:D:58:PHE:O	1:D:213:GLY:CA	2.61	0.48
1:C:269:ASP:HB2	1:F:210:ILE:HB	1.97	0.47
1:B:268:LEU:HB3	1:D:210:ILE:HD13	1.96	0.47
1:C:327:LYS:HD3	1:C:334:TRP:CZ3	2.49	0.47
1:A:57:THR:OG1	1:A:209:PHE:HE2	1.98	0.47
1:C:15:ILE:HG21	1:C:81:GLY:HA2	1.95	0.47
1:E:327:LYS:HD3	1:E:334:TRP:CZ3	2.50	0.47
1:F:292:LYS:HG3	1:F:293:GLY:N	2.30	0.47
1:B:159:ASN:OD1	1:D:211:SER:OG	2.19	0.47
1:C:64:VAL:HG13	1:C:209:PHE:HE1	1.78	0.47
1:B:152:MET:HG3	1:B:192:VAL:HG22	1.97	0.47
1:D:58:PHE:O	1:D:213:GLY:HA2	2.15	0.47
1:D:211:SER:C	1:D:213:GLY:H	2.17	0.47
1:A:65:ALA:CA	1:A:209:PHE:HZ	2.28	0.46
1:F:58:PHE:O	1:F:213:GLY:CA	2.63	0.46
1:C:64:VAL:HG23	1:C:207:GLU:OE2	2.15	0.46
1:C:60:THR:HG22	1:C:214:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HG	1:B:209:PHE:N	2.27	0.46
1:A:268:LEU:HG	1:C:210:ILE:CG1	2.45	0.46
1:D:40:LYS:HG3	1:D:221:TRP:CE2	2.51	0.46
1:C:196:PHE:O	1:C:204:GLU:HA	2.16	0.46
1:D:56:ASP:HB3	1:D:380:PHE:CD2	2.51	0.46
1:B:269:ASP:O	1:D:210:ILE:CG2	2.64	0.46
1:F:65:ALA:CA	1:F:209:PHE:HZ	2.29	0.45
1:A:88:ALA:HB1	1:A:207:GLU:OE1	2.17	0.45
1:B:137:ALA:HB2	1:B:155:ARG:NE	2.32	0.45
1:C:363:ILE:O	1:C:363:ILE:HG22	2.16	0.45
1:A:268:LEU:HB3	1:C:210:ILE:HD11	1.98	0.45
1:D:64:VAL:CG1	1:D:209:PHE:CE1	3.00	0.45
1:F:64:VAL:HG12	1:F:209:PHE:CE1	2.51	0.44
1:B:15:ILE:HG21	1:B:81:GLY:HA2	1.99	0.44
1:B:268:LEU:O	1:D:210:ILE:HB	2.17	0.44
1:E:57:THR:OG1	1:E:209:PHE:HE2	2.01	0.44
1:E:345:TRP:CD2	1:E:361:GLY:HA3	2.53	0.44
1:A:208:LEU:HD13	1:F:372:GLY:N	2.31	0.44
1:A:181:TYR:CZ	1:A:248:LEU:HD22	2.52	0.44
1:B:64:VAL:HB	1:B:209:PHE:HE1	1.83	0.44
1:D:40:LYS:HA	1:D:40:LYS:HD2	1.88	0.44
1:E:54:GLU:OE2	1:E:56:ASP:OD2	2.35	0.44
1:A:62:GLY:O	1:A:363:ILE:HG21	2.18	0.44
1:F:230:MET:SD	1:F:230:MET:C	2.96	0.44
1:C:191:SER:HB2	1:C:211:SER:HA	1.99	0.44
1:B:17:SER:O	1:B:17:SER:OG	2.29	0.43
1:D:15:ILE:HG21	1:D:81:GLY:HA2	2.01	0.43
1:D:170:ASP:O	1:D:174:GLN:HG3	2.17	0.43
1:D:64:VAL:HG12	1:D:209:PHE:CE1	2.53	0.43
1:C:95:HIS:CG	1:C:344:VAL:O	2.71	0.43
1:F:64:VAL:O	1:F:209:PHE:CZ	2.72	0.43
1:B:210:ILE:C	1:B:212:SER:N	2.69	0.43
1:C:268:LEU:O	1:F:210:ILE:CB	2.65	0.43
1:D:59:ASP:C	1:D:212:SER:O	2.57	0.43
1:C:52:LEU:HD13	1:C:71:TYR:CE1	2.54	0.43
1:B:208:LEU:O	1:B:209:PHE:HD1	2.02	0.43
1:C:64:VAL:C	1:C:209:PHE:HE1	2.22	0.43
1:D:259:LYS:HD3	1:D:259:LYS:HA	1.84	0.43
1:A:40:LYS:HA	1:A:40:LYS:HD2	1.78	0.42
1:A:176:CYS:HB2	1:A:177:PRO:HD2	2.00	0.42
1:B:268:LEU:HD23	1:D:210:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:THR:HG22	1:F:212:SER:O	2.17	0.42
1:F:342:ARG:HB2	1:F:363:ILE:HB	2.00	0.42
1:B:40:LYS:HG3	1:B:221:TRP:CE2	2.55	0.42
1:B:280:VAL:HG11	1:B:297:ARG:HH21	1.83	0.42
1:A:271:SER:HB2	1:C:210:ILE:HD12	0.65	0.42
1:F:89:LEU:HD23	1:F:363:ILE:HG13	2.01	0.42
1:D:64:VAL:HG12	1:D:209:PHE:CZ	2.55	0.42
1:C:273:VAL:CB	1:F:208:LEU:HD22	2.49	0.42
1:B:57:THR:HG1	1:B:209:PHE:HE2	1.58	0.42
1:D:60:THR:OG1	1:D:212:SER:HB2	2.20	0.42
1:E:280:VAL:CG2	1:E:297:ARG:HB2	2.49	0.42
1:E:367:SER:HA	1:E:375:TYR:O	2.18	0.42
1:B:342:ARG:HD3	1:B:363:ILE:HG21	2.00	0.42
1:C:327:LYS:HD3	1:C:334:TRP:HZ3	1.85	0.42
1:A:268:LEU:CG	1:C:210:ILE:HG12	2.50	0.41
1:C:122:LYS:HA	1:C:122:LYS:HE2	2.02	0.41
1:D:271:SER:OG	1:E:210:ILE:HD12	2.20	0.41
1:D:269:ASP:O	1:E:210:ILE:HG21	2.21	0.41
1:D:66:PHE:HB2	1:D:207:GLU:OE2	2.20	0.41
1:A:190:THR:OG1	1:A:213:GLY:CA	2.68	0.41
1:B:27:PRO:HB3	1:B:41:PHE:CZ	2.54	0.41
1:D:45:ILE:HD11	1:D:77:VAL:HG21	2.01	0.41
1:D:56:ASP:HB3	1:D:380:PHE:HD2	1.86	0.41
1:D:329:ASP:O	1:E:204:GLU:OE2	2.39	0.41
1:E:40:LYS:HG3	1:E:221:TRP:CE2	2.56	0.41
1:F:230:MET:SD	1:F:230:MET:O	2.79	0.41
1:D:60:THR:HG22	1:D:214:TYR:CE2	2.56	0.41
1:E:363:ILE:O	1:E:363:ILE:HG22	2.21	0.41
1:C:269:ASP:O	1:F:210:ILE:HG21	2.22	0.40
1:E:210:ILE:O	1:E:212:SER:N	2.54	0.40
1:E:227:PRO:HB3	1:E:388:VAL:HG21	2.02	0.40
1:A:271:SER:CB	1:C:210:ILE:HG23	2.52	0.40
1:E:58:PHE:HA	1:E:209:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/389 (95%)	357 (96%)	12 (3%)	1 (0%)	41	37
1	B	371/389 (95%)	356 (96%)	14 (4%)	1 (0%)	41	37
1	C	371/389 (95%)	355 (96%)	15 (4%)	1 (0%)	41	37
1	D	370/389 (95%)	353 (95%)	15 (4%)	2 (0%)	29	23
1	E	371/389 (95%)	359 (97%)	10 (3%)	2 (0%)	29	23
1	F	370/389 (95%)	355 (96%)	13 (4%)	2 (0%)	29	23
All	All	2223/2334 (95%)	2135 (96%)	79 (4%)	9 (0%)	34	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	211	SER
1	C	211	SER
1	D	211	SER
1	E	211	SER
1	E	212	SER
1	F	211	SER
1	F	214	TYR
1	D	212	SER
1	A	212	SER

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/313 (96%)	294 (98%)	7 (2%)	50	53
1	B	302/313 (96%)	298 (99%)	4 (1%)	69	74
1	C	302/313 (96%)	301 (100%)	1 (0%)	92	95
1	D	301/313 (96%)	300 (100%)	1 (0%)	92	95
1	E	302/313 (96%)	300 (99%)	2 (1%)	84	88
1	F	301/313 (96%)	299 (99%)	2 (1%)	84	88
All	All	1809/1878 (96%)	1792 (99%)	17 (1%)	78	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	206	ARG
1	A	210	ILE
1	A	211	SER
1	A	212	SER
1	A	249	ARG
1	A	332	HIS
1	B	204	GLU
1	B	206	ARG
1	B	249	ARG
1	B	364	GLU
1	C	249	ARG
1	D	364	GLU
1	E	212	SER
1	E	244	MET
1	F	181	TYR
1	F	244	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	374/389 (96%)	0.02	26 (6%)	16 15	15, 23, 43, 67	0
1	B	375/389 (96%)	-0.04	17 (4%)	33 32	14, 22, 42, 81	0
1	C	375/389 (96%)	-0.07	27 (7%)	15 14	13, 21, 42, 74	0
1	D	374/389 (96%)	-0.06	23 (6%)	21 20	13, 20, 42, 80	0
1	E	375/389 (96%)	-0.02	20 (5%)	26 25	14, 21, 44, 79	0
1	F	374/389 (96%)	0.02	22 (5%)	22 21	14, 23, 43, 83	0
All	All	2247/2334 (96%)	-0.03	135 (6%)	21 20	13, 22, 43, 83	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	SER	13.8
1	B	211	SER	11.3
1	E	211	SER	10.8
1	E	202	ASN	10.0
1	C	211	SER	9.8
1	F	212	SER	9.4
1	D	202	ASN	8.9
1	A	202	ASN	8.4
1	F	213	GLY	8.3
1	C	202	ASN	8.3
1	A	210	ILE	8.1
1	F	202	ASN	7.6
1	F	211	SER	7.4
1	E	329	ASP	7.4
1	A	211	SER	7.3
1	F	210	ILE	7.2
1	B	202	ASN	7.1
1	F	292	LYS	7.1
1	B	282	ASP	6.8

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Mol	Chain	Res	Type	RSRZ
1	E	159	ASN	6.8
1	D	329	ASP	6.6
1	A	212	SER	6.4
1	F	329	ASP	6.3
1	B	329	ASP	6.0
1	F	281	GLY	5.9
1	B	281	GLY	5.9
1	A	213	GLY	5.8
1	A	329	ASP	5.7
1	C	281	GLY	5.6
1	E	158	ALA	5.6
1	E	292	LYS	5.5
1	E	281	GLY	5.5
1	F	159	ASN	5.3
1	E	331	GLU	5.1
1	E	212	SER	5.0
1	D	5	SER	4.9
1	B	212	SER	4.9
1	A	332	HIS	4.9
1	D	157	HIS	4.8
1	D	281	GLY	4.8
1	F	6	GLU	4.8
1	C	332	HIS	4.7
1	D	330	SER	4.6
1	A	201	ALA	4.6
1	C	159	ASN	4.6
1	C	329	ASP	4.3
1	E	5	SER	4.3
1	D	210	ILE	4.3
1	C	5	SER	4.3
1	C	292	LYS	4.2
1	E	201	ALA	4.2
1	C	212	SER	4.2
1	A	281	GLY	4.1
1	D	213	GLY	4.1
1	C	201	ALA	4.1
1	A	157	HIS	4.0
1	F	332	HIS	4.0
1	B	159	ASN	3.9
1	B	5	SER	3.9
1	D	158	ALA	3.8
1	C	200	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	209	PHE	3.8
1	A	159	ASN	3.8
1	E	157	HIS	3.7
1	A	331	GLU	3.7
1	E	332	HIS	3.6
1	D	211	SER	3.6
1	D	328	LYS	3.6
1	C	328	LYS	3.6
1	E	200	GLY	3.5
1	C	210	ILE	3.5
1	A	158	ALA	3.5
1	D	201	ALA	3.5
1	C	331	GLU	3.4
1	D	18	ASN	3.4
1	A	5	SER	3.3
1	A	203	GLY	3.3
1	F	209	PHE	3.2
1	F	214	TYR	3.2
1	F	201	ALA	3.2
1	C	6	GLU	3.1
1	A	363	ILE	3.1
1	D	332	HIS	3.1
1	B	18	ASN	3.1
1	A	328	LYS	3.1
1	E	6	GLU	3.1
1	B	122	LYS	3.1
1	B	210	ILE	3.1
1	D	214	TYR	3.0
1	F	330	SER	3.0
1	A	204	GLU	3.0
1	F	328	LYS	3.0
1	B	363	ILE	3.0
1	D	122	LYS	2.9
1	A	209	PHE	2.9
1	C	205	SER	2.9
1	F	331	GLU	2.9
1	E	203	GLY	2.9
1	A	122	LYS	2.9
1	C	204	GLU	2.9
1	F	293	GLY	2.9
1	B	331	GLU	2.9
1	B	201	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	331	GLU	2.8
1	A	18	ASN	2.8
1	B	6	GLU	2.8
1	F	157	HIS	2.8
1	D	159	ASN	2.8
1	D	124	GLY	2.8
1	B	328	LYS	2.8
1	D	203	GLY	2.7
1	E	160	VAL	2.7
1	F	190	THR	2.7
1	A	123	ASP	2.6
1	C	199	VAL	2.6
1	C	157	HIS	2.5
1	E	293	GLY	2.5
1	E	209	PHE	2.5
1	C	124	GLY	2.4
1	C	203	GLY	2.4
1	D	6	GLU	2.4
1	D	160	VAL	2.3
1	C	363	ILE	2.3
1	C	18	ASN	2.3
1	A	17	SER	2.3
1	E	210	ILE	2.2
1	A	330	SER	2.2
1	C	330	SER	2.2
1	C	160	VAL	2.2
1	C	123	ASP	2.1
1	B	354	PRO	2.1
1	F	122	LYS	2.1
1	F	357	THR	2.1
1	A	206	ARG	2.0
1	A	354	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.