Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:10 PM EDT

PDB ID	:	1OQE
Title	:	Crystal structure of sTALL-1 with BAFF-R
Authors	:	Zhang, G.
Deposited on	:	2003-03-07
Resolution	:	2.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

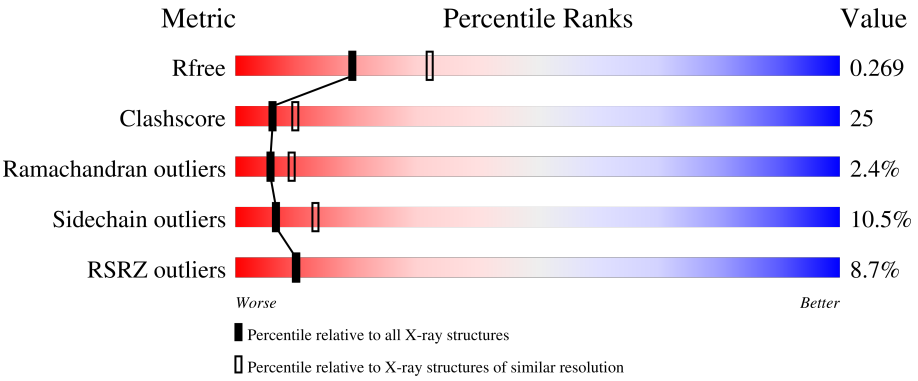
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	144	% 58% 35% 7%
1	B	144	61% 31% 8%
1	C	144	57% 35% 8%
1	D	144	64% 28% 8%
1	E	144	59% 33% 8%

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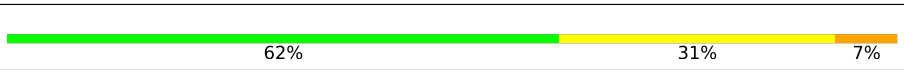
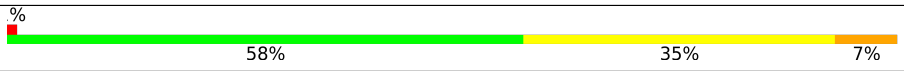
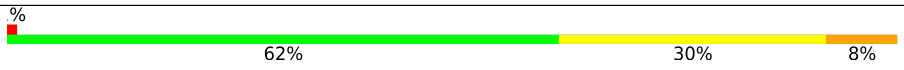
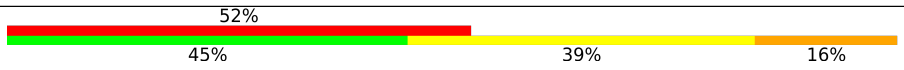
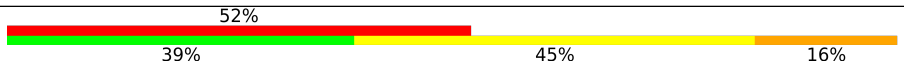
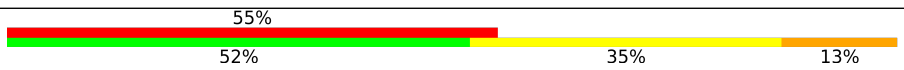
Mol	Chain	Length	Quality of chain
1	F	144	
1	G	144	
1	H	144	
1	I	144	
1	J	144	
2	K	31	
2	L	31	
2	M	31	
2	N	31	
2	O	31	
2	P	31	
2	Q	31	
2	R	31	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13240 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 Tumor necrosis factor ligand superfamily member 13B, soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	B	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	C	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	D	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	E	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	F	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	G	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	H	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	I	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	J	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 13C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	31	Total	C	N	O	S	0	0	0
			233	148	43	38	4			
2	L	31	Total	C	N	O	S	0	0	0
			233	148	43	38	4			
2	M	31	Total	C	N	O	S	0	0	0
			233	148	43	38	4			
2	N	24	Total	C	N	O	S	0	0	0
			179	114	32	29	4			

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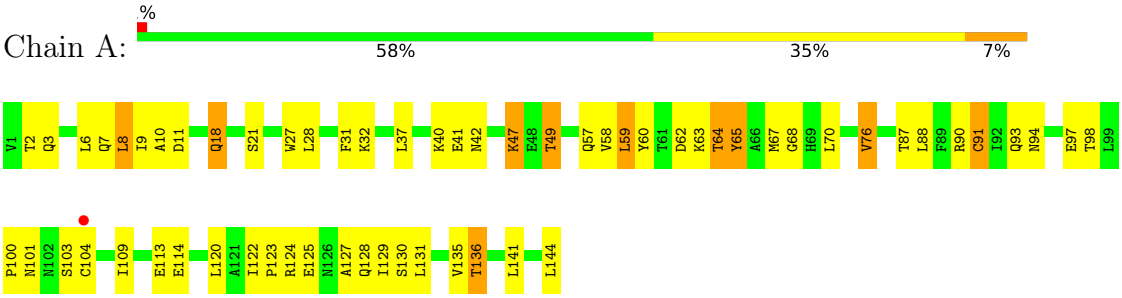
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	31	Total	C	N	O	S	0	0	0
			233	148	43	38	4			
2	P	31	Total	C	N	O	S	0	0	0
			233	148	43	38	4			
2	Q	31	Total	C	N	O	S	0	0	0
			233	148	43	38	4			
2	R	31	Total	C	N	O	S	0	0	0
			233	148	43	38	4			

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.

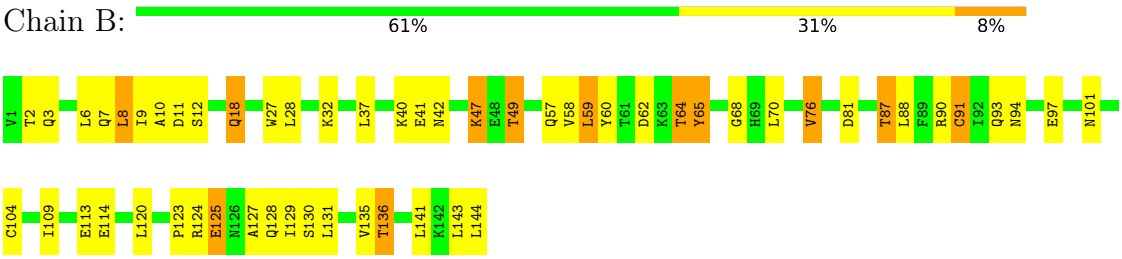
• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

Chain A:



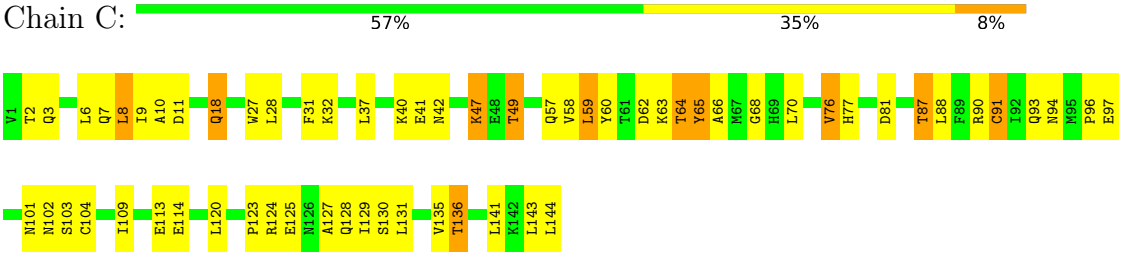
• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

Chain B:



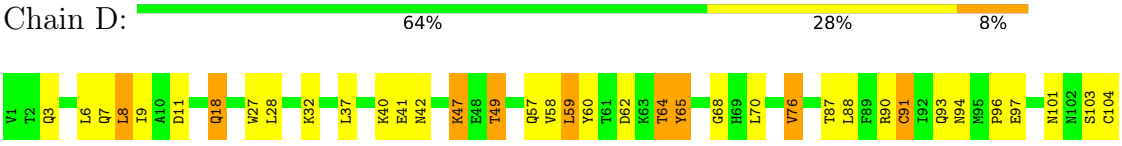
• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

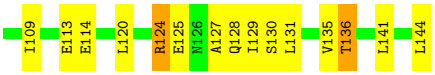
Chain C:



• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

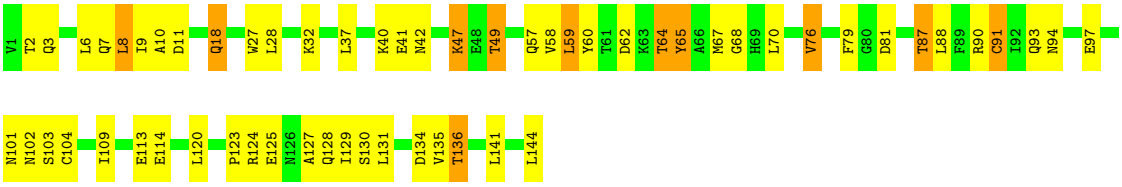
Chain D:





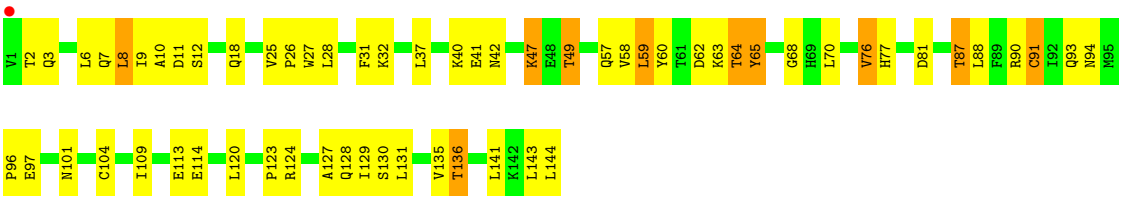
• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

Chain E:



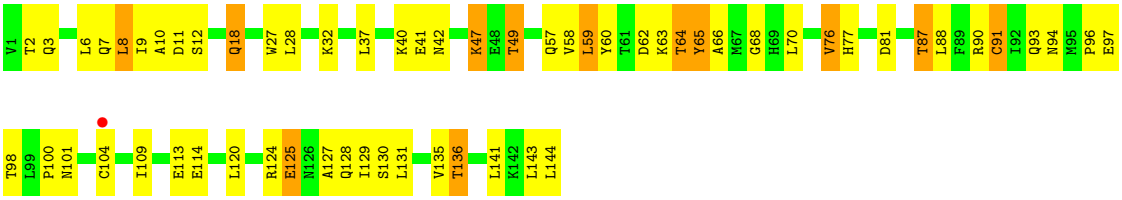
• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

Chain F:



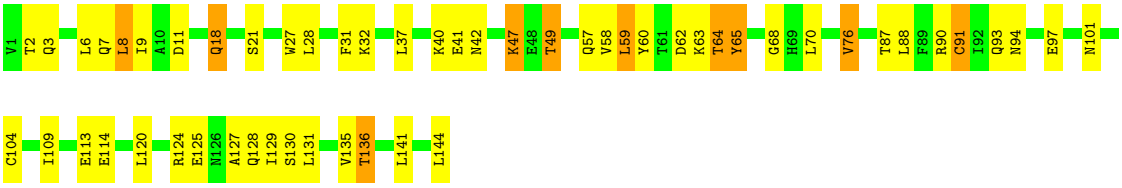
• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

Chain G:



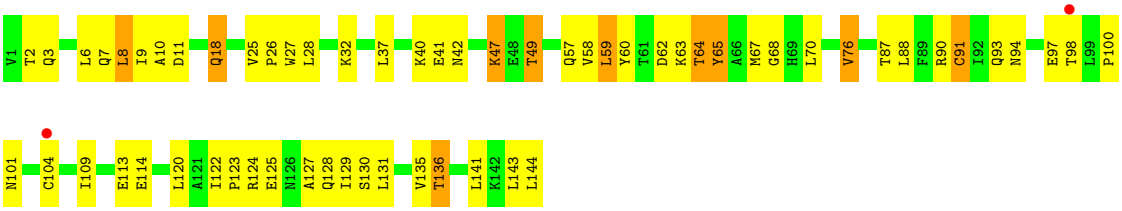
• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

Chain H:

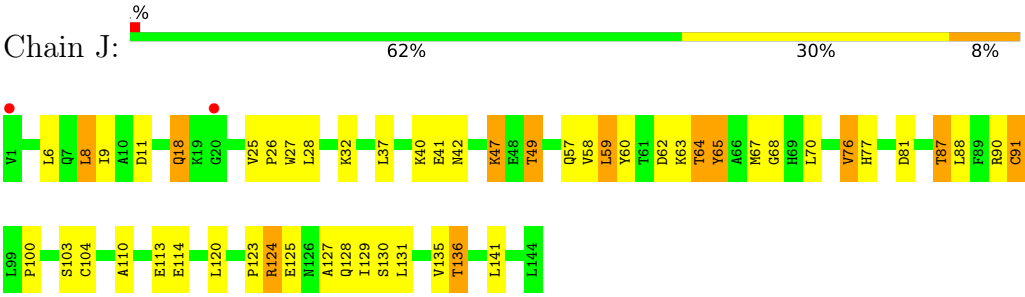


• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form

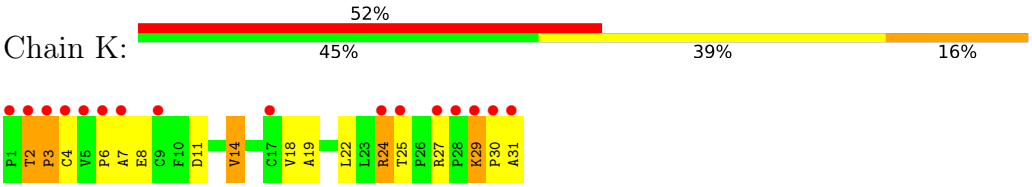
Chain I:



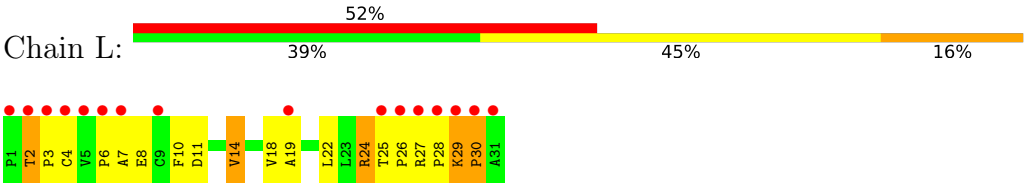
• Molecule 1: Tumor necrosis factor ligand superfamily member 13B, soluble form



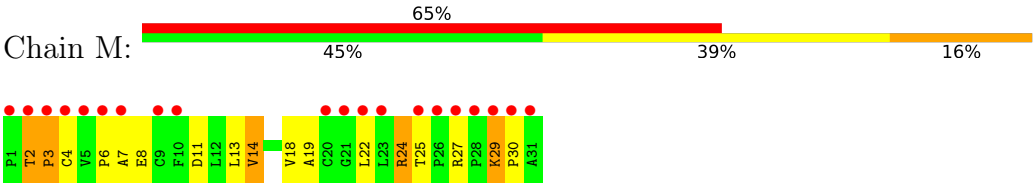
• Molecule 2: Tumor necrosis factor receptor superfamily member 13C



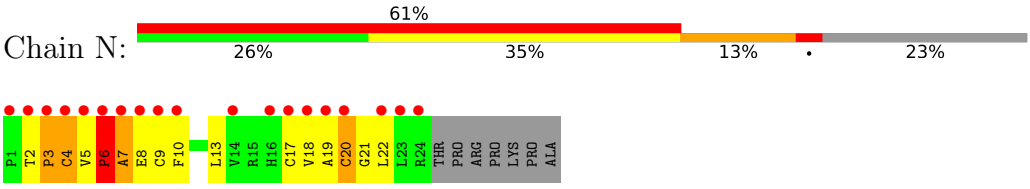
• Molecule 2: Tumor necrosis factor receptor superfamily member 13C



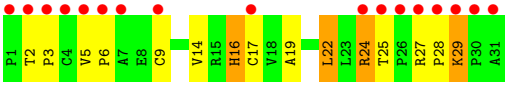
• Molecule 2: Tumor necrosis factor receptor superfamily member 13C



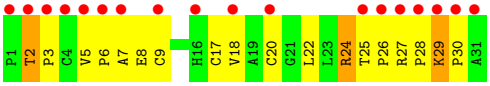
• Molecule 2: Tumor necrosis factor receptor superfamily member 13C



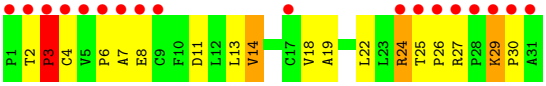
• Molecule 2: Tumor necrosis factor receptor superfamily member 13C



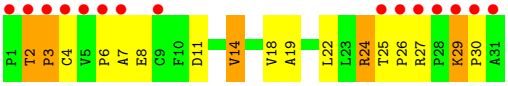
• Molecule 2: Tumor necrosis factor receptor superfamily member 13C



• Molecule 2: Tumor necrosis factor receptor superfamily member 13C



• Molecule 2: Tumor necrosis factor receptor superfamily member 13C



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	233.26Å 233.26Å 211.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 49.50 – 2.45	Depositor EDS
% Data completeness (in resolution range)	85.2 (20.00-2.50) 87.8 (49.50-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.244 , 0.259 0.253 , 0.269	Depositor DCC
R_{free} test set	2150 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13240	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.43	0/1165	0.72	1/1574 (0.1%)
1	B	0.42	0/1165	0.72	1/1574 (0.1%)
1	C	0.43	0/1165	0.72	1/1574 (0.1%)
1	D	0.43	0/1165	0.73	1/1574 (0.1%)
1	E	0.43	0/1165	0.72	1/1574 (0.1%)
1	F	0.43	0/1165	0.72	1/1574 (0.1%)
1	G	0.45	0/1165	0.72	1/1574 (0.1%)
1	H	0.43	0/1165	0.73	1/1574 (0.1%)
1	I	0.44	0/1165	0.73	1/1574 (0.1%)
1	J	0.43	0/1165	0.72	1/1574 (0.1%)
2	K	0.70	0/240	0.67	0/327
2	L	0.71	0/240	0.71	0/327
2	M	0.67	0/240	0.67	0/327
2	N	0.83	0/183	0.79	0/249
2	O	0.74	0/240	0.77	0/327
2	P	0.69	0/240	0.68	0/327
2	Q	0.70	0/240	0.68	0/327
2	R	0.71	0/240	0.66	0/327
All	All	0.48	0/13513	0.72	10/18278 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	91	CYS	CA-CB-SG	5.96	124.72	114.00
1	F	91	CYS	CA-CB-SG	5.78	124.40	114.00
1	H	91	CYS	CA-CB-SG	5.72	124.29	114.00
1	J	91	CYS	CA-CB-SG	5.62	124.12	114.00
1	I	91	CYS	CA-CB-SG	5.60	124.09	114.00
1	C	91	CYS	CA-CB-SG	5.60	124.07	114.00
1	D	91	CYS	CA-CB-SG	5.57	124.03	114.00
1	E	91	CYS	CA-CB-SG	5.50	123.91	114.00
1	B	91	CYS	CA-CB-SG	5.43	123.78	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	CYS	CA-CB-SG	5.22	123.39	114.00

There are no chirality outliers.

There are no planarity outliers.

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	1143	0	1148	66	0
1	B	1143	0	1148	59	0
1	C	1143	0	1148	64	0
1	D	1143	0	1148	64	0
1	E	1143	0	1148	64	0
1	F	1143	0	1148	64	0
1	G	1143	0	1148	62	0
1	H	1143	0	1148	58	0
1	I	1143	0	1148	66	0
1	J	1143	0	1148	49	0
2	K	233	0	241	22	0
2	L	233	0	241	22	0
2	M	233	0	241	20	0
2	N	179	0	182	20	0
2	O	233	0	241	9	0
2	P	233	0	241	18	0
2	Q	233	0	241	19	0
2	R	233	0	241	16	0
All	All	13240	0	13349	653	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 25.

All (653) 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:49:THR:HG22	1:B:114:GLU:H	1.20	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:THR:HG22	1:E:114:GLU:H	1.19	1.05
1:D:49:THR:HG22	1:D:114:GLU:H	1.20	1.04
1:F:49:THR:HG22	1:F:114:GLU:H	1.20	1.04
1:I:49:THR:HG22	1:I:114:GLU:H	1.21	1.04
1:G:49:THR:HG22	1:G:114:GLU:H	1.20	1.03
1:C:49:THR:HG22	1:C:114:GLU:H	1.21	1.03
2:P:2:THR:H	2:P:3:PRO:HD3	1.18	1.03
1:A:49:THR:HG22	1:A:114:GLU:H	1.18	1.02
1:H:49:THR:HG22	1:H:114:GLU:H	1.20	1.02
2:R:24:ARG:HB2	2:R:24:ARG:HH11	1.26	1.01
1:J:49:THR:HG22	1:J:114:GLU:H	1.21	1.00
2:K:24:ARG:HH11	2:K:24:ARG:HB2	1.27	0.99
1:H:94:ASN:HD21	1:I:101:ASN:H	1.00	0.98
2:M:24:ARG:HH11	2:M:24:ARG:HB2	1.27	0.98
1:B:27:TRP:H	1:B:42:ASN:HD21	1.11	0.97
1:A:101:ASN:H	1:C:94:ASN:HD21	1.13	0.96
1:J:27:TRP:H	1:J:42:ASN:HD21	1.14	0.96
1:E:94:ASN:HD21	1:F:101:ASN:H	1.11	0.96
1:D:27:TRP:H	1:D:42:ASN:HD21	1.13	0.95
2:L:24:ARG:HH11	2:L:24:ARG:HB2	1.28	0.95
2:Q:24:ARG:HB2	2:Q:24:ARG:HH11	1.27	0.95
2:R:2:THR:H	2:R:3:PRO:HD3	1.29	0.95
1:B:94:ASN:HD21	1:C:101:ASN:H	1.15	0.94
1:G:101:ASN:H	1:I:94:ASN:HD21	1.12	0.94
1:G:94:ASN:HD21	1:H:101:ASN:H	1.10	0.94
1:A:94:ASN:HD21	1:B:101:ASN:H	1.01	0.94
1:C:27:TRP:H	1:C:42:ASN:HD21	1.13	0.94
2:R:2:THR:H	2:R:3:PRO:CD	1.81	0.94
1:D:94:ASN:HD21	1:E:101:ASN:H	0.95	0.93
1:F:27:TRP:H	1:F:42:ASN:HD21	1.14	0.92
1:G:27:TRP:H	1:G:42:ASN:HD21	1.13	0.92
1:E:27:TRP:H	1:E:42:ASN:HD21	1.14	0.92
1:I:27:TRP:H	1:I:42:ASN:HD21	1.14	0.91
1:D:3:GLN:HE21	1:F:144:LEU:H	1.18	0.91
2:O:24:ARG:HB2	2:O:24:ARG:HH11	1.33	0.91
1:D:101:ASN:H	1:F:94:ASN:HD21	1.14	0.90
1:H:27:TRP:H	1:H:42:ASN:HD21	1.14	0.90
2:K:24:ARG:HB2	2:K:24:ARG:NH1	1.87	0.90
1:A:27:TRP:H	1:A:42:ASN:HD21	1.14	0.90
2:R:24:ARG:HB2	2:R:24:ARG:NH1	1.86	0.90
2:M:24:ARG:HB2	2:M:24:ARG:NH1	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:24:ARG:HB2	2:L:24:ARG:NH1	1.88	0.89
2:Q:24:ARG:HB2	2:Q:24:ARG:NH1	1.87	0.88
1:E:144:LEU:H	1:F:3:GLN:HE21	1.21	0.87
1:A:67:MET:SD	1:A:124:ARG:HD2	2.13	0.87
1:B:144:LEU:H	1:C:3:GLN:HE21	1.22	0.86
2:O:24:ARG:HB2	2:O:24:ARG:NH1	1.91	0.85
1:D:94:ASN:ND2	1:E:101:ASN:H	1.75	0.84
2:P:2:THR:H	2:P:3:PRO:CD	1.90	0.84
1:D:64:THR:O	1:D:64:THR:HG22	1.77	0.84
1:A:124:ARG:HG2	1:A:124:ARG:HH11	1.43	0.83
1:H:94:ASN:ND2	1:I:101:ASN:H	1.77	0.83
1:F:123:PRO:O	1:F:124:ARG:HD3	1.78	0.82
1:D:7:GLN:HE22	1:F:109:ILE:H	1.25	0.82
1:G:144:LEU:H	1:H:3:GLN:HE21	1.26	0.82
1:H:109:ILE:H	1:I:7:GLN:HE22	1.28	0.82
1:A:3:GLN:HE21	1:C:144:LEU:H	1.26	0.82
1:A:21:SER:HA	1:A:125:GLU:OE2	1.80	0.82
1:B:123:PRO:O	1:B:124:ARG:HD3	1.79	0.82
1:E:81:ASP:OD2	1:J:87:THR:HG23	1.80	0.81
1:A:94:ASN:ND2	1:B:101:ASN:H	1.78	0.81
1:G:7:GLN:HE22	1:I:109:ILE:H	1.25	0.81
1:E:109:ILE:H	1:F:7:GLN:HE22	1.29	0.81
1:A:64:THR:O	1:A:64:THR:HG22	1.82	0.80
1:H:64:THR:HG22	1:H:64:THR:O	1.81	0.80
1:G:64:THR:HG22	1:G:64:THR:O	1.81	0.80
1:H:21:SER:HA	1:H:125:GLU:HG2	1.64	0.80
1:H:144:LEU:H	1:I:3:GLN:HE21	1.26	0.80
2:K:2:THR:H	2:K:3:PRO:CD	1.93	0.80
1:I:64:THR:O	1:I:64:THR:HG22	1.82	0.80
2:M:2:THR:H	2:M:3:PRO:HD3	1.46	0.79
1:A:109:ILE:H	1:B:7:GLN:HE22	1.29	0.79
1:J:64:THR:HG22	1:J:64:THR:O	1.82	0.79
1:G:49:THR:HG22	1:G:114:GLU:N	1.98	0.79
2:N:2:THR:HG23	2:N:10:PHE:HB2	1.63	0.79
1:C:64:THR:HG22	1:C:64:THR:O	1.81	0.79
1:C:123:PRO:O	1:C:124:ARG:HD3	1.81	0.79
1:E:64:THR:HG22	1:E:64:THR:O	1.82	0.78
1:F:64:THR:O	1:F:64:THR:HG22	1.82	0.78
1:B:64:THR:HG22	1:B:64:THR:O	1.82	0.77
1:G:3:GLN:HE21	1:I:144:LEU:H	1.31	0.77
1:B:109:ILE:H	1:C:7:GLN:HE22	1.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:22:LEU:HD22	2:N:22:LEU:H	1.48	0.77
1:F:49:THR:HG22	1:F:114:GLU:N	1.99	0.76
2:L:29:LYS:H	2:L:30:PRO:CD	1.99	0.76
1:J:49:THR:HG22	1:J:114:GLU:N	2.00	0.75
1:J:60:TYR:CD2	1:J:129:ILE:HD11	2.21	0.75
1:I:123:PRO:O	1:I:124:ARG:HG2	1.86	0.75
1:G:109:ILE:H	1:H:7:GLN:HE22	1.34	0.75
1:A:7:GLN:HE22	1:C:109:ILE:H	1.34	0.75
1:A:144:LEU:H	1:B:3:GLN:HE21	1.34	0.75
1:B:49:THR:HG22	1:B:114:GLU:N	1.99	0.74
1:C:49:THR:HG22	1:C:114:GLU:N	2.00	0.74
1:D:49:THR:HG22	1:D:114:GLU:N	2.00	0.74
1:H:49:THR:HG22	1:H:114:GLU:N	2.00	0.74
1:D:144:LEU:H	1:E:3:GLN:HE21	1.33	0.74
1:A:49:THR:HG22	1:A:114:GLU:N	1.98	0.73
2:O:5:VAL:HG12	2:O:6:PRO:O	1.88	0.73
2:P:24:ARG:HH11	2:P:24:ARG:HB2	1.53	0.73
1:H:60:TYR:CD2	1:H:129:ILE:HD11	2.23	0.73
1:D:109:ILE:H	1:E:7:GLN:HE22	1.37	0.73
1:I:49:THR:HG22	1:I:114:GLU:N	2.00	0.72
1:E:49:THR:HG22	1:E:114:GLU:N	1.99	0.72
1:G:101:ASN:H	1:I:94:ASN:ND2	1.88	0.72
1:E:94:ASN:ND2	1:F:101:ASN:H	1.88	0.71
1:A:123:PRO:O	1:A:124:ARG:HG2	1.91	0.71
1:J:124:ARG:HG2	1:J:124:ARG:HH11	1.56	0.70
1:I:60:TYR:CD2	1:I:129:ILE:HD11	2.27	0.70
1:D:59:LEU:H	1:D:136:THR:HG22	1.57	0.70
1:D:101:ASN:H	1:F:94:ASN:ND2	1.88	0.70
2:P:28:PRO:O	2:P:29:LYS:HD2	1.91	0.70
1:D:94:ASN:HD21	1:E:101:ASN:N	1.80	0.69
2:N:4:CYS:HB3	2:N:8:GLU:O	1.92	0.69
1:D:60:TYR:CD2	1:D:129:ILE:HD11	2.28	0.69
2:L:2:THR:HG23	2:L:10:PHE:HB2	1.75	0.68
1:G:94:ASN:ND2	1:H:101:ASN:H	1.89	0.68
1:H:94:ASN:HD21	1:I:101:ASN:N	1.84	0.68
1:C:49:THR:HB	1:C:113:GLU:HA	1.76	0.68
1:E:123:PRO:O	1:E:124:ARG:HD3	1.94	0.68
2:M:2:THR:O	2:M:4:CYS:N	2.27	0.68
1:A:49:THR:HB	1:A:113:GLU:HA	1.76	0.67
1:B:59:LEU:H	1:B:136:THR:HG22	1.59	0.67
1:H:59:LEU:H	1:H:136:THR:HG22	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TYR:CD2	1:A:129:ILE:HD11	2.29	0.67
1:J:59:LEU:H	1:J:136:THR:HG22	1.59	0.67
2:R:2:THR:N	2:R:3:PRO:CD	2.57	0.67
1:H:49:THR:HB	1:H:113:GLU:HA	1.77	0.67
2:K:19:ALA:HB3	2:K:22:LEU:CD2	2.25	0.67
1:G:49:THR:HB	1:G:113:GLU:HA	1.77	0.66
1:E:49:THR:HB	1:E:113:GLU:HA	1.77	0.66
1:E:60:TYR:CD2	1:E:129:ILE:HD11	2.31	0.66
1:I:49:THR:HB	1:I:113:GLU:HA	1.77	0.66
2:L:19:ALA:HB3	2:L:22:LEU:CD2	2.25	0.66
2:M:19:ALA:HB3	2:M:22:LEU:CD2	2.26	0.66
1:D:49:THR:HB	1:D:113:GLU:HA	1.78	0.65
1:J:123:PRO:O	1:J:124:ARG:HG2	1.95	0.65
1:G:60:TYR:CD2	1:G:129:ILE:HD11	2.31	0.65
1:B:49:THR:HB	1:B:113:GLU:HA	1.78	0.65
1:D:18:GLN:NE2	1:D:125:GLU:O	2.30	0.65
2:Q:19:ALA:HB3	2:Q:22:LEU:CD2	2.25	0.65
2:R:19:ALA:HB3	2:R:22:LEU:CD2	2.26	0.65
1:J:49:THR:HB	1:J:113:GLU:HA	1.79	0.65
2:K:29:LYS:HB2	2:K:30:PRO:HD3	1.77	0.65
1:F:49:THR:HB	1:F:113:GLU:HA	1.78	0.65
1:A:101:ASN:H	1:C:94:ASN:ND2	1.90	0.64
2:N:2:THR:N	2:N:3:PRO:HD3	2.12	0.64
2:N:19:ALA:HB3	2:N:22:LEU:CD2	2.28	0.64
1:A:59:LEU:H	1:A:136:THR:HG22	1.62	0.64
1:H:62:ASP:HB2	1:H:128:GLN:HB2	1.78	0.64
1:J:62:ASP:HB2	1:J:128:GLN:HB2	1.80	0.64
2:N:18:VAL:HG12	2:N:22:LEU:HD23	1.80	0.63
2:P:2:THR:N	2:P:3:PRO:HD3	2.02	0.63
1:A:94:ASN:HD21	1:B:101:ASN:N	1.85	0.63
1:E:62:ASP:HB2	1:E:128:GLN:HB2	1.78	0.63
1:C:59:LEU:H	1:C:136:THR:HG22	1.63	0.63
1:F:60:TYR:CD2	1:F:129:ILE:HD11	2.34	0.63
2:P:24:ARG:HB2	2:P:24:ARG:NH1	2.12	0.63
1:B:60:TYR:CD2	1:B:129:ILE:HD11	2.34	0.62
1:E:59:LEU:H	1:E:136:THR:HG22	1.64	0.62
1:B:94:ASN:ND2	1:C:101:ASN:H	1.92	0.62
1:H:60:TYR:CE2	1:H:129:ILE:HD11	2.33	0.62
1:F:59:LEU:H	1:F:136:THR:HG22	1.65	0.62
2:L:2:THR:N	2:L:3:PRO:HD3	2.15	0.62
1:C:87:THR:HG23	1:G:81:ASP:OD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:29:LYS:H	2:Q:30:PRO:CD	2.12	0.62
1:C:60:TYR:CD2	1:C:129:ILE:HD11	2.35	0.62
1:E:18:GLN:NE2	1:E:125:GLU:O	2.33	0.61
2:Q:6:PRO:O	2:Q:7:ALA:HB3	2.00	0.61
2:K:6:PRO:O	2:K:7:ALA:HB3	2.01	0.61
2:M:27:ARG:HG2	2:M:29:LYS:HE3	1.83	0.61
2:R:6:PRO:O	2:R:7:ALA:HB3	2.01	0.61
1:E:87:THR:HG23	1:J:81:ASP:OD2	2.00	0.61
2:Q:27:ARG:HG2	2:Q:29:LYS:HE3	1.83	0.61
2:M:6:PRO:O	2:M:7:ALA:HB3	2.00	0.61
1:A:124:ARG:HG2	1:A:124:ARG:NH1	2.11	0.60
1:D:64:THR:O	1:D:64:THR:CG2	2.49	0.60
1:A:62:ASP:HB2	1:A:128:GLN:HB2	1.83	0.60
1:D:62:ASP:HB2	1:D:128:GLN:HB2	1.83	0.60
1:J:60:TYR:CE2	1:J:129:ILE:HD11	2.36	0.60
1:G:59:LEU:H	1:G:136:THR:HG22	1.66	0.60
2:L:6:PRO:O	2:L:7:ALA:HB3	2.02	0.59
1:C:124:ARG:NH2	2:M:13:LEU:HD23	2.17	0.59
1:H:62:ASP:CB	1:H:128:GLN:HB2	2.32	0.59
1:I:135:VAL:HG23	1:I:136:THR:HG23	1.83	0.59
1:I:67:MET:SD	1:I:124:ARG:HD2	2.42	0.59
1:C:135:VAL:HG23	1:C:136:THR:HG23	1.85	0.59
1:D:135:VAL:HG23	1:D:136:THR:HG23	1.84	0.59
1:J:135:VAL:HG23	1:J:136:THR:HG23	1.85	0.58
2:R:27:ARG:HG2	2:R:29:LYS:HE3	1.85	0.58
1:J:62:ASP:CB	1:J:128:GLN:HB2	2.32	0.58
2:O:28:PRO:O	2:O:29:LYS:HG3	2.03	0.58
1:I:59:LEU:H	1:I:136:THR:HG22	1.67	0.58
1:E:135:VAL:HG23	1:E:136:THR:HG23	1.85	0.58
2:P:6:PRO:O	2:P:7:ALA:HB3	2.03	0.58
1:A:135:VAL:HG23	1:A:136:THR:HG23	1.84	0.58
1:B:76:VAL:HG21	1:B:114:GLU:O	2.04	0.58
1:E:60:TYR:CE2	1:E:129:ILE:HD11	2.39	0.58
1:H:135:VAL:HG23	1:H:136:THR:HG23	1.86	0.58
2:K:2:THR:H	2:K:3:PRO:HD3	1.69	0.57
2:K:2:THR:N	2:K:3:PRO:CD	2.67	0.57
2:L:27:ARG:HG2	2:L:29:LYS:HE3	1.85	0.57
2:P:2:THR:O	2:P:2:THR:HG22	2.03	0.57
2:P:2:THR:N	2:P:3:PRO:CD	2.64	0.57
1:E:124:ARG:NH2	2:N:13:LEU:HD23	2.20	0.57
2:M:2:THR:N	2:M:3:PRO:CD	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:VAL:HG21	1:G:114:GLU:O	2.05	0.57
2:K:27:ARG:HG2	2:K:29:LYS:HE3	1.86	0.57
1:A:76:VAL:HG21	1:A:114:GLU:O	2.05	0.57
1:C:76:VAL:HG21	1:C:114:GLU:O	2.04	0.57
2:M:2:THR:N	2:M:3:PRO:HD3	2.18	0.57
2:N:22:LEU:HD22	2:N:22:LEU:N	2.19	0.57
2:R:2:THR:N	2:R:3:PRO:HD3	2.12	0.57
1:G:135:VAL:HG12	1:I:90:ARG:HG2	1.85	0.57
1:J:76:VAL:HG21	1:J:114:GLU:O	2.05	0.57
1:G:135:VAL:HG23	1:G:136:THR:HG23	1.87	0.57
2:L:2:THR:HG23	2:L:10:PHE:CB	2.34	0.57
1:D:76:VAL:HG21	1:D:114:GLU:O	2.05	0.56
2:K:2:THR:O	2:K:4:CYS:N	2.38	0.56
1:B:135:VAL:HG23	1:B:136:THR:HG23	1.86	0.56
1:G:62:ASP:HB2	1:G:128:GLN:HB2	1.86	0.56
1:I:62:ASP:HB2	1:I:128:GLN:HB2	1.86	0.56
2:P:18:VAL:HG12	2:P:22:LEU:HD23	1.87	0.56
1:D:60:TYR:CE2	1:D:129:ILE:HD11	2.40	0.56
1:E:76:VAL:HG21	1:E:114:GLU:O	2.05	0.56
2:L:29:LYS:H	2:L:30:PRO:HD3	1.70	0.56
2:N:22:LEU:H	2:N:22:LEU:CD2	2.18	0.56
1:A:64:THR:O	1:A:64:THR:CG2	2.53	0.56
1:E:127:ALA:HB1	1:E:129:ILE:HD13	1.88	0.56
1:E:144:LEU:OXT	1:F:2:THR:HG22	2.05	0.56
1:H:76:VAL:HG21	1:H:114:GLU:O	2.05	0.56
1:F:76:VAL:HG21	1:F:114:GLU:O	2.05	0.56
1:I:76:VAL:HG21	1:I:114:GLU:O	2.05	0.56
1:A:60:TYR:CE2	1:A:129:ILE:HD11	2.41	0.56
1:F:135:VAL:HG23	1:F:136:THR:HG23	1.87	0.56
2:M:2:THR:H	2:M:3:PRO:CD	2.16	0.56
1:C:62:ASP:HB2	1:C:128:GLN:HB2	1.88	0.55
1:J:127:ALA:HB1	1:J:129:ILE:HD13	1.88	0.55
1:I:60:TYR:CE2	1:I:129:ILE:HD11	2.41	0.55
1:F:127:ALA:HB1	1:F:129:ILE:HD13	1.88	0.55
1:A:40:LYS:HE2	1:A:41:GLU:OE1	2.06	0.55
1:D:144:LEU:OXT	1:E:2:THR:HG22	2.06	0.55
1:F:64:THR:O	1:F:65:TYR:CD2	2.60	0.55
1:F:141:LEU:C	1:F:141:LEU:HD23	2.27	0.55
2:O:19:ALA:O	2:O:22:LEU:HB2	2.06	0.55
1:G:127:ALA:HB1	1:G:129:ILE:HD13	1.89	0.55
1:C:64:THR:O	1:C:64:THR:CG2	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:2:THR:O	2:N:2:THR:HG22	2.07	0.55
1:E:62:ASP:CB	1:E:128:GLN:HB2	2.37	0.55
1:B:127:ALA:HB1	1:B:129:ILE:HD13	1.89	0.55
1:H:40:LYS:HE2	1:H:41:GLU:OE1	2.07	0.54
1:D:70:LEU:HD23	1:D:90:ARG:HB2	1.89	0.54
1:I:141:LEU:C	1:I:141:LEU:HD23	2.28	0.54
1:A:144:LEU:OXT	1:B:2:THR:HG22	2.06	0.54
1:E:11:ASP:HB2	1:E:28:LEU:HB2	1.89	0.54
1:J:141:LEU:HD23	1:J:141:LEU:C	2.28	0.54
1:C:64:THR:O	1:C:65:TYR:CD2	2.61	0.54
1:G:141:LEU:HD23	1:G:141:LEU:C	2.28	0.54
1:H:64:THR:OG1	1:H:124:ARG:NH1	2.41	0.54
1:C:81:ASP:OD2	1:G:87:THR:HG23	2.08	0.54
1:C:127:ALA:HB1	1:C:129:ILE:HD13	1.90	0.54
1:I:127:ALA:HB1	1:I:129:ILE:HD13	1.90	0.54
2:Q:29:LYS:H	2:Q:30:PRO:HD3	1.72	0.54
1:A:141:LEU:C	1:A:141:LEU:HD23	2.28	0.54
1:B:11:ASP:HB2	1:B:28:LEU:HB2	1.90	0.54
1:C:18:GLN:NE2	1:C:125:GLU:O	2.41	0.54
1:A:127:ALA:HB1	1:A:129:ILE:HD13	1.88	0.54
1:C:141:LEU:C	1:C:141:LEU:HD23	2.28	0.53
1:D:62:ASP:CB	1:D:128:GLN:HB2	2.37	0.53
1:D:127:ALA:HB1	1:D:129:ILE:HD13	1.90	0.53
1:I:123:PRO:C	1:I:124:ARG:HG2	2.28	0.53
1:B:62:ASP:HB2	1:B:128:GLN:HB2	1.89	0.53
1:D:40:LYS:HE2	1:D:41:GLU:OE1	2.08	0.53
1:F:40:LYS:HE2	1:F:41:GLU:OE1	2.08	0.53
1:D:11:ASP:HB2	1:D:28:LEU:HB2	1.90	0.53
1:D:141:LEU:C	1:D:141:LEU:HD23	2.28	0.53
1:E:90:ARG:HG2	1:F:135:VAL:HG12	1.91	0.53
1:G:135:VAL:CG1	1:I:90:ARG:HG2	2.39	0.53
2:K:2:THR:H	2:K:3:PRO:HD2	1.73	0.53
2:N:5:VAL:O	2:N:6:PRO:C	2.46	0.53
1:A:62:ASP:CB	1:A:128:GLN:HB2	2.38	0.53
1:B:141:LEU:HD23	1:B:141:LEU:C	2.29	0.53
1:H:90:ARG:HG2	1:I:135:VAL:HG12	1.90	0.53
1:I:11:ASP:HB2	1:I:28:LEU:HB2	1.91	0.53
1:H:70:LEU:HD23	1:H:90:ARG:HB2	1.91	0.53
1:I:18:GLN:NE2	1:I:125:GLU:O	2.41	0.53
2:N:2:THR:C	2:N:4:CYS:H	2.12	0.53
1:A:70:LEU:HD23	1:A:90:ARG:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:HG2	1:C:135:VAL:HG12	1.89	0.53
1:I:40:LYS:HE2	1:I:41:GLU:OE1	2.08	0.53
1:H:127:ALA:HB1	1:H:129:ILE:HD13	1.91	0.53
1:B:64:THR:O	1:B:65:TYR:CD2	2.61	0.53
1:E:64:THR:O	1:E:65:TYR:CD2	2.62	0.53
1:F:11:ASP:HB2	1:F:28:LEU:HB2	1.90	0.53
1:F:62:ASP:HB2	1:F:128:GLN:HB2	1.91	0.53
1:I:64:THR:O	1:I:65:TYR:CD2	2.62	0.53
1:J:64:THR:O	1:J:65:TYR:CD2	2.62	0.53
1:D:57:GLN:O	1:D:136:THR:HA	2.10	0.52
1:H:11:ASP:HB2	1:H:28:LEU:HB2	1.91	0.52
1:A:70:LEU:CD2	1:A:90:ARG:HB2	2.40	0.52
1:B:70:LEU:CD2	1:B:90:ARG:HB2	2.40	0.52
1:G:70:LEU:HD23	1:G:90:ARG:HB2	1.91	0.52
1:A:64:THR:O	1:A:65:TYR:CD2	2.62	0.52
1:C:40:LYS:HE2	1:C:41:GLU:OE1	2.08	0.52
1:E:40:LYS:HE2	1:E:41:GLU:OE1	2.09	0.52
2:N:6:PRO:O	2:N:7:ALA:CB	2.57	0.52
1:E:64:THR:O	1:E:64:THR:CG2	2.53	0.52
1:G:64:THR:O	1:G:65:TYR:CD2	2.62	0.52
1:F:64:THR:O	1:F:64:THR:CG2	2.54	0.52
1:I:70:LEU:HD23	1:I:90:ARG:HB2	1.90	0.52
1:H:64:THR:O	1:H:65:TYR:CD2	2.63	0.52
1:I:64:THR:O	1:I:64:THR:CG2	2.53	0.52
1:J:40:LYS:HE2	1:J:41:GLU:OE1	2.08	0.52
1:B:70:LEU:HD23	1:B:90:ARG:HB2	1.91	0.52
1:D:70:LEU:CD2	1:D:90:ARG:HB2	2.40	0.52
1:A:11:ASP:HB2	1:A:28:LEU:HB2	1.92	0.52
1:G:11:ASP:HB2	1:G:28:LEU:HB2	1.92	0.52
1:H:70:LEU:CD2	1:H:90:ARG:HB2	2.40	0.52
1:B:40:LYS:HE2	1:B:41:GLU:OE1	2.10	0.51
1:C:70:LEU:HD23	1:C:90:ARG:HB2	1.91	0.51
1:D:64:THR:O	1:D:65:TYR:CD2	2.64	0.51
1:H:141:LEU:C	1:H:141:LEU:HD23	2.30	0.51
1:B:18:GLN:NE2	1:B:125:GLU:O	2.43	0.51
1:E:70:LEU:HD23	1:E:90:ARG:HB2	1.91	0.51
1:G:60:TYR:CE2	1:G:129:ILE:HD11	2.45	0.51
1:I:70:LEU:CD2	1:I:90:ARG:HB2	2.41	0.51
2:M:2:THR:O	2:M:2:THR:HG22	2.11	0.51
1:J:11:ASP:HB2	1:J:28:LEU:HB2	1.92	0.51
1:G:70:LEU:CD2	1:G:90:ARG:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:ASP:CA	1:J:128:GLN:HB2	2.41	0.51
1:J:70:LEU:HD23	1:J:90:ARG:HB2	1.92	0.51
2:K:2:THR:O	2:K:3:PRO:C	2.49	0.51
1:C:11:ASP:HB2	1:C:28:LEU:HB2	1.91	0.51
1:G:64:THR:O	1:G:64:THR:CG2	2.52	0.51
1:D:3:GLN:NE2	1:F:144:LEU:H	1.99	0.51
1:E:70:LEU:CD2	1:E:90:ARG:HB2	2.41	0.51
1:E:141:LEU:HD23	1:E:141:LEU:C	2.30	0.51
1:F:70:LEU:HD23	1:F:90:ARG:HB2	1.91	0.51
1:J:70:LEU:CD2	1:J:90:ARG:HB2	2.41	0.51
1:C:70:LEU:CD2	1:C:90:ARG:HB2	2.40	0.51
1:J:59:LEU:HB3	1:J:130:SER:HB3	1.93	0.51
2:O:9:CYS:O	2:O:17:CYS:HA	2.11	0.51
1:J:124:ARG:HG2	1:J:124:ARG:NH1	2.22	0.50
1:F:70:LEU:CD2	1:F:90:ARG:HB2	2.41	0.50
1:G:40:LYS:HE2	1:G:41:GLU:OE1	2.09	0.50
1:E:57:GLN:O	1:E:136:THR:HA	2.11	0.50
1:H:18:GLN:NE2	1:H:125:GLU:O	2.44	0.50
1:B:64:THR:O	1:B:64:THR:CG2	2.54	0.50
1:J:67:MET:SD	1:J:124:ARG:HD2	2.51	0.50
1:C:60:TYR:CE2	1:C:129:ILE:HD11	2.47	0.50
1:H:90:ARG:HG2	1:I:135:VAL:CG1	2.41	0.50
1:G:144:LEU:OXT	1:H:2:THR:HG22	2.12	0.49
2:P:18:VAL:CG1	2:P:22:LEU:HD23	2.41	0.49
1:F:60:TYR:CE2	1:F:129:ILE:HD11	2.47	0.49
1:H:57:GLN:O	1:H:136:THR:HA	2.13	0.49
1:I:62:ASP:CB	1:I:128:GLN:HB2	2.41	0.49
1:D:101:ASN:N	1:F:94:ASN:HD21	1.96	0.49
1:B:90:ARG:HG2	1:C:135:VAL:CG1	2.42	0.49
1:D:6:LEU:HD21	1:D:8:LEU:HD13	1.94	0.49
1:D:135:VAL:HG12	1:F:90:ARG:HG2	1.94	0.49
2:L:29:LYS:H	2:L:30:PRO:HD2	1.77	0.49
2:P:27:ARG:HD3	2:P:28:PRO:CD	2.43	0.49
1:J:58:VAL:HA	1:J:136:THR:HB	1.94	0.49
1:A:59:LEU:HB3	1:A:130:SER:HB3	1.95	0.49
1:H:58:VAL:HA	1:H:136:THR:HB	1.95	0.49
1:H:64:THR:O	1:H:64:THR:CG2	2.53	0.49
1:D:96:PRO:HG2	1:F:94:ASN:CG	2.33	0.48
1:J:129:ILE:HG22	1:J:131:LEU:CD1	2.43	0.48
2:M:4:CYS:HB3	2:M:8:GLU:O	2.13	0.48
1:C:66:ALA:O	1:C:124:ARG:NH2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:VAL:HA	1:D:136:THR:HB	1.96	0.48
1:B:6:LEU:HD21	1:B:8:LEU:HD13	1.96	0.48
1:D:90:ARG:HG2	1:E:135:VAL:HG12	1.95	0.48
1:E:6:LEU:HD21	1:E:8:LEU:HD13	1.95	0.48
1:H:59:LEU:HB3	1:H:130:SER:HB3	1.95	0.48
1:B:60:TYR:CE2	1:B:129:ILE:HD11	2.47	0.48
1:C:129:ILE:HG22	1:C:131:LEU:CD1	2.44	0.48
1:F:128:GLN:O	1:F:129:ILE:HD12	2.13	0.48
1:H:6:LEU:HD21	1:H:8:LEU:HD13	1.96	0.48
1:I:125:GLU:OE1	2:Q:27:ARG:CB	2.62	0.48
1:G:62:ASP:CB	1:G:128:GLN:HB2	2.43	0.48
1:G:2:THR:HG22	1:I:144:LEU:OXT	2.13	0.48
1:C:57:GLN:O	1:C:136:THR:HA	2.14	0.48
1:F:6:LEU:HD21	1:F:8:LEU:HD13	1.95	0.48
1:B:129:ILE:HG22	1:B:131:LEU:CD1	2.44	0.47
1:I:6:LEU:HD21	1:I:8:LEU:HD13	1.96	0.47
1:C:6:LEU:HD21	1:C:8:LEU:HD13	1.95	0.47
1:E:90:ARG:HG2	1:F:135:VAL:CG1	2.44	0.47
1:E:129:ILE:HG22	1:E:131:LEU:CD1	2.44	0.47
1:A:129:ILE:HG22	1:A:131:LEU:CD1	2.44	0.47
2:L:2:THR:O	2:L:2:THR:HG22	2.15	0.47
2:K:11:ASP:CG	2:K:14:VAL:HG23	2.34	0.47
2:L:11:ASP:CG	2:L:14:VAL:HG23	2.35	0.47
1:A:18:GLN:NE2	1:A:125:GLU:O	2.48	0.47
1:H:68:GLY:HA3	1:H:91:CYS:O	2.15	0.47
2:M:29:LYS:H	2:M:30:PRO:CD	2.28	0.47
2:Q:2:THR:N	2:Q:3:PRO:CD	2.77	0.47
2:R:4:CYS:HB3	2:R:8:GLU:O	2.14	0.47
1:A:57:GLN:O	1:A:136:THR:HA	2.14	0.47
1:E:94:ASN:HD21	1:F:101:ASN:N	1.95	0.47
1:G:6:LEU:HD21	1:G:8:LEU:HD13	1.97	0.47
1:J:57:GLN:O	1:J:136:THR:HA	2.15	0.47
1:A:6:LEU:HD21	1:A:8:LEU:HD13	1.96	0.47
1:G:18:GLN:NE2	1:G:125:GLU:O	2.47	0.47
1:B:144:LEU:OXT	1:C:2:THR:HG22	2.15	0.47
2:L:4:CYS:HB3	2:L:8:GLU:O	2.15	0.47
2:L:29:LYS:N	2:L:30:PRO:CD	2.69	0.47
1:A:2:THR:HG22	1:C:144:LEU:OXT	2.14	0.47
1:B:47:LYS:O	1:B:114:GLU:HG2	2.15	0.47
1:B:62:ASP:CB	1:B:128:GLN:HB2	2.45	0.47
1:A:68:GLY:HA3	1:A:91:CYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:ILE:H	1:I:7:GLN:NE2	2.06	0.46
1:E:59:LEU:HB3	1:E:130:SER:HB3	1.97	0.46
1:G:7:GLN:NE2	1:I:109:ILE:H	2.04	0.46
1:D:68:GLY:HA3	1:D:91:CYS:O	2.15	0.46
1:D:129:ILE:HG22	1:D:131:LEU:CD1	2.45	0.46
1:E:109:ILE:H	1:F:7:GLN:NE2	2.06	0.46
1:F:68:GLY:HA3	1:F:91:CYS:O	2.16	0.46
1:I:129:ILE:HG22	1:I:131:LEU:CD1	2.46	0.46
1:J:64:THR:O	1:J:64:THR:CG2	2.53	0.46
2:M:11:ASP:CG	2:M:14:VAL:HG23	2.35	0.46
2:N:19:ALA:O	2:N:20:CYS:C	2.54	0.46
1:E:47:LYS:O	1:E:114:GLU:HG2	2.16	0.46
1:F:129:ILE:HG22	1:F:131:LEU:CD1	2.46	0.46
1:G:129:ILE:HG22	1:G:131:LEU:CD1	2.46	0.46
2:M:6:PRO:O	2:M:7:ALA:CB	2.63	0.46
2:Q:2:THR:O	2:Q:3:PRO:C	2.54	0.46
1:A:47:LYS:O	1:A:114:GLU:HG2	2.16	0.46
1:G:47:LYS:O	1:G:114:GLU:HG2	2.15	0.46
1:J:68:GLY:HA3	1:J:91:CYS:O	2.15	0.46
1:A:31:PHE:HA	1:G:77:HIS:CD2	2.51	0.46
1:I:68:GLY:HA3	1:I:91:CYS:O	2.16	0.46
2:P:9:CYS:O	2:P:17:CYS:HA	2.16	0.46
2:R:6:PRO:O	2:R:7:ALA:CB	2.64	0.46
2:R:11:ASP:CG	2:R:14:VAL:HG23	2.36	0.46
1:A:58:VAL:HA	1:A:136:THR:HB	1.97	0.46
1:A:128:GLN:O	1:A:129:ILE:HD12	2.15	0.46
1:B:68:GLY:HA3	1:B:91:CYS:O	2.16	0.46
1:D:59:LEU:HB3	1:D:130:SER:HB3	1.98	0.46
1:E:68:GLY:HA3	1:E:91:CYS:O	2.15	0.46
1:J:6:LEU:HD21	1:J:8:LEU:HD13	1.97	0.46
1:C:62:ASP:CB	1:C:128:GLN:HB2	2.47	0.45
1:D:135:VAL:CG1	1:F:90:ARG:HG2	2.46	0.45
1:I:47:LYS:O	1:I:114:GLU:HG2	2.16	0.45
2:K:4:CYS:HB3	2:K:8:GLU:O	2.16	0.45
1:A:90:ARG:HG2	1:B:135:VAL:HG12	1.98	0.45
1:C:47:LYS:O	1:C:114:GLU:HG2	2.15	0.45
1:D:59:LEU:N	1:D:136:THR:HG22	2.29	0.45
1:G:128:GLN:O	1:G:129:ILE:HD12	2.16	0.45
2:K:2:THR:O	2:K:4:CYS:SG	2.74	0.45
1:H:47:LYS:O	1:H:114:GLU:HG2	2.17	0.45
1:C:93:GLN:HG2	1:C:104:CYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:PRO:HG2	1:I:94:ASN:CG	2.37	0.45
1:H:129:ILE:HG22	1:H:131:LEU:CD1	2.45	0.45
1:C:128:GLN:O	1:C:129:ILE:HD12	2.15	0.45
2:R:19:ALA:HB3	2:R:22:LEU:HD22	1.98	0.45
1:E:128:GLN:O	1:E:129:ILE:HD12	2.16	0.45
1:G:68:GLY:HA3	1:G:91:CYS:O	2.16	0.45
2:K:6:PRO:O	2:K:7:ALA:CB	2.64	0.45
1:D:64:THR:OG1	1:D:124:ARG:NE	2.46	0.45
1:D:90:ARG:HG2	1:E:135:VAL:CG1	2.47	0.45
1:F:10:ALA:HB2	1:F:136:THR:OG1	2.17	0.45
1:F:47:LYS:O	1:F:114:GLU:HG2	2.16	0.45
1:H:49:THR:CB	1:H:113:GLU:HA	2.47	0.45
1:J:128:GLN:O	1:J:129:ILE:HD12	2.17	0.45
2:L:18:VAL:HG12	2:L:22:LEU:HD23	1.98	0.45
1:B:59:LEU:HB3	1:B:130:SER:HB3	1.99	0.45
1:E:49:THR:CB	1:E:113:GLU:HA	2.47	0.45
1:I:63:LYS:HE2	1:I:63:LYS:HB3	1.83	0.45
1:E:93:GLN:HG2	1:E:104:CYS:HB2	1.98	0.44
1:G:66:ALA:O	1:G:124:ARG:NH2	2.43	0.44
1:I:10:ALA:HB2	1:I:136:THR:OG1	2.18	0.44
1:E:79:PHE:CE2	1:J:110:ALA:HA	2.52	0.44
2:Q:11:ASP:CG	2:Q:14:VAL:HG23	2.37	0.44
1:C:68:GLY:HA3	1:C:91:CYS:O	2.17	0.44
1:C:124:ARG:HH12	2:M:11:ASP:CG	2.21	0.44
1:D:124:ARG:HH11	1:D:124:ARG:HG2	1.83	0.44
1:F:62:ASP:CB	1:F:128:GLN:HB2	2.47	0.44
1:F:93:GLN:HG2	1:F:104:CYS:HB2	1.99	0.44
1:E:10:ALA:HB2	1:E:136:THR:OG1	2.17	0.44
1:H:93:GLN:HG2	1:H:104:CYS:HB2	2.00	0.44
2:L:6:PRO:O	2:L:7:ALA:CB	2.65	0.44
2:R:18:VAL:HG12	2:R:22:LEU:HD23	1.99	0.44
1:A:109:ILE:H	1:B:7:GLN:NE2	2.06	0.44
1:B:93:GLN:HG2	1:B:104:CYS:HB2	1.99	0.44
1:D:93:GLN:HE22	1:E:93:GLN:HE22	1.65	0.44
1:D:141:LEU:HD11	1:F:143:LEU:HD22	1.98	0.44
1:F:57:GLN:O	1:F:136:THR:HA	2.17	0.44
1:I:59:LEU:HB3	1:I:130:SER:HB3	1.99	0.44
2:K:19:ALA:HB3	2:K:22:LEU:HD22	1.98	0.44
1:B:81:ASP:OD2	1:F:87:THR:HG23	2.17	0.44
1:B:128:GLN:O	1:B:129:ILE:HD12	2.17	0.44
2:K:2:THR:O	2:K:2:THR:CG2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLN:O	1:B:136:THR:HA	2.18	0.44
1:C:49:THR:CB	1:C:113:GLU:HA	2.46	0.44
1:I:128:GLN:O	1:I:129:ILE:HD12	2.17	0.44
2:M:19:ALA:HB3	2:M:22:LEU:HD22	1.98	0.44
1:G:10:ALA:HB2	1:G:136:THR:OG1	2.17	0.44
1:G:32:LYS:HE3	1:G:37:LEU:O	2.17	0.44
2:N:2:THR:H	2:N:3:PRO:HD3	1.82	0.44
1:A:90:ARG:HG2	1:B:135:VAL:CG1	2.47	0.44
1:C:10:ALA:HB2	1:C:136:THR:OG1	2.17	0.44
1:D:59:LEU:HB2	1:D:135:VAL:HB	2.00	0.44
1:H:128:GLN:O	1:H:129:ILE:HD12	2.18	0.44
2:Q:18:VAL:HG12	2:Q:22:LEU:HD23	1.99	0.44
1:F:31:PHE:HA	1:J:77:HIS:CD2	2.53	0.43
1:G:57:GLN:O	1:G:136:THR:HA	2.18	0.43
1:G:144:LEU:HD12	1:H:144:LEU:HD12	1.99	0.43
2:N:18:VAL:HG11	2:N:22:LEU:HB2	2.00	0.43
1:A:141:LEU:HD11	1:C:143:LEU:HD22	1.99	0.43
1:B:58:VAL:HA	1:B:136:THR:HB	1.99	0.43
1:C:77:HIS:CD2	1:H:31:PHE:HA	2.53	0.43
1:D:93:GLN:HG2	1:D:104:CYS:HB2	1.99	0.43
1:F:32:LYS:HE3	1:F:37:LEU:O	2.18	0.43
1:G:58:VAL:HA	1:G:136:THR:HB	2.00	0.43
2:N:19:ALA:O	2:N:21:GLY:N	2.51	0.43
1:A:93:GLN:HE22	1:B:93:GLN:HE22	1.67	0.43
1:A:135:VAL:HG12	1:C:90:ARG:HG2	2.00	0.43
1:D:130:SER:O	1:D:136:THR:HG21	2.19	0.43
1:G:130:SER:O	1:G:136:THR:HG21	2.18	0.43
1:I:124:ARG:HH22	2:Q:13:LEU:HB3	1.83	0.43
2:M:18:VAL:HG12	2:M:22:LEU:HD23	2.00	0.43
1:A:101:ASN:N	1:C:94:ASN:HD21	1.96	0.43
1:B:49:THR:CB	1:B:113:GLU:HA	2.47	0.43
1:J:47:LYS:O	1:J:114:GLU:HG2	2.18	0.43
1:C:59:LEU:HB3	1:C:130:SER:HB3	1.99	0.43
1:I:93:GLN:HG2	1:I:104:CYS:HB2	2.01	0.43
2:K:2:THR:N	2:K:3:PRO:HD3	2.32	0.43
2:R:18:VAL:CG1	2:R:22:LEU:HD23	2.49	0.43
1:C:58:VAL:HA	1:C:136:THR:HB	2.01	0.43
1:G:144:LEU:HD12	1:H:144:LEU:CD1	2.49	0.43
1:I:49:THR:CB	1:I:113:GLU:HA	2.46	0.43
2:O:27:ARG:HA	2:O:27:ARG:HD3	1.75	0.43
1:B:10:ALA:HB2	1:B:136:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:THR:CB	1:F:113:GLU:HA	2.48	0.43
2:M:18:VAL:CG1	2:M:22:LEU:HD23	2.49	0.43
1:D:47:LYS:O	1:D:114:GLU:HG2	2.18	0.43
1:G:93:GLN:HE22	1:I:93:GLN:HE22	1.67	0.43
2:L:19:ALA:HB3	2:L:22:LEU:HD22	1.98	0.43
2:Q:4:CYS:HB3	2:Q:8:GLU:O	2.18	0.43
1:B:32:LYS:HE3	1:B:37:LEU:O	2.19	0.42
1:B:94:ASN:CG	1:C:96:PRO:HG2	2.39	0.42
1:F:58:VAL:HA	1:F:136:THR:HB	2.00	0.42
2:N:18:VAL:CG1	2:N:22:LEU:HB2	2.49	0.42
1:A:93:GLN:HG2	1:A:104:CYS:HB2	2.00	0.42
1:H:62:ASP:CA	1:H:128:GLN:HB2	2.49	0.42
1:B:143:LEU:HD22	1:C:141:LEU:HD11	2.01	0.42
1:F:25:VAL:HA	1:F:26:PRO:HD3	1.87	0.42
1:F:59:LEU:HB3	1:F:130:SER:HB3	2.01	0.42
1:H:59:LEU:N	1:H:136:THR:HG22	2.30	0.42
1:J:63:LYS:HB3	1:J:63:LYS:HE2	1.84	0.42
1:G:8:LEU:HG	1:G:27:TRP:HB3	2.01	0.42
1:G:98:THR:O	1:G:100:PRO:HD3	2.19	0.42
1:I:8:LEU:HG	1:I:27:TRP:HB3	2.01	0.42
2:L:18:VAL:CG1	2:L:22:LEU:HD23	2.49	0.42
1:D:90:ARG:HH11	1:E:134:ASP:CG	2.21	0.42
1:E:32:LYS:HE3	1:E:37:LEU:O	2.19	0.42
1:F:12:SER:HA	1:F:131:LEU:HB3	2.02	0.42
1:A:49:THR:CB	1:A:113:GLU:HA	2.45	0.42
1:A:63:LYS:HE2	1:A:63:LYS:HB3	1.84	0.42
1:A:130:SER:O	1:A:136:THR:HG21	2.19	0.42
1:I:122:ILE:HA	1:I:123:PRO:HD3	1.87	0.42
1:I:130:SER:O	1:I:136:THR:HG21	2.20	0.42
1:J:59:LEU:N	1:J:136:THR:HG22	2.30	0.42
2:O:14:VAL:HG11	2:O:16:HIS:CE1	2.54	0.42
2:P:29:LYS:H	2:P:30:PRO:CD	2.33	0.42
1:A:59:LEU:N	1:A:136:THR:HG22	2.32	0.42
1:F:130:SER:O	1:F:136:THR:HG21	2.19	0.42
1:G:59:LEU:HB3	1:G:130:SER:HB3	2.01	0.42
1:G:143:LEU:HD22	1:H:141:LEU:HD11	2.00	0.42
1:A:135:VAL:CG1	1:C:90:ARG:HG2	2.49	0.42
1:G:93:GLN:HG2	1:G:104:CYS:HB2	2.00	0.42
1:H:144:LEU:OXT	1:I:2:THR:HG22	2.18	0.42
2:L:29:LYS:N	2:L:30:PRO:HD3	2.31	0.42
2:P:27:ARG:HD3	2:P:28:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:19:ALA:HB3	2:Q:22:LEU:HD22	1.98	0.42
1:A:10:ALA:HB2	1:A:136:THR:OG1	2.20	0.42
1:B:8:LEU:HG	1:B:27:TRP:HB3	2.02	0.42
1:D:109:ILE:H	1:E:7:GLN:NE2	2.12	0.42
1:E:67:MET:C	2:N:13:LEU:HD21	2.40	0.42
1:H:32:LYS:HE3	1:H:37:LEU:O	2.19	0.42
1:H:63:LYS:HB3	1:H:63:LYS:HE2	1.83	0.42
1:I:58:VAL:HA	1:I:136:THR:HB	2.01	0.42
1:J:8:LEU:HG	1:J:27:TRP:HB3	2.02	0.42
1:J:59:LEU:H	1:J:136:THR:CG2	2.32	0.42
1:J:93:GLN:HG2	1:J:104:CYS:HB2	2.01	0.42
2:Q:18:VAL:CG1	2:Q:22:LEU:HD23	2.49	0.42
1:C:32:LYS:HE3	1:C:37:LEU:O	2.20	0.42
1:D:32:LYS:HE3	1:D:37:LEU:O	2.20	0.42
1:D:128:GLN:O	1:D:129:ILE:HD12	2.20	0.42
1:I:32:LYS:HE3	1:I:37:LEU:O	2.20	0.42
1:J:32:LYS:HE3	1:J:37:LEU:O	2.20	0.42
2:K:18:VAL:CG1	2:K:22:LEU:HD23	2.50	0.42
2:Q:6:PRO:O	2:Q:7:ALA:CB	2.63	0.42
1:D:62:ASP:CA	1:D:128:GLN:HB2	2.50	0.41
1:H:130:SER:O	1:H:136:THR:HG21	2.20	0.41
1:I:62:ASP:CA	1:I:128:GLN:HB2	2.49	0.41
1:J:58:VAL:O	1:J:103:SER:HA	2.20	0.41
2:P:25:THR:HA	2:P:26:PRO:HD3	1.86	0.41
1:E:58:VAL:HA	1:E:136:THR:HB	2.00	0.41
2:R:29:LYS:HB2	2:R:30:PRO:HD3	2.01	0.41
1:A:8:LEU:HG	1:A:27:TRP:HB3	2.03	0.41
1:A:32:LYS:HE3	1:A:37:LEU:O	2.20	0.41
1:B:94:ASN:HD22	1:C:102:ASN:ND2	2.18	0.41
1:G:49:THR:CB	1:G:113:GLU:HA	2.47	0.41
1:H:8:LEU:HG	1:H:27:TRP:HB3	2.01	0.41
2:K:18:VAL:HG12	2:K:22:LEU:HD23	2.02	0.41
2:P:29:LYS:H	2:P:30:PRO:HD2	1.86	0.41
1:C:31:PHE:HA	1:F:77:HIS:CD2	2.55	0.41
1:D:94:ASN:HD22	1:E:102:ASN:ND2	2.17	0.41
1:J:18:GLN:NE2	1:J:125:GLU:O	2.53	0.41
1:C:130:SER:O	1:C:136:THR:HG21	2.19	0.41
1:F:8:LEU:HG	1:F:27:TRP:HB3	2.02	0.41
1:I:57:GLN:O	1:I:136:THR:HA	2.21	0.41
1:J:98:THR:O	1:J:100:PRO:HD3	2.20	0.41
2:K:30:PRO:O	2:K:31:ALA:OXT	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:9:CYS:O	2:N:17:CYS:HA	2.21	0.41
1:A:62:ASP:CA	1:A:128:GLN:HB2	2.51	0.41
1:A:98:THR:O	1:A:100:PRO:HD3	2.21	0.41
1:C:63:LYS:HB3	1:C:63:LYS:HE2	1.85	0.41
1:D:58:VAL:O	1:D:103:SER:HA	2.21	0.41
1:E:8:LEU:HG	1:E:27:TRP:HB3	2.01	0.41
1:G:12:SER:HA	1:G:131:LEU:HB3	2.01	0.41
2:L:2:THR:N	2:L:3:PRO:CD	2.82	0.41
2:P:5:VAL:O	2:P:8:GLU:HB2	2.20	0.41
1:C:58:VAL:O	1:C:103:SER:HA	2.21	0.41
1:D:8:LEU:HG	1:D:27:TRP:HB3	2.02	0.41
1:G:141:LEU:HD11	1:I:143:LEU:HD22	2.02	0.41
1:I:125:GLU:OE1	2:Q:27:ARG:HB2	2.20	0.41
1:E:93:GLN:HE22	1:F:93:GLN:HE22	1.68	0.41
1:F:63:LYS:HE2	1:F:63:LYS:HB3	1.85	0.41
1:A:58:VAL:O	1:A:103:SER:HA	2.21	0.41
1:E:94:ASN:CG	1:F:96:PRO:HG2	2.40	0.41
1:G:27:TRP:H	1:G:42:ASN:ND2	1.97	0.41
1:I:98:THR:O	1:I:100:PRO:HD3	2.21	0.41
1:J:25:VAL:HA	1:J:26:PRO:HD3	1.86	0.41
2:Q:29:LYS:N	2:Q:30:PRO:HD3	2.36	0.41
1:B:130:SER:O	1:B:136:THR:HG21	2.21	0.41
1:G:63:LYS:HE2	1:G:63:LYS:HB3	1.84	0.41
1:J:130:SER:O	1:J:136:THR:HG21	2.20	0.41
1:B:12:SER:HA	1:B:131:LEU:HB3	2.03	0.40
1:H:59:LEU:HB2	1:H:135:VAL:HB	2.02	0.40
1:A:122:ILE:HA	1:A:123:PRO:HD3	1.88	0.40
1:B:87:THR:HG23	1:F:81:ASP:OD2	2.22	0.40
1:C:8:LEU:HG	1:C:27:TRP:HB3	2.02	0.40
1:J:59:LEU:HD12	1:J:135:VAL:HG21	2.03	0.40
1:D:6:LEU:CD2	1:D:8:LEU:HD13	2.52	0.40
1:D:49:THR:CB	1:D:113:GLU:HA	2.47	0.40
1:D:103:SER:OG	1:F:91:CYS:HB2	2.21	0.40
1:E:58:VAL:O	1:E:103:SER:HA	2.21	0.40
1:I:25:VAL:HA	1:I:26:PRO:HD3	1.85	0.40
2:L:28:PRO:O	2:L:29:LYS:HG2	2.22	0.40
2:O:16:HIS:C	2:O:16:HIS:CD2	2.95	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	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	22	39
1	B	142/144 (99%)	135 (95%)	5 (4%)	2 (1%)	11	20
1	C	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	22	39
1	D	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	22	39
1	E	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	22	39
1	F	142/144 (99%)	133 (94%)	8 (6%)	1 (1%)	22	39
1	G	142/144 (99%)	134 (94%)	6 (4%)	2 (1%)	11	20
1	H	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	22	39
1	I	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	22	39
1	J	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	22	39
2	K	29/31 (94%)	20 (69%)	6 (21%)	3 (10%)	0	0
2	L	29/31 (94%)	20 (69%)	5 (17%)	4 (14%)	0	0
2	M	29/31 (94%)	20 (69%)	6 (21%)	3 (10%)	0	0
2	N	22/31 (71%)	14 (64%)	3 (14%)	5 (23%)	0	0
2	O	29/31 (94%)	22 (76%)	4 (14%)	3 (10%)	0	0
2	P	29/31 (94%)	17 (59%)	9 (31%)	3 (10%)	0	0
2	Q	29/31 (94%)	21 (72%)	5 (17%)	3 (10%)	0	0
2	R	29/31 (94%)	21 (72%)	4 (14%)	4 (14%)	0	0
All	All	1645/1688 (98%)	1498 (91%)	107 (6%)	40 (2%)	6	9

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	2	THR
2	L	29	LYS
2	M	29	LYS
2	N	7	ALA

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Mol	Chain	Res	Type
2	O	29	LYS
2	P	2	THR
2	Q	29	LYS
2	R	2	THR
2	M	3	PRO
2	N	4	CYS
2	O	2	THR
2	Q	3	PRO
2	R	29	LYS
1	B	125	GLU
1	G	64	THR
1	J	64	THR
2	K	3	PRO
2	K	29	LYS
2	P	29	LYS
2	R	3	PRO
1	A	64	THR
1	B	64	THR
1	C	64	THR
1	D	64	THR
1	E	64	THR
1	F	64	THR
1	H	64	THR
1	I	64	THR
2	L	30	PRO
2	M	2	THR
2	N	20	CYS
1	G	125	GLU
2	N	6	PRO
2	O	3	PRO
2	P	20	CYS
2	L	2	THR
2	N	3	PRO
2	L	26	PRO
2	Q	26	PRO
2	R	26	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	126/126 (100%)	113 (90%)	13 (10%)	7 14
1	B	126/126 (100%)	113 (90%)	13 (10%)	7 14
1	C	126/126 (100%)	113 (90%)	13 (10%)	7 14
1	D	126/126 (100%)	112 (89%)	14 (11%)	6 11
1	E	126/126 (100%)	113 (90%)	13 (10%)	7 14
1	F	126/126 (100%)	113 (90%)	13 (10%)	7 14
1	G	126/126 (100%)	113 (90%)	13 (10%)	7 14
1	H	126/126 (100%)	113 (90%)	13 (10%)	7 14
1	I	126/126 (100%)	113 (90%)	13 (10%)	7 14
1	J	126/126 (100%)	112 (89%)	14 (11%)	6 11
2	K	27/27 (100%)	24 (89%)	3 (11%)	6 11
2	L	27/27 (100%)	24 (89%)	3 (11%)	6 11
2	M	27/27 (100%)	24 (89%)	3 (11%)	6 11
2	N	21/27 (78%)	20 (95%)	1 (5%)	25 48
2	O	27/27 (100%)	23 (85%)	4 (15%)	3 5
2	P	27/27 (100%)	26 (96%)	1 (4%)	34 60
2	Q	27/27 (100%)	23 (85%)	4 (15%)	3 5
2	R	27/27 (100%)	24 (89%)	3 (11%)	6 11
All	All	1470/1476 (100%)	1316 (90%)	154 (10%)	7 13

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	ILE
1	A	18	GLN
1	A	47	LYS
1	A	49	THR
1	A	59	LEU
1	A	65	TYR
1	A	76	VAL
1	A	87	THR
1	A	88	LEU
1	A	97	GLU

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Mol	Chain	Res	Type
1	A	120	LEU
1	A	136	THR
1	B	8	LEU
1	B	9	ILE
1	B	18	GLN
1	B	47	LYS
1	B	49	THR
1	B	59	LEU
1	B	65	TYR
1	B	76	VAL
1	B	87	THR
1	B	88	LEU
1	B	97	GLU
1	B	120	LEU
1	B	136	THR
1	C	8	LEU
1	C	9	ILE
1	C	18	GLN
1	C	47	LYS
1	C	49	THR
1	C	59	LEU
1	C	65	TYR
1	C	76	VAL
1	C	87	THR
1	C	88	LEU
1	C	97	GLU
1	C	120	LEU
1	C	136	THR
1	D	8	LEU
1	D	9	ILE
1	D	18	GLN
1	D	47	LYS
1	D	49	THR
1	D	59	LEU
1	D	65	TYR
1	D	76	VAL
1	D	87	THR
1	D	88	LEU
1	D	97	GLU
1	D	120	LEU
1	D	124	ARG
1	D	136	THR

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Mol	Chain	Res	Type
1	E	8	LEU
1	E	9	ILE
1	E	18	GLN
1	E	47	LYS
1	E	49	THR
1	E	59	LEU
1	E	65	TYR
1	E	76	VAL
1	E	87	THR
1	E	88	LEU
1	E	97	GLU
1	E	120	LEU
1	E	136	THR
1	F	8	LEU
1	F	9	ILE
1	F	18	GLN
1	F	47	LYS
1	F	49	THR
1	F	59	LEU
1	F	65	TYR
1	F	76	VAL
1	F	87	THR
1	F	88	LEU
1	F	97	GLU
1	F	120	LEU
1	F	136	THR
1	G	8	LEU
1	G	9	ILE
1	G	18	GLN
1	G	47	LYS
1	G	49	THR
1	G	59	LEU
1	G	65	TYR
1	G	76	VAL
1	G	87	THR
1	G	88	LEU
1	G	97	GLU
1	G	120	LEU
1	G	136	THR
1	H	8	LEU
1	H	9	ILE
1	H	18	GLN

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Mol	Chain	Res	Type
1	H	47	LYS
1	H	49	THR
1	H	59	LEU
1	H	65	TYR
1	H	76	VAL
1	H	87	THR
1	H	88	LEU
1	H	97	GLU
1	H	120	LEU
1	H	136	THR
1	I	8	LEU
1	I	9	ILE
1	I	18	GLN
1	I	47	LYS
1	I	49	THR
1	I	59	LEU
1	I	65	TYR
1	I	76	VAL
1	I	87	THR
1	I	88	LEU
1	I	97	GLU
1	I	120	LEU
1	I	136	THR
1	J	8	LEU
1	J	9	ILE
1	J	18	GLN
1	J	47	LYS
1	J	49	THR
1	J	59	LEU
1	J	65	TYR
1	J	76	VAL
1	J	87	THR
1	J	88	LEU
1	J	97	GLU
1	J	120	LEU
1	J	124	ARG
1	J	136	THR
2	K	14	VAL
2	K	24	ARG
2	K	25	THR
2	L	14	VAL
2	L	24	ARG

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Mol	Chain	Res	Type
2	L	25	THR
2	M	14	VAL
2	M	24	ARG
2	M	25	THR
2	N	6	PRO
2	O	16	HIS
2	O	22	LEU
2	O	24	ARG
2	O	25	THR
2	P	24	ARG
2	Q	3	PRO
2	Q	14	VAL
2	Q	24	ARG
2	Q	25	THR
2	R	14	VAL
2	R	24	ARG
2	R	25	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	GLN
1	A	18	GLN
1	A	42	ASN
1	A	93	GLN
1	A	94	ASN
1	A	119	GLN
1	B	3	GLN
1	B	7	GLN
1	B	18	GLN
1	B	42	ASN
1	B	93	GLN
1	B	94	ASN
1	B	119	GLN
1	C	3	GLN
1	C	7	GLN
1	C	18	GLN
1	C	42	ASN
1	C	77	HIS
1	C	93	GLN
1	C	94	ASN

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Mol	Chain	Res	Type
1	C	119	GLN
1	D	3	GLN
1	D	7	GLN
1	D	18	GLN
1	D	42	ASN
1	D	93	GLN
1	D	94	ASN
1	D	119	GLN
1	E	3	GLN
1	E	7	GLN
1	E	18	GLN
1	E	42	ASN
1	E	93	GLN
1	E	94	ASN
1	E	119	GLN
1	E	126	ASN
1	F	3	GLN
1	F	7	GLN
1	F	18	GLN
1	F	42	ASN
1	F	77	HIS
1	F	93	GLN
1	F	94	ASN
1	F	119	GLN
1	G	3	GLN
1	G	7	GLN
1	G	18	GLN
1	G	42	ASN
1	G	77	HIS
1	G	93	GLN
1	G	94	ASN
1	G	119	GLN
1	H	3	GLN
1	H	7	GLN
1	H	18	GLN
1	H	42	ASN
1	H	93	GLN
1	H	94	ASN
1	H	119	GLN
1	I	3	GLN
1	I	7	GLN
1	I	18	GLN

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Mol	Chain	Res	Type
1	I	42	ASN
1	I	93	GLN
1	I	94	ASN
1	I	119	GLN
1	J	7	GLN
1	J	18	GLN
1	J	42	ASN
1	J	77	HIS
1	J	119	GLN
2	N	16	HIS
2	O	16	HIS

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 monosaccharides 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	144/144 (100%)	0.09	1 (0%) 87 89	20, 34, 55, 68	0
1	B	144/144 (100%)	-0.06	0 100 100	16, 32, 54, 74	0
1	C	144/144 (100%)	-0.15	0 100 100	18, 30, 52, 63	0
1	D	144/144 (100%)	-0.22	0 100 100	16, 29, 50, 63	0
1	E	144/144 (100%)	-0.21	0 100 100	19, 28, 47, 57	0
1	F	144/144 (100%)	-0.18	1 (0%) 87 89	17, 29, 49, 61	0
1	G	144/144 (100%)	0.19	1 (0%) 87 89	14, 28, 51, 61	0
1	H	144/144 (100%)	-0.12	0 100 100	16, 27, 46, 57	0
1	I	144/144 (100%)	0.13	2 (1%) 75 77	17, 29, 51, 62	0
1	J	144/144 (100%)	-0.03	2 (1%) 75 77	16, 31, 53, 65	0
2	K	31/31 (100%)	3.33	16 (51%) 0 0	54, 88, 134, 140	0
2	L	31/31 (100%)	3.31	16 (51%) 0 0	54, 87, 131, 136	0
2	M	31/31 (100%)	3.31	20 (64%) 0 0	48, 86, 134, 140	0
2	N	24/31 (77%)	5.18	19 (79%) 0 0	82, 104, 134, 140	0
2	O	31/31 (100%)	2.67	17 (54%) 0 0	43, 70, 132, 140	0
2	P	31/31 (100%)	3.26	18 (58%) 0 0	40, 74, 124, 131	0
2	Q	31/31 (100%)	3.75	18 (58%) 0 0	39, 79, 140, 144	0
2	R	31/31 (100%)	3.29	15 (48%) 0 0	43, 84, 129, 137	0
All	All	1681/1688 (99%)	0.45	146 (8%) 10 10	14, 32, 107, 144	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	30	PRO	13.9
2	N	1	PRO	13.8
2	L	31	ALA	12.6

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Mol	Chain	Res	Type	RSRZ
2	N	4	CYS	12.4
2	N	2	THR	11.9
2	R	30	PRO	11.0
2	L	30	PRO	10.6
2	L	2	THR	10.6
2	M	1	PRO	10.3
2	O	30	PRO	10.3
2	N	5	VAL	9.6
2	Q	27	ARG	9.3
2	K	30	PRO	9.3
2	P	30	PRO	9.2
2	O	31	ALA	9.2
2	K	2	THR	9.2
2	N	3	PRO	9.0
2	P	31	ALA	8.9
2	R	1	PRO	8.8
2	Q	31	ALA	8.8
2	Q	28	PRO	8.8
2	N	6	PRO	8.4
2	K	28	PRO	8.2
2	M	31	ALA	8.2
2	K	29	LYS	8.2
2	R	31	ALA	8.1
2	L	1	PRO	8.0
2	P	1	PRO	7.9
2	O	1	PRO	7.8
2	M	30	PRO	7.7
2	R	28	PRO	7.6
2	K	27	ARG	7.4
2	R	2	THR	7.3
2	Q	1	PRO	7.3
2	Q	5	VAL	7.1
2	R	3	PRO	7.0
2	K	31	ALA	6.9
2	N	7	ALA	6.7
2	L	29	LYS	6.7
2	L	28	PRO	6.7
2	P	2	THR	6.7
2	O	2	THR	6.6
2	Q	2	THR	6.5
2	K	1	PRO	6.5
2	P	27	ARG	6.4

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Mol	Chain	Res	Type	RSRZ
2	Q	29	LYS	6.3
2	Q	6	PRO	6.2
2	M	3	PRO	6.2
2	Q	26	PRO	6.2
2	R	27	ARG	6.1
2	N	22	LEU	6.1
2	M	6	PRO	6.0
2	M	28	PRO	6.0
2	O	29	LYS	5.9
2	P	28	PRO	5.7
2	L	27	ARG	5.5
2	M	29	LYS	5.4
2	M	2	THR	5.3
2	R	29	LYS	5.2
2	K	5	VAL	5.2
2	M	5	VAL	5.2
2	M	4	CYS	5.1
2	P	7	ALA	5.1
2	Q	3	PRO	5.0
2	N	9	CYS	4.9
2	O	27	ARG	4.8
2	K	7	ALA	4.8
2	R	7	ALA	4.6
2	K	6	PRO	4.6
2	P	6	PRO	4.6
2	P	3	PRO	4.5
2	O	28	PRO	4.5
2	O	5	VAL	4.4
2	L	7	ALA	4.3
2	R	26	PRO	4.3
2	Q	9	CYS	4.3
2	P	29	LYS	4.3
2	K	4	CYS	4.3
2	L	6	PRO	4.2
2	P	4	CYS	4.2
2	N	19	ALA	4.1
2	P	5	VAL	4.1
2	Q	4	CYS	4.1
2	N	24	ARG	4.0
2	M	7	ALA	4.0
2	N	18	VAL	4.0
2	R	6	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
2	R	5	VAL	3.8
2	N	8	GLU	3.8
2	M	9	CYS	3.7
2	L	4	CYS	3.7
2	O	3	PRO	3.6
2	L	9	CYS	3.5
2	M	27	ARG	3.5
2	K	25	THR	3.5
2	N	17	CYS	3.4
2	N	20	CYS	3.4
2	R	25	THR	3.4
2	O	6	PRO	3.3
2	R	4	CYS	3.3
2	O	4	CYS	3.3
2	M	26	PRO	3.3
2	P	20	CYS	3.2
2	P	26	PRO	3.2
1	I	104	CYS	3.1
1	J	20	GLY	3.1
2	N	23	LEU	3.1
2	Q	7	ALA	3.1
2	K	17	CYS	3.1
2	P	9	CYS	3.0
2	K	3	PRO	3.0
2	O	26	PRO	3.0
2	L	3	PRO	3.0
2	N	10	PHE	2.9
2	L	19	ALA	2.9
2	L	5	VAL	2.8
2	P	18	VAL	2.8
2	R	9	CYS	2.8
2	O	7	ALA	2.8
2	O	25	THR	2.8
2	P	25	THR	2.7
2	Q	25	THR	2.6
2	K	9	CYS	2.6
2	M	22	LEU	2.5
2	N	16	HIS	2.5
2	L	26	PRO	2.5
1	J	1	VAL	2.4
1	I	98	THR	2.4
2	O	17	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	104	CYS	2.3
2	O	9	CYS	2.2
2	Q	17	CYS	2.2
2	Q	24	ARG	2.2
2	Q	8	GLU	2.2
2	P	16	HIS	2.2
2	N	14	VAL	2.2
2	L	25	THR	2.2
2	M	23	LEU	2.2
2	M	25	THR	2.1
2	O	24	ARG	2.1
2	M	10	PHE	2.1
2	K	24	ARG	2.1
1	F	1	VAL	2.1
2	M	20	CYS	2.1
2	M	21	GLY	2.0
1	G	104	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 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.