Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 07:42 AM GMT

PDB ID	:	3BTU
Title	:	Crystal structure of the super-repressor mutant of Gal80p from Saccharomyces cerevisiae; Gal80(S2) [E351K]
Authors	:	Kumar, P.R.; Joshua-Tor, L.
Deposited on	:	2007-12-30
Resolution	:	2.85 Å(reported)

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

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

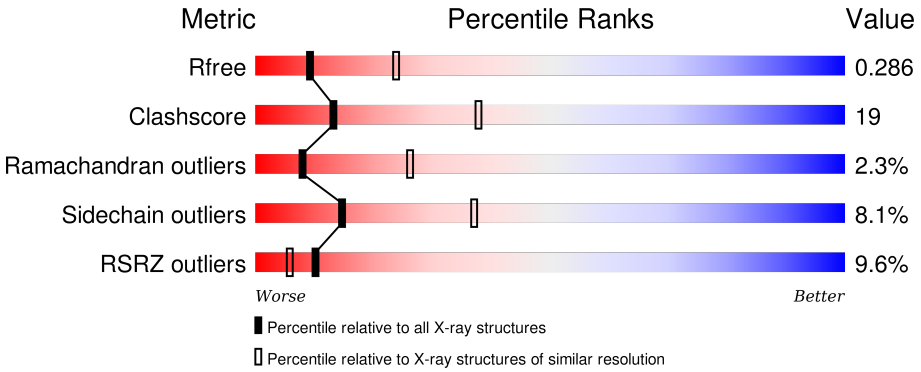
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	438	5% 57% 28% • 11%
1	B	438	3% 58% 26% • 11%
1	C	438	6% 57% 27% • 11%
1	D	438	2% 59% 25% 5% 11%
1	E	438	13% 46% 37% 5% 12%

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Mol	Chain	Length	Quality of chain
1	F	438	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18389 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3088	1987	518	572	11			
1	B	389	Total	C	N	O	S	0	0	0
			3065	1975	513	566	11			
1	C	388	Total	C	N	O	S	0	0	0
			3057	1969	511	566	11			
1	D	392	Total	C	N	O	S	0	0	0
			3087	1987	518	571	11			
1	E	387	Total	C	N	O	S	0	0	0
			3046	1960	512	563	11			
1	F	387	Total	C	N	O	S	0	0	0
			3046	1960	512	563	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P04387
A	-1	SER	-	EXPRESSION TAG	UNP P04387
A	0	HIS	-	EXPRESSION TAG	UNP P04387
A	351	LYS	GLU	ENGINEERED	UNP P04387
B	-2	GLY	-	EXPRESSION TAG	UNP P04387
B	-1	SER	-	EXPRESSION TAG	UNP P04387
B	0	HIS	-	EXPRESSION TAG	UNP P04387
B	351	LYS	GLU	ENGINEERED	UNP P04387
C	-2	GLY	-	EXPRESSION TAG	UNP P04387
C	-1	SER	-	EXPRESSION TAG	UNP P04387
C	0	HIS	-	EXPRESSION TAG	UNP P04387
C	351	LYS	GLU	ENGINEERED	UNP P04387
D	-2	GLY	-	EXPRESSION TAG	UNP P04387
D	-1	SER	-	EXPRESSION TAG	UNP P04387
D	0	HIS	-	EXPRESSION TAG	UNP P04387
D	351	LYS	GLU	ENGINEERED	UNP P04387
E	-2	GLY	-	EXPRESSION TAG	UNP P04387

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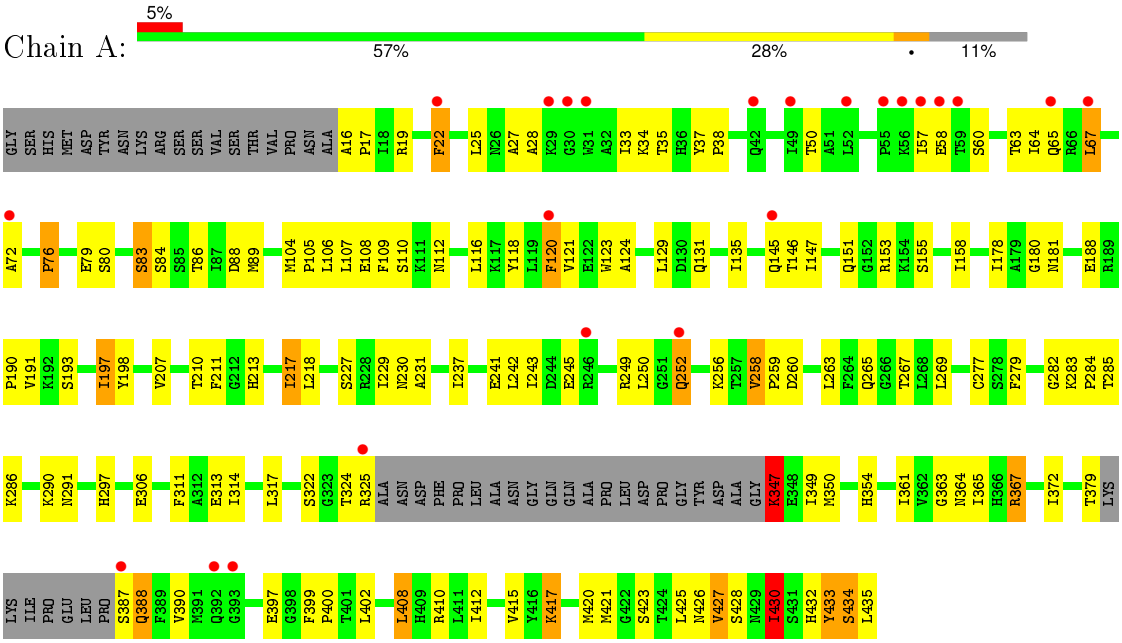
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	EXPRESSION TAG	UNP P04387
E	0	HIS	-	EXPRESSION TAG	UNP P04387
E	351	LYS	GLU	ENGINEERED	UNP P04387
F	-2	GLY	-	EXPRESSION TAG	UNP P04387
F	-1	SER	-	EXPRESSION TAG	UNP P04387
F	0	HIS	-	EXPRESSION TAG	UNP P04387
F	351	LYS	GLU	ENGINEERED	UNP P04387

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.

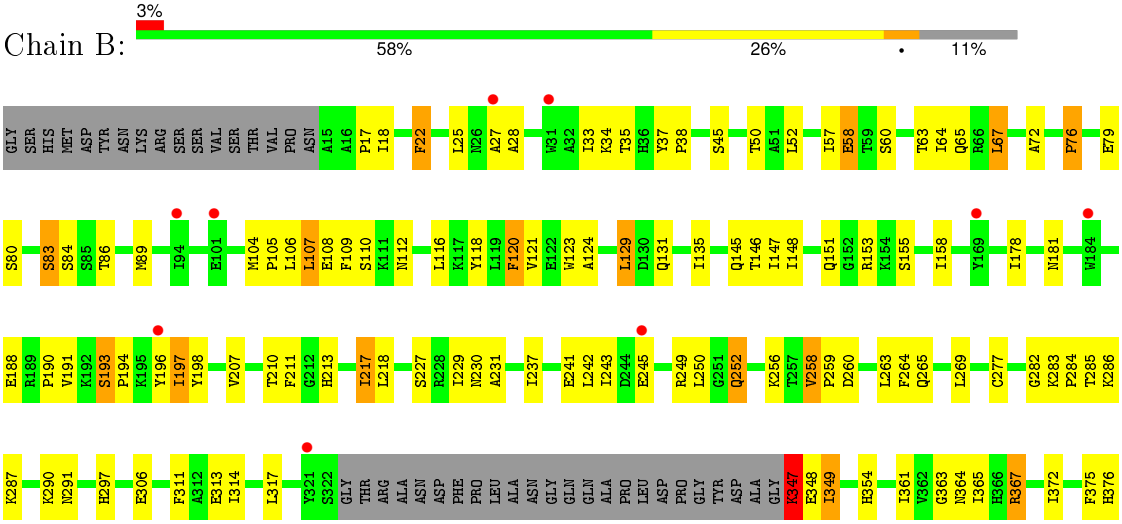
- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

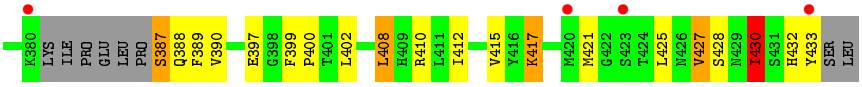
Chain A:



- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

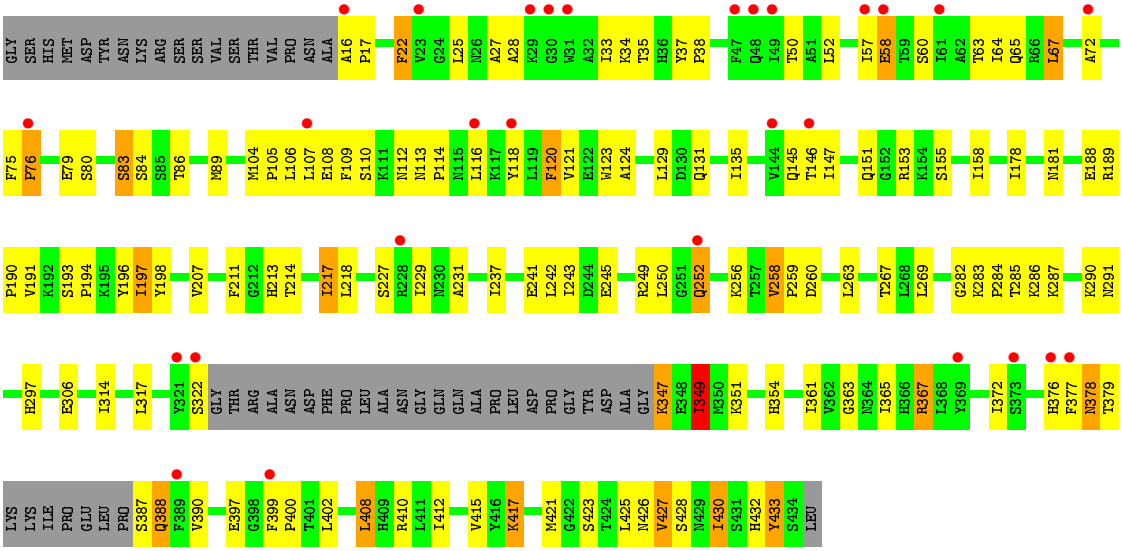
Chain B:





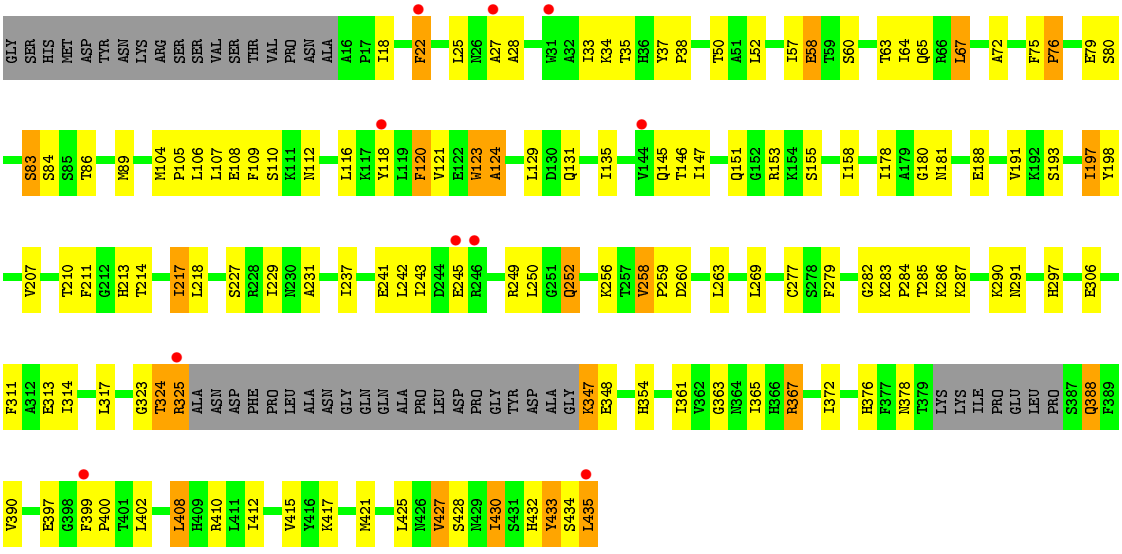
• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

Chain C:



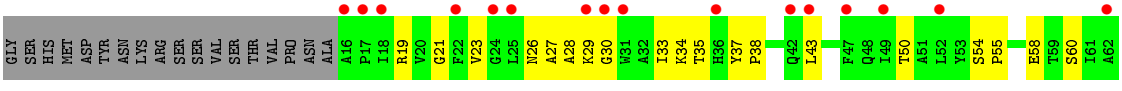
• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

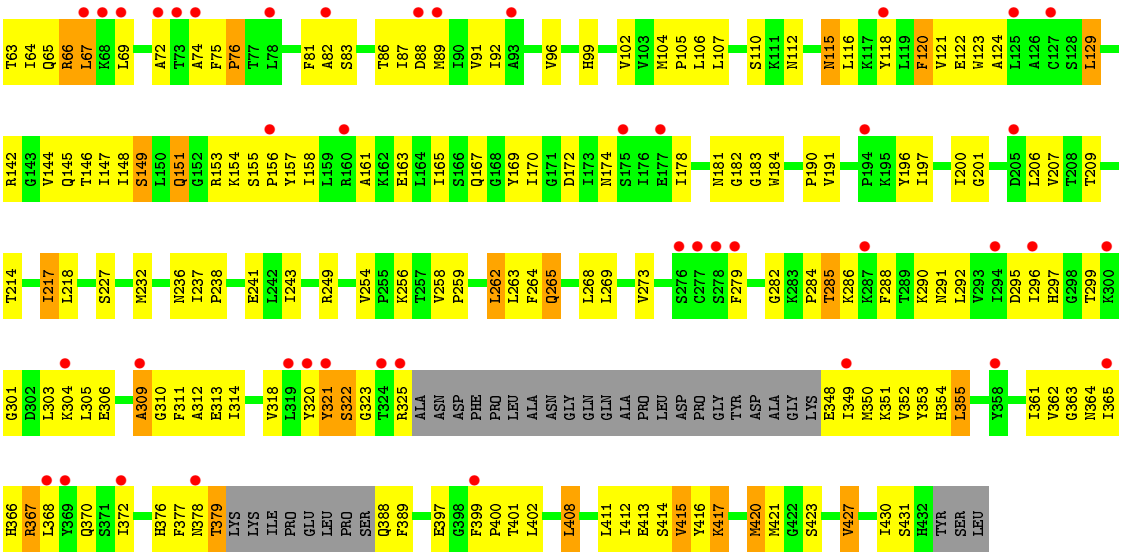
Chain D:



• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

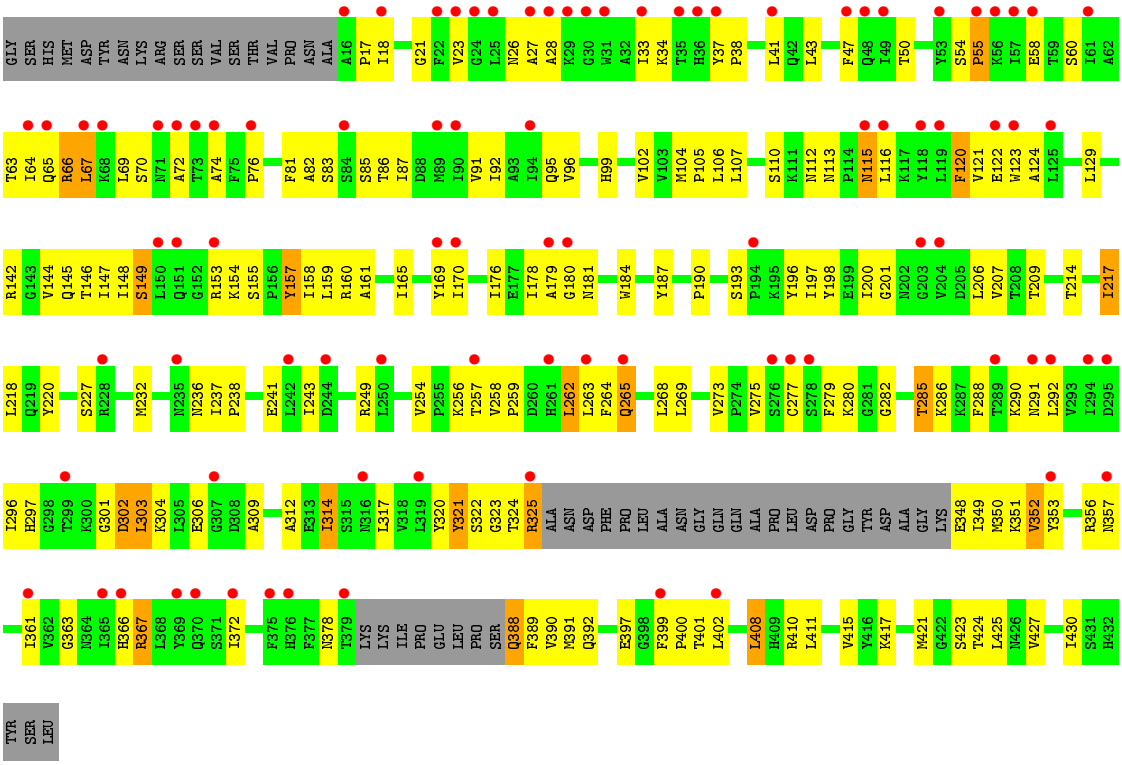
Chain E:





- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	495.32Å 84.86Å 66.46Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 48.39 – 2.85	Depositor EDS
% Data completeness (in resolution range)	85.6 (50.00-2.85) 85.6 (48.39-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.86Å)	Xtriage
Refinement program	PHENIX.REFINE	Depositor
R, R_{free}	0.228 , 0.278 0.244 , 0.286	Depositor DCC
R_{free} test set	5495 reflections (10.08%)	DCC
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.7	EDS
Estimated twinning fraction	0.040 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 54552 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18389	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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	0.34	0/3155	0.51	1/4270 (0.0%)
1	B	0.35	0/3132	0.52	1/4240 (0.0%)
1	C	0.34	0/3124	0.53	2/4230 (0.0%)
1	D	0.36	0/3154	0.51	0/4270
1	E	0.28	0/3112	0.47	0/4214
1	F	0.28	0/3112	0.47	0/4214
All	All	0.33	0/18789	0.50	4/25438 (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	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	347	LYS	N-CA-C	-10.61	82.37	111.00
1	B	347	LYS	N-CA-C	-10.35	83.05	111.00
1	C	379	THR	N-CA-C	-6.64	93.06	111.00
1	A	347	LYS	N-CA-C	-5.91	95.06	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	123	TRP	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	3088	0	3101	108	0
1	B	3065	0	3080	106	0
1	C	3057	0	3067	111	0
1	D	3087	0	3101	107	0
1	E	3046	0	3058	160	0
1	F	3046	0	3058	151	0
All	All	18389	0	18465	698	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 19.

All (698) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:LYS:N	1:D:348:GLU:CA	1.70	1.34
1:E:155:SER:HB3	1:E:158:ILE:HD13	1.41	1.03
1:B:347:LYS:HD2	1:B:347:LYS:O	1.59	0.99
1:C:349:ILE:HD11	1:C:351:LYS:HE3	1.48	0.94
1:D:347:LYS:N	1:D:348:GLU:HA	0.77	0.92
1:F:427:VAL:HG13	1:F:430:ILE:HG13	1.51	0.92
1:E:263:LEU:HB3	1:F:265:GLN:HE21	1.35	0.91
1:D:347:LYS:HG3	1:D:347:LYS:O	1.72	0.90
1:F:292:LEU:HD21	1:F:312:ALA:HB2	1.55	0.88
1:D:410:ARG:HB3	1:D:430:ILE:HD12	1.53	0.87
1:B:410:ARG:HB3	1:B:430:ILE:HD12	1.57	0.86
1:E:304:LYS:HG2	1:E:305:LEU:H	1.40	0.86
1:A:410:ARG:HB3	1:A:430:ILE:HD12	1.57	0.86
1:E:265:GLN:HE21	1:F:263:LEU:HB3	1.41	0.85
1:C:410:ARG:HB3	1:C:430:ILE:HD12	1.58	0.85
1:E:427:VAL:HG12	1:E:430:ILE:HG13	1.60	0.82
1:E:151:GLN:HG2	1:E:365:ILE:HD13	1.60	0.82
1:F:361:ILE:HD12	1:F:361:ILE:H	1.45	0.81
1:A:153:ARG:HD2	1:A:400:PRO:HG3	1.63	0.81
1:C:153:ARG:HD2	1:C:400:PRO:HG3	1.63	0.80
1:E:427:VAL:HG12	1:E:430:ILE:CG1	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:GLN:NE2	1:F:263:LEU:HB3	1.97	0.79
1:C:27:ALA:HB1	1:C:67:LEU:HD21	1.65	0.78
1:E:263:LEU:HB3	1:F:265:GLN:NE2	1.98	0.78
1:D:324:THR:O	1:D:324:THR:HG22	1.83	0.78
1:B:347:LYS:HD2	1:B:347:LYS:C	2.05	0.77
1:D:153:ARG:HD2	1:D:400:PRO:HG3	1.66	0.77
1:F:268:LEU:HB2	1:F:273:VAL:HB	1.67	0.77
1:E:258:VAL:HG13	1:E:259:PRO:HD2	1.67	0.77
1:B:27:ALA:HB1	1:B:67:LEU:HD21	1.67	0.77
1:E:268:LEU:HB2	1:E:273:VAL:HB	1.66	0.76
1:D:27:ALA:HB1	1:D:67:LEU:HD21	1.66	0.76
1:C:349:ILE:O	1:C:349:ILE:HD13	1.85	0.76
1:A:27:ALA:HB1	1:A:67:LEU:HD21	1.68	0.76
1:E:146:THR:HB	1:E:402:LEU:HG	1.67	0.76
1:C:79:GLU:O	1:C:83:SER:HB2	1.86	0.75
1:A:79:GLU:O	1:A:83:SER:HB2	1.86	0.75
1:D:79:GLU:O	1:D:83:SER:HB2	1.87	0.75
1:E:145:GLN:HE21	1:E:388:GLN:HG3	1.50	0.75
1:F:206:LEU:HD11	1:F:279:PHE:HB3	1.69	0.74
1:F:258:VAL:HG13	1:F:259:PRO:HD2	1.69	0.74
1:F:176:ILE:HD13	1:F:218:LEU:HD11	1.70	0.74
1:B:153:ARG:HD2	1:B:400:PRO:HG3	1.68	0.74
1:E:376:HIS:HD2	1:E:377:PHE:CE1	2.06	0.74
1:E:145:GLN:NE2	1:E:388:GLN:HG3	2.01	0.74
1:C:50:THR:HG21	1:C:86:THR:HB	1.69	0.73
1:B:79:GLU:O	1:B:83:SER:HB2	1.87	0.73
1:E:292:LEU:HD21	1:E:312:ALA:HB2	1.71	0.73
1:B:50:THR:HG21	1:B:86:THR:HB	1.69	0.73
1:E:206:LEU:HD11	1:E:279:PHE:HB3	1.69	0.73
1:F:352:VAL:HG12	1:F:353:TYR:N	2.03	0.73
1:F:64:ILE:HG23	1:F:72:ALA:HB3	1.71	0.72
1:B:241:GLU:HG2	1:B:249:ARG:HD3	1.71	0.72
1:A:241:GLU:HG2	1:A:249:ARG:HD3	1.71	0.72
1:D:241:GLU:HG2	1:D:249:ARG:HD3	1.70	0.72
1:A:57:ILE:HD12	1:A:76:PRO:HA	1.71	0.72
1:E:37:TYR:HB3	1:E:38:PRO:HD3	1.70	0.72
1:E:64:ILE:HG23	1:E:72:ALA:HB3	1.71	0.72
1:F:146:THR:HB	1:F:402:LEU:HG	1.69	0.72
1:D:50:THR:HG21	1:D:86:THR:HB	1.71	0.72
1:C:57:ILE:HD12	1:C:76:PRO:HA	1.70	0.72
1:C:104:MET:HB2	1:C:105:PRO:HD3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:MET:HE1	1:C:372:ILE:HG21	1.72	0.72
1:E:170:ILE:HB	1:E:301:GLY:O	1.89	0.72
1:A:50:THR:HG21	1:A:86:THR:HB	1.70	0.72
1:A:104:MET:HB2	1:A:105:PRO:HD3	1.72	0.71
1:C:27:ALA:HB2	1:C:63:THR:HG23	1.73	0.71
1:E:161:ALA:O	1:E:165:ILE:HG13	1.90	0.71
1:D:22:PHE:CD2	1:D:25:LEU:HB2	2.25	0.71
1:D:57:ILE:HD12	1:D:76:PRO:HA	1.71	0.71
1:C:241:GLU:HG2	1:C:249:ARG:HD3	1.71	0.71
1:A:417:LYS:HG3	1:C:417:LYS:HZ3	1.54	0.71
1:B:104:MET:HB2	1:B:105:PRO:HD3	1.72	0.70
1:D:131:GLN:O	1:D:135:ILE:HG13	1.90	0.70
1:E:157:TYR:OH	1:E:355:LEU:HB2	1.92	0.70
1:D:104:MET:HB2	1:D:105:PRO:HD3	1.73	0.70
1:B:22:PHE:CD2	1:B:25:LEU:HB2	2.27	0.70
1:E:297:HIS:NE2	1:F:286:LYS:HD3	2.06	0.70
1:E:288:PHE:CE2	1:F:320:TYR:HB3	2.26	0.70
1:C:285:THR:HB	1:C:291:ASN:HD21	1.57	0.70
1:B:27:ALA:HB2	1:B:63:THR:HG23	1.74	0.69
1:F:37:TYR:HB3	1:F:38:PRO:HD3	1.73	0.69
1:F:352:VAL:HG12	1:F:353:TYR:H	1.56	0.69
1:C:131:GLN:O	1:C:135:ILE:HG13	1.92	0.69
1:B:57:ILE:HD12	1:B:76:PRO:HA	1.75	0.69
1:B:89:MET:HE1	1:B:372:ILE:HG21	1.75	0.69
1:F:83:SER:OG	1:F:112:ASN:HB2	1.93	0.68
1:C:22:PHE:CD2	1:C:25:LEU:HB2	2.29	0.68
1:D:89:MET:HE1	1:D:372:ILE:HG21	1.76	0.67
1:B:131:GLN:O	1:B:135:ILE:HG13	1.94	0.67
1:A:22:PHE:CD2	1:A:25:LEU:HB2	2.29	0.67
1:E:83:SER:OG	1:E:112:ASN:HB2	1.95	0.67
1:E:207:VAL:HG22	1:E:262:LEU:HD22	1.77	0.67
1:A:158:ILE:HG12	1:A:217:ILE:HG21	1.77	0.67
1:E:155:SER:HA	1:E:364:ASN:ND2	2.10	0.66
1:A:27:ALA:HB2	1:A:63:THR:HG23	1.76	0.66
1:F:67:LEU:O	1:F:69:LEU:HG	1.95	0.66
1:C:145:GLN:HE21	1:C:388:GLN:HG3	1.58	0.66
1:D:237:ILE:O	1:D:256:LYS:NZ	2.26	0.66
1:E:67:LEU:O	1:E:69:LEU:HG	1.96	0.66
1:E:145:GLN:HE22	1:E:389:PHE:H	1.44	0.66
1:D:123:TRP:CH2	1:D:408:LEU:HD13	2.30	0.65
1:A:131:GLN:O	1:A:135:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ALA:HB2	1:D:63:THR:HG23	1.78	0.65
1:A:285:THR:HB	1:A:291:ASN:HD21	1.62	0.65
1:A:397:GLU:H	1:A:397:GLU:CD	2.00	0.65
1:F:153:ARG:HD2	1:F:400:PRO:HG3	1.77	0.65
1:B:178:ILE:HD11	1:B:218:LEU:HD22	1.77	0.65
1:D:158:ILE:HG12	1:D:217:ILE:HG21	1.78	0.64
1:B:158:ILE:HG12	1:B:217:ILE:HG21	1.79	0.64
1:A:363:GLY:O	1:A:367:ARG:HD2	1.97	0.64
1:B:397:GLU:CD	1:B:397:GLU:H	2.01	0.64
1:C:377:PHE:O	1:C:378:ASN:C	2.36	0.64
1:E:286:LYS:HD3	1:F:297:HIS:NE2	2.12	0.64
1:C:349:ILE:CD1	1:C:351:LYS:HE3	2.24	0.64
1:F:207:VAL:HG22	1:F:262:LEU:HD22	1.79	0.64
1:F:352:VAL:CG1	1:F:353:TYR:H	2.10	0.64
1:F:322:SER:HB2	1:F:350:MET:HG2	1.79	0.64
1:B:227:SER:HB2	1:B:269:LEU:HD12	1.80	0.64
1:F:256:LYS:HE2	1:F:258:VAL:O	1.98	0.64
1:C:158:ILE:HG12	1:C:217:ILE:HG21	1.79	0.64
1:F:123:TRP:CD2	1:F:124:ALA:N	2.64	0.63
1:C:237:ILE:O	1:C:256:LYS:NZ	2.29	0.63
1:B:285:THR:HB	1:B:291:ASN:HD21	1.63	0.63
1:C:397:GLU:CD	1:C:397:GLU:H	2.01	0.63
1:D:285:THR:HB	1:D:291:ASN:HD21	1.62	0.63
1:E:21:GLY:HA3	1:E:87:ILE:HD13	1.80	0.63
1:E:408:LEU:O	1:E:412:ILE:HG12	1.99	0.63
1:E:43:LEU:HD11	1:E:366:HIS:CD2	2.33	0.63
1:E:142:ARG:HG3	1:E:144:VAL:HG13	1.81	0.63
1:D:123:TRP:CG	1:D:124:ALA:N	2.66	0.63
1:E:389:PHE:HE1	1:E:401:THR:CG2	2.13	0.62
1:F:262:LEU:HD12	1:F:263:LEU:O	2.00	0.62
1:E:303:LEU:HD23	1:E:304:LYS:N	2.15	0.62
1:E:120:PHE:HZ	1:E:368:LEU:HD23	1.65	0.62
1:F:123:TRP:CG	1:F:124:ALA:N	2.67	0.62
1:A:297:HIS:CE1	1:B:286:LYS:HD3	2.35	0.62
1:D:363:GLY:O	1:D:367:ARG:HD2	2.00	0.62
1:D:427:VAL:HG13	1:D:427:VAL:O	2.00	0.62
1:B:290:LYS:HG3	1:B:306:GLU:HB3	1.80	0.62
1:F:142:ARG:HG3	1:F:144:VAL:HG13	1.82	0.61
1:E:313:GLU:HG2	1:E:314:ILE:HG23	1.82	0.61
1:A:290:LYS:HG3	1:A:306:GLU:HB3	1.82	0.61
1:F:21:GLY:HA3	1:F:87:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:GLN:HE21	1:F:388:GLN:HG3	1.65	0.61
1:D:434:SER:O	1:D:435:LEU:HD22	2.00	0.61
1:D:178:ILE:HD11	1:D:218:LEU:HD22	1.83	0.61
1:A:347:LYS:HA	1:A:347:LYS:HE3	1.82	0.61
1:C:297:HIS:NE2	1:D:286:LYS:HD3	2.16	0.61
1:E:123:TRP:CG	1:E:124:ALA:N	2.68	0.60
1:D:145:GLN:HE21	1:D:388:GLN:HG3	1.65	0.60
1:D:397:GLU:H	1:D:397:GLU:CD	2.02	0.60
1:A:146:THR:HB	1:A:402:LEU:HG	1.82	0.60
1:F:321:TYR:CG	1:F:321:TYR:O	2.54	0.60
1:E:320:TYR:HB3	1:F:288:PHE:CE2	2.36	0.60
1:F:352:VAL:CG1	1:F:353:TYR:N	2.64	0.60
1:C:178:ILE:HD11	1:C:218:LEU:HD22	1.81	0.60
1:E:26:ASN:O	1:E:33:ILE:HB	2.02	0.60
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.37	0.60
1:D:60:SER:O	1:D:64:ILE:HG13	2.02	0.60
1:E:155:SER:HA	1:E:364:ASN:HD21	1.67	0.59
1:B:146:THR:HB	1:B:402:LEU:HG	1.83	0.59
1:C:123:TRP:CD2	1:C:124:ALA:HA	2.37	0.59
1:B:17:PRO:HG3	1:B:45:SER:O	2.02	0.59
1:E:104:MET:HB2	1:E:105:PRO:HD3	1.84	0.59
1:C:363:GLY:O	1:C:367:ARG:HD2	2.02	0.59
1:C:146:THR:HB	1:C:402:LEU:HG	1.84	0.59
1:E:196:TYR:CE1	1:E:197:ILE:HG22	2.38	0.59
1:A:237:ILE:O	1:A:256:LYS:NZ	2.30	0.59
1:F:110:SER:HB2	1:F:116:LEU:HD22	1.84	0.59
1:C:227:SER:HB2	1:C:269:LEU:HD12	1.83	0.59
1:C:33:ILE:HG23	1:C:34:LYS:HG3	1.85	0.59
1:D:213:HIS:O	1:D:217:ILE:HG12	2.03	0.59
1:E:320:TYR:O	1:E:321:TYR:HB3	2.01	0.59
1:A:227:SER:HB2	1:A:269:LEU:HD12	1.84	0.59
1:D:227:SER:HB2	1:D:269:LEU:HD12	1.83	0.59
1:A:123:TRP:CZ2	1:A:408:LEU:HD13	2.37	0.59
1:B:237:ILE:O	1:B:256:LYS:NZ	2.30	0.59
1:C:290:LYS:HG3	1:C:306:GLU:HB3	1.85	0.59
1:A:421:MET:CE	1:A:425:LEU:HD21	2.33	0.59
1:E:363:GLY:O	1:E:367:ARG:HD2	2.02	0.59
1:E:91:VAL:HG22	1:E:120:PHE:HB3	1.85	0.59
1:E:311:PHE:HB3	1:E:314:ILE:HG13	1.84	0.59
1:E:110:SER:HB2	1:E:116:LEU:HD22	1.84	0.58
1:D:146:THR:HB	1:D:402:LEU:HG	1.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD11	1:A:218:LEU:HD22	1.84	0.58
1:F:363:GLY:O	1:F:367:ARG:HD2	2.03	0.58
1:C:213:HIS:O	1:C:217:ILE:HG12	2.03	0.58
1:E:156:PRO:HG3	1:E:367:ARG:NH1	2.18	0.58
1:D:33:ILE:HG23	1:D:34:LYS:HG3	1.84	0.58
1:E:227:SER:HB2	1:E:269:LEU:HD12	1.85	0.58
1:B:213:HIS:O	1:B:217:ILE:HG12	2.04	0.58
1:A:19:ARG:HG3	1:A:88:ASP:OD2	2.03	0.58
1:F:146:THR:OG1	1:F:401:THR:HB	2.03	0.58
1:A:213:HIS:O	1:A:217:ILE:HG12	2.04	0.58
1:D:290:LYS:HG3	1:D:306:GLU:HB3	1.84	0.58
1:F:104:MET:HB2	1:F:105:PRO:HD3	1.85	0.58
1:E:27:ALA:HB2	1:E:63:THR:HG23	1.86	0.58
1:F:26:ASN:O	1:F:33:ILE:HB	2.03	0.58
1:A:286:LYS:HD3	1:B:297:HIS:CE1	2.38	0.58
1:F:27:ALA:HB2	1:F:63:THR:HG23	1.86	0.58
1:B:347:LYS:C	1:B:347:LYS:CD	2.72	0.57
1:F:91:VAL:HG22	1:F:120:PHE:HB3	1.86	0.57
1:A:89:MET:HE1	1:A:372:ILE:HG21	1.85	0.57
1:F:18:ILE:HD12	1:F:47:PHE:CE2	2.39	0.57
1:D:410:ARG:HH22	1:D:433:TYR:HD1	1.53	0.57
1:E:35:THR:HA	1:E:362:VAL:HG22	1.86	0.57
1:D:347:LYS:N	1:D:348:GLU:CB	2.64	0.57
1:F:320:TYR:O	1:F:321:TYR:HB3	2.03	0.57
1:E:121:VAL:O	1:E:148:ILE:HD12	2.04	0.57
1:B:427:VAL:O	1:B:427:VAL:HG13	2.02	0.57
1:F:153:ARG:HG2	1:F:220:TYR:CG	2.39	0.57
1:A:33:ILE:HG23	1:A:34:LYS:HG3	1.85	0.57
1:B:123:TRP:CZ2	1:B:408:LEU:HD13	2.40	0.57
1:E:314:ILE:HD12	1:E:314:ILE:O	2.04	0.57
1:B:123:TRP:CD2	1:B:124:ALA:HA	2.39	0.57
1:C:27:ALA:CB	1:C:67:LEU:HD21	2.35	0.57
1:C:256:LYS:HE3	1:C:260:ASP:HB3	1.87	0.57
1:F:285:THR:HB	1:F:291:ASN:HD21	1.68	0.57
1:E:145:GLN:NE2	1:E:389:PHE:H	2.03	0.57
1:C:123:TRP:CZ2	1:C:408:LEU:HD13	2.39	0.57
1:B:421:MET:CE	1:B:425:LEU:HD21	2.35	0.56
1:C:297:HIS:CE1	1:D:286:LYS:HD3	2.40	0.56
1:E:411:LEU:O	1:E:415:VAL:HG23	2.05	0.56
1:E:147:ILE:HD13	1:E:372:ILE:HD13	1.86	0.56
1:E:423:SER:HA	1:F:423:SER:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:VAL:HG13	1:A:427:VAL:O	2.04	0.56
1:C:188:GLU:HB3	1:C:243:ILE:HG12	1.87	0.56
1:E:153:ARG:O	1:E:154:LYS:HD3	2.05	0.56
1:D:18:ILE:HD11	1:D:376:HIS:CG	2.40	0.56
1:E:256:LYS:HE2	1:E:258:VAL:O	2.05	0.56
1:D:421:MET:CE	1:D:425:LEU:HD21	2.35	0.56
1:E:377:PHE:O	1:E:379:THR:N	2.39	0.56
1:E:262:LEU:HD12	1:E:263:LEU:O	2.05	0.56
1:F:176:ILE:HB	1:F:275:VAL:HG22	1.87	0.56
1:C:421:MET:CE	1:C:425:LEU:HD21	2.35	0.56
1:D:18:ILE:HD11	1:D:376:HIS:CD2	2.41	0.56
1:F:121:VAL:O	1:F:148:ILE:HD12	2.06	0.56
1:E:309:ALA:O	1:E:311:PHE:N	2.39	0.56
1:D:145:GLN:NE2	1:D:388:GLN:HG3	2.20	0.56
1:A:37:TYR:HB3	1:A:38:PRO:HD3	1.88	0.56
1:C:60:SER:O	1:C:64:ILE:HG13	2.06	0.56
1:D:317:LEU:O	1:D:354:HIS:HD2	1.89	0.56
1:E:191:VAL:HG23	1:E:243:ILE:O	2.06	0.56
1:B:363:GLY:O	1:B:367:ARG:HD2	2.06	0.56
1:A:297:HIS:NE2	1:B:286:LYS:HD3	2.21	0.55
1:B:33:ILE:HG23	1:B:34:LYS:HG3	1.88	0.55
1:E:96:VAL:HA	1:E:99:HIS:CD2	2.41	0.55
1:E:285:THR:HB	1:E:291:ASN:HD21	1.70	0.55
1:E:304:LYS:HG2	1:E:305:LEU:N	2.16	0.55
1:D:27:ALA:CB	1:D:67:LEU:HD21	2.36	0.55
1:A:60:SER:O	1:A:64:ILE:HG13	2.05	0.55
1:F:227:SER:HB2	1:F:269:LEU:HD12	1.89	0.55
1:F:122:GLU:HA	1:F:149:SER:HB3	1.88	0.55
1:B:60:SER:O	1:B:64:ILE:HG13	2.07	0.55
1:D:37:TYR:HB3	1:D:38:PRO:HD3	1.88	0.55
1:E:290:LYS:HG3	1:E:306:GLU:HB3	1.88	0.55
1:F:410:ARG:HB3	1:F:430:ILE:HD12	1.89	0.55
1:E:146:THR:OG1	1:E:401:THR:HB	2.07	0.55
1:B:64:ILE:HG23	1:B:72:ALA:HB3	1.88	0.55
1:D:155:SER:HB3	1:D:158:ILE:HD13	1.88	0.54
1:F:96:VAL:HA	1:F:99:HIS:CD2	2.42	0.54
1:E:413:GLU:O	1:E:417:LYS:HB2	2.07	0.54
1:E:297:HIS:CE1	1:F:286:LYS:HG2	2.42	0.54
1:E:322:SER:OG	1:E:323:GLY:N	2.41	0.54
1:B:375:PHE:CZ	1:B:387:SER:O	2.60	0.54
1:F:236:ASN:O	1:F:238:PRO:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG22	1:A:259:PRO:CD	2.38	0.54
1:A:256:LYS:HD2	1:A:258:VAL:HG12	1.89	0.54
1:B:256:LYS:HG2	1:B:258:VAL:H	1.73	0.54
1:E:264:PHE:O	1:E:265:GLN:HB2	2.06	0.53
1:D:256:LYS:HD2	1:D:258:VAL:HG12	1.90	0.53
1:E:153:ARG:HD2	1:E:400:PRO:HG3	1.90	0.53
1:B:375:PHE:HZ	1:B:387:SER:O	1.91	0.53
1:D:188:GLU:HB3	1:D:243:ILE:HG12	1.90	0.53
1:B:256:LYS:HE3	1:B:260:ASP:HB3	1.90	0.53
1:C:37:TYR:HB3	1:C:38:PRO:HD3	1.91	0.53
1:B:120:PHE:HD2	1:B:121:VAL:N	2.07	0.53
1:F:96:VAL:HG13	1:F:124:ALA:O	2.08	0.53
1:E:96:VAL:HG13	1:E:124:ALA:O	2.08	0.53
1:B:256:LYS:HD2	1:B:258:VAL:HG12	1.90	0.53
1:C:155:SER:HB3	1:C:158:ILE:HD13	1.90	0.53
1:F:82:ALA:HB2	1:F:106:LEU:HG	1.91	0.53
1:F:264:PHE:CG	1:F:265:GLN:N	2.77	0.53
1:C:57:ILE:HD12	1:C:76:PRO:CA	2.36	0.53
1:F:361:ILE:CD1	1:F:361:ILE:H	2.20	0.53
1:E:190:PRO:HA	1:E:243:ILE:HD12	1.90	0.53
1:A:64:ILE:HG23	1:A:72:ALA:HB3	1.91	0.53
1:E:262:LEU:HD12	1:E:262:LEU:C	2.29	0.53
1:E:123:TRP:CH2	1:E:408:LEU:HD13	2.43	0.53
1:A:317:LEU:O	1:A:354:HIS:HD2	1.92	0.53
1:C:287:LYS:HE3	1:D:348:GLU:OE1	2.09	0.53
1:E:427:VAL:HG12	1:E:430:ILE:HG12	1.88	0.53
1:D:427:VAL:CG1	1:D:427:VAL:O	2.57	0.53
1:B:283:LYS:HA	1:B:284:PRO:C	2.28	0.53
1:E:122:GLU:HA	1:E:149:SER:HB3	1.90	0.52
1:F:262:LEU:HD12	1:F:262:LEU:C	2.28	0.52
1:F:264:PHE:O	1:F:265:GLN:HB2	2.08	0.52
1:A:57:ILE:HD12	1:A:76:PRO:CA	2.37	0.52
1:C:427:VAL:O	1:C:427:VAL:HG13	2.09	0.52
1:A:242:LEU:HD12	1:A:252:GLN:HG2	1.92	0.52
1:A:188:GLU:HB3	1:A:243:ILE:HG12	1.92	0.52
1:B:155:SER:HB3	1:B:158:ILE:HD13	1.91	0.52
1:D:361:ILE:H	1:D:361:ILE:HD12	1.75	0.52
1:D:324:THR:O	1:D:324:THR:CG2	2.55	0.52
1:E:92:ILE:HB	1:E:121:VAL:HG22	1.92	0.52
1:D:432:HIS:O	1:D:433:TYR:HB2	2.09	0.52
1:F:123:TRP:CH2	1:F:408:LEU:HD13	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:PHE:HD2	1:D:121:VAL:N	2.07	0.51
1:B:37:TYR:HB3	1:B:38:PRO:HD3	1.92	0.51
1:D:258:VAL:HG22	1:D:259:PRO:CD	2.41	0.51
1:F:161:ALA:O	1:F:165:ILE:HG13	2.10	0.51
1:B:188:GLU:HB3	1:B:243:ILE:HG12	1.92	0.51
1:C:256:LYS:HG2	1:C:258:VAL:H	1.75	0.51
1:A:256:LYS:HE3	1:A:260:ASP:HB3	1.92	0.51
1:E:169:TYR:CE2	1:E:323:GLY:HA3	2.46	0.51
1:E:82:ALA:HB2	1:E:106:LEU:HG	1.93	0.51
1:C:64:ILE:HG23	1:C:72:ALA:HB3	1.92	0.51
1:A:426:ASN:HB3	1:C:423:SER:CB	2.40	0.51
1:D:256:LYS:HG2	1:D:258:VAL:H	1.75	0.51
1:C:286:LYS:HD3	1:D:297:HIS:CE1	2.46	0.51
1:F:155:SER:HB3	1:F:158:ILE:HB	1.92	0.51
1:E:350:MET:O	1:E:351:LYS:HG3	2.10	0.51
1:B:27:ALA:CB	1:B:67:LEU:HD21	2.37	0.51
1:D:57:ILE:HD12	1:D:76:PRO:CA	2.38	0.51
1:F:349:ILE:HG22	1:F:350:MET:N	2.25	0.51
1:F:427:VAL:CG1	1:F:427:VAL:O	2.58	0.51
1:C:317:LEU:O	1:C:354:HIS:HD2	1.93	0.51
1:A:120:PHE:HD2	1:A:121:VAL:N	2.09	0.51
1:E:361:ILE:HD12	1:E:361:ILE:H	1.76	0.51
1:F:427:VAL:HG12	1:F:427:VAL:O	2.10	0.51
1:F:153:ARG:HG2	1:F:220:TYR:CD1	2.45	0.51
1:A:256:LYS:HG2	1:A:258:VAL:H	1.75	0.51
1:C:120:PHE:HD2	1:C:121:VAL:N	2.09	0.51
1:E:54:SER:HB3	1:E:55:PRO:HD2	1.93	0.51
1:E:236:ASN:O	1:E:238:PRO:HD3	2.10	0.51
1:E:123:TRP:CZ2	1:E:408:LEU:HD13	2.46	0.51
1:E:408:LEU:HD22	1:E:412:ILE:HD11	1.92	0.51
1:A:16:ALA:N	1:A:17:PRO:HD3	2.26	0.51
1:D:35:THR:HB	1:D:365:ILE:HG13	1.93	0.51
1:E:264:PHE:CG	1:E:265:GLN:N	2.78	0.50
1:F:303:LEU:HD23	1:F:304:LYS:N	2.25	0.50
1:E:258:VAL:HG13	1:E:259:PRO:CD	2.40	0.50
1:E:413:GLU:HA	1:E:413:GLU:OE1	2.11	0.50
1:D:283:LYS:HA	1:D:284:PRO:C	2.32	0.50
1:C:256:LYS:HD2	1:C:258:VAL:HG12	1.93	0.50
1:D:123:TRP:CZ2	1:D:408:LEU:HD13	2.46	0.50
1:E:169:TYR:HE2	1:E:322:SER:O	1.94	0.50
1:B:361:ILE:HD12	1:B:361:ILE:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:THR:O	1:A:325:ARG:C	2.50	0.50
1:B:18:ILE:HD11	1:B:376:HIS:CG	2.46	0.50
1:A:417:LYS:HZ3	1:C:417:LYS:HG3	1.76	0.50
1:A:155:SER:HB3	1:A:158:ILE:HD13	1.93	0.50
1:D:256:LYS:HE3	1:D:260:ASP:HB3	1.92	0.50
1:B:35:THR:HB	1:B:365:ILE:HG13	1.94	0.50
1:B:258:VAL:HG22	1:B:259:PRO:CD	2.42	0.50
1:E:106:LEU:C	1:E:106:LEU:HD23	2.32	0.50
1:A:27:ALA:CB	1:A:67:LEU:HD21	2.37	0.50
1:B:178:ILE:CD1	1:B:218:LEU:HD22	2.41	0.50
1:E:320:TYR:HB3	1:F:288:PHE:CD2	2.47	0.50
1:B:242:LEU:HD12	1:B:252:GLN:HG2	1.94	0.50
1:D:64:ILE:HG23	1:D:72:ALA:HB3	1.93	0.49
1:F:102:VAL:O	1:F:105:PRO:HD2	2.11	0.49
1:A:35:THR:HB	1:A:365:ILE:HG13	1.93	0.49
1:A:79:GLU:HG3	1:A:109:PHE:CD2	2.46	0.49
1:F:145:GLN:HE22	1:F:389:PHE:H	1.60	0.49
1:E:102:VAL:O	1:E:105:PRO:HD2	2.12	0.49
1:D:323:GLY:O	1:D:324:THR:C	2.50	0.49
1:F:322:SER:CB	1:F:350:MET:HG2	2.43	0.49
1:E:65:GLN:O	1:E:66:ARG:C	2.51	0.49
1:F:390:VAL:HG13	1:F:391:MET:HG2	1.94	0.49
1:B:427:VAL:O	1:B:427:VAL:CG1	2.60	0.49
1:F:21:GLY:H	1:F:87:ILE:HG23	1.78	0.49
1:F:123:TRP:CZ2	1:F:408:LEU:HD13	2.47	0.49
1:F:54:SER:HB3	1:F:55:PRO:HD2	1.93	0.49
1:B:317:LEU:O	1:B:354:HIS:HD2	1.95	0.49
1:C:408:LEU:O	1:C:412:ILE:HG12	2.13	0.49
1:C:35:THR:HB	1:C:365:ILE:HG13	1.95	0.49
1:E:182:GLY:O	1:E:184:TRP:N	2.39	0.49
1:B:57:ILE:HD12	1:B:76:PRO:CA	2.42	0.49
1:C:258:VAL:HG22	1:C:259:PRO:CD	2.42	0.49
1:F:351:LYS:O	1:F:352:VAL:HG23	2.12	0.49
1:A:158:ILE:HG12	1:A:217:ILE:CG2	2.41	0.49
1:F:155:SER:HB3	1:F:158:ILE:HD13	1.94	0.48
1:C:207:VAL:O	1:C:211:PHE:HB3	2.13	0.48
1:A:197:ILE:HG12	1:A:198:TYR:CE1	2.48	0.48
1:F:60:SER:HB3	1:F:74:ALA:HB1	1.95	0.48
1:A:427:VAL:CG1	1:A:427:VAL:O	2.62	0.48
1:F:258:VAL:HG13	1:F:259:PRO:CD	2.42	0.48
1:C:158:ILE:HG12	1:C:217:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG22	1:A:259:PRO:HD3	1.95	0.48
1:B:145:GLN:HE21	1:B:388:GLN:HG3	1.78	0.48
1:A:123:TRP:CH2	1:A:408:LEU:HD13	2.49	0.48
1:A:322:SER:HB3	1:A:350:MET:HG2	1.96	0.48
1:C:242:LEU:HD12	1:C:252:GLN:HG2	1.95	0.48
1:C:322:SER:OG	1:D:287:LYS:HG3	2.13	0.48
1:E:295:ASP:OD1	1:E:304:LYS:HE2	2.14	0.48
1:E:354:HIS:CD2	1:E:355:LEU:N	2.82	0.48
1:F:302:ASP:O	1:F:303:LEU:HB2	2.14	0.48
1:F:65:GLN:O	1:F:66:ARG:C	2.51	0.48
1:C:123:TRP:CH2	1:C:408:LEU:HD13	2.48	0.48
1:B:408:LEU:O	1:B:412:ILE:HG12	2.13	0.48
1:F:106:LEU:C	1:F:106:LEU:HD23	2.34	0.48
1:A:433:TYR:C	1:A:435:LEU:H	2.17	0.48
1:A:387:SER:O	1:A:388:GLN:C	2.51	0.48
1:C:361:ILE:HD12	1:C:361:ILE:H	1.79	0.48
1:D:158:ILE:HG12	1:D:217:ILE:CG2	2.43	0.48
1:E:123:TRP:CD2	1:E:124:ALA:N	2.65	0.48
1:F:179:ALA:HB1	1:F:286:LYS:NZ	2.29	0.48
1:D:258:VAL:HG22	1:D:259:PRO:HD3	1.96	0.48
1:A:283:LYS:HA	1:A:284:PRO:C	2.34	0.48
1:E:352:VAL:CG1	1:E:353:TYR:N	2.76	0.48
1:F:363:GLY:O	1:F:366:HIS:HB3	2.14	0.48
1:C:283:LYS:HA	1:C:284:PRO:C	2.34	0.48
1:E:286:LYS:HG2	1:F:297:HIS:CE1	2.49	0.47
1:F:147:ILE:HD13	1:F:372:ILE:HD13	1.96	0.47
1:D:242:LEU:HD12	1:D:252:GLN:HG2	1.96	0.47
1:B:197:ILE:HG12	1:B:198:TYR:CE1	2.49	0.47
1:D:108:GLU:OE2	1:D:108:GLU:HA	2.14	0.47
1:F:349:ILE:HD12	1:F:349:ILE:H	1.79	0.47
1:B:231:ALA:CB	1:B:415:VAL:HG13	2.44	0.47
1:D:76:PRO:HD2	1:D:80:SER:OG	2.15	0.47
1:E:243:ILE:HD12	1:E:243:ILE:O	2.14	0.47
1:B:106:LEU:C	1:B:106:LEU:HD23	2.34	0.47
1:F:314:ILE:HD12	1:F:314:ILE:O	2.14	0.47
1:F:361:ILE:HD12	1:F:361:ILE:N	2.22	0.47
1:A:417:LYS:NZ	1:C:417:LYS:HG3	2.29	0.47
1:B:217:ILE:H	1:B:217:ILE:HG12	1.45	0.47
1:B:417:LYS:O	1:B:421:MET:HG3	2.15	0.47
1:E:174:ASN:ND2	1:F:187:TYR:CE1	2.83	0.47
1:C:79:GLU:HG3	1:C:109:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:SER:O	1:C:388:GLN:C	2.53	0.47
1:F:349:ILE:CG2	1:F:350:MET:N	2.77	0.47
1:E:367:ARG:O	1:E:370:GLN:HB3	2.15	0.47
1:A:423:SER:CB	1:C:426:ASN:HB3	2.45	0.47
1:C:181:ASN:OD1	1:C:282:GLY:HA2	2.15	0.47
1:F:181:ASN:ND2	1:F:280:LYS:HB3	2.29	0.47
1:C:314:ILE:HD12	1:C:314:ILE:O	2.15	0.47
1:C:145:GLN:NE2	1:C:388:GLN:HG3	2.29	0.47
1:A:265:GLN:NE2	1:B:265:GLN:HB2	2.30	0.47
1:F:237:ILE:O	1:F:256:LYS:NZ	2.48	0.47
1:E:376:HIS:CD2	1:E:377:PHE:CE1	2.96	0.47
1:A:434:SER:O	1:A:435:LEU:C	2.53	0.47
1:F:147:ILE:HG21	1:F:372:ILE:HD11	1.97	0.47
1:E:174:ASN:HD22	1:F:187:TYR:HE1	1.62	0.47
1:A:286:LYS:HD3	1:B:297:HIS:NE2	2.30	0.46
1:A:361:ILE:H	1:A:361:ILE:HD12	1.79	0.46
1:B:145:GLN:NE2	1:B:388:GLN:HG3	2.30	0.46
1:F:181:ASN:OD1	1:F:282:GLY:HA2	2.15	0.46
1:E:349:ILE:HD12	1:E:349:ILE:N	2.30	0.46
1:A:283:LYS:HB3	1:A:284:PRO:HA	1.97	0.46
1:F:23:VAL:HG23	1:F:81:PHE:CZ	2.51	0.46
1:D:256:LYS:HE2	1:D:258:VAL:O	2.15	0.46
1:F:153:ARG:HD3	1:F:392:GLN:OE1	2.14	0.46
1:E:363:GLY:O	1:E:366:HIS:HB3	2.15	0.46
1:F:200:ILE:HG12	1:F:201:GLY:N	2.30	0.46
1:B:158:ILE:HG12	1:B:217:ILE:CG2	2.44	0.46
1:F:27:ALA:CB	1:F:67:LEU:HD21	2.46	0.46
1:F:147:ILE:HD13	1:F:372:ILE:CD1	2.45	0.46
1:E:181:ASN:OD1	1:E:282:GLY:HA2	2.16	0.46
1:E:21:GLY:H	1:E:87:ILE:HG23	1.80	0.46
1:F:122:GLU:HA	1:F:149:SER:CB	2.45	0.46
1:B:349:ILE:O	1:B:349:ILE:HG22	2.15	0.46
1:E:27:ALA:CB	1:E:67:LEU:HD21	2.46	0.46
1:C:231:ALA:CB	1:C:415:VAL:HG13	2.46	0.46
1:F:306:GLU:O	1:F:317:LEU:HD22	2.16	0.46
1:A:430:ILE:HA	1:A:430:ILE:HD13	1.66	0.46
1:E:122:GLU:HA	1:E:149:SER:CB	2.46	0.46
1:E:200:ILE:HG12	1:E:201:GLY:N	2.31	0.46
1:D:106:LEU:HD23	1:D:106:LEU:C	2.36	0.46
1:E:237:ILE:O	1:E:256:LYS:NZ	2.49	0.46
1:C:256:LYS:HE2	1:C:258:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:ILE:HB	1:F:121:VAL:HG22	1.97	0.46
1:A:108:GLU:HA	1:A:108:GLU:OE2	2.16	0.46
1:F:264:PHE:CD2	1:F:265:GLN:N	2.84	0.45
1:F:320:TYR:CD2	1:F:352:VAL:HG22	2.51	0.45
1:A:197:ILE:HG12	1:A:198:TYR:CD1	2.51	0.45
1:B:207:VAL:O	1:B:211:PHE:HB3	2.14	0.45
1:B:79:GLU:HG3	1:B:109:PHE:CD2	2.51	0.45
1:A:147:ILE:HG12	1:A:399:PHE:CE2	2.51	0.45
1:F:147:ILE:HG12	1:F:399:PHE:CE2	2.51	0.45
1:E:232:MET:HB2	1:E:263:LEU:HB2	1.98	0.45
1:B:76:PRO:HD2	1:B:80:SER:OG	2.17	0.45
1:F:96:VAL:HG11	1:F:124:ALA:HB1	1.98	0.45
1:A:408:LEU:O	1:A:412:ILE:HG12	2.17	0.45
1:F:178:ILE:HB	1:F:277:CYS:SG	2.57	0.45
1:A:313:GLU:HG2	1:A:314:ILE:HG23	1.99	0.45
1:D:408:LEU:O	1:D:412:ILE:HG12	2.15	0.45
1:C:197:ILE:O	1:C:197:ILE:HG13	2.16	0.45
1:E:60:SER:HB3	1:E:74:ALA:HB1	1.97	0.45
1:D:181:ASN:OD1	1:D:282:GLY:HA2	2.16	0.45
1:C:178:ILE:CD1	1:C:218:LEU:HD22	2.45	0.45
1:B:256:LYS:HE2	1:B:258:VAL:O	2.16	0.45
1:B:210:THR:HG1	1:B:311:PHE:HE1	1.64	0.45
1:D:313:GLU:HG2	1:D:314:ILE:HG23	1.98	0.45
1:D:58:GLU:HG3	1:D:58:GLU:H	1.48	0.45
1:D:83:SER:OG	1:D:112:ASN:HB2	2.16	0.45
1:B:123:TRP:CH2	1:B:408:LEU:HD13	2.51	0.45
1:B:197:ILE:HG12	1:B:198:TYR:CD1	2.51	0.45
1:B:197:ILE:O	1:B:197:ILE:HG13	2.17	0.45
1:D:207:VAL:O	1:D:211:PHE:HB3	2.16	0.45
1:E:163:GLU:O	1:E:167:GLN:HG3	2.16	0.45
1:C:58:GLU:H	1:C:58:GLU:HG3	1.51	0.45
1:F:236:ASN:C	1:F:238:PRO:HD3	2.36	0.45
1:C:83:SER:OG	1:C:112:ASN:HB2	2.17	0.45
1:B:145:GLN:HE22	1:B:389:PHE:H	1.64	0.45
1:B:108:GLU:HA	1:B:108:GLU:OE2	2.17	0.45
1:A:83:SER:OG	1:A:112:ASN:HB2	2.17	0.45
1:E:311:PHE:HD1	1:E:313:GLU:OE2	2.00	0.45
1:D:197:ILE:HG12	1:D:198:TYR:CE1	2.51	0.45
1:D:283:LYS:HB3	1:D:284:PRO:HA	1.97	0.45
1:B:181:ASN:OD1	1:B:282:GLY:HA2	2.16	0.45
1:F:157:TYR:CD1	1:F:157:TYR:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD23	1:A:106:LEU:C	2.38	0.45
1:E:236:ASN:C	1:E:238:PRO:HD3	2.37	0.44
1:F:60:SER:HB3	1:F:74:ALA:CB	2.46	0.44
1:B:83:SER:OG	1:B:112:ASN:HB2	2.17	0.44
1:E:147:ILE:HG21	1:E:372:ILE:HD11	1.99	0.44
1:A:322:SER:OG	1:B:287:LYS:HG3	2.18	0.44
1:C:432:HIS:O	1:C:433:TYR:O	2.35	0.44
1:F:170:ILE:HB	1:F:301:GLY:O	2.17	0.44
1:C:106:LEU:C	1:C:106:LEU:HD23	2.37	0.44
1:C:108:GLU:HA	1:C:108:GLU:OE2	2.16	0.44
1:D:197:ILE:HG12	1:D:198:TYR:CD1	2.52	0.44
1:F:411:LEU:O	1:F:415:VAL:HG23	2.17	0.44
1:A:417:LYS:HG3	1:C:417:LYS:NZ	2.30	0.44
1:A:417:LYS:O	1:A:421:MET:HG3	2.17	0.44
1:F:190:PRO:HA	1:F:243:ILE:HD12	1.99	0.44
1:C:76:PRO:HD2	1:C:80:SER:OG	2.18	0.44
1:A:89:MET:HB2	1:A:118:TYR:HB2	2.00	0.44
1:A:197:ILE:O	1:A:197:ILE:HG13	2.18	0.44
1:B:193:SER:HA	1:B:194:PRO:HD3	1.75	0.44
1:E:23:VAL:HG23	1:E:81:PHE:CZ	2.51	0.44
1:F:262:LEU:O	1:F:262:LEU:HG	2.17	0.44
1:E:156:PRO:HG3	1:E:367:ARG:CZ	2.48	0.44
1:B:258:VAL:HG22	1:B:259:PRO:HD3	1.99	0.44
1:C:110:SER:HB2	1:C:116:LEU:HD22	1.99	0.44
1:C:376:HIS:HD2	1:C:377:PHE:CD1	2.36	0.44
1:E:129:LEU:HD12	1:E:413:GLU:HG2	1.99	0.44
1:C:427:VAL:O	1:C:427:VAL:CG1	2.65	0.44
1:B:110:SER:HB2	1:B:116:LEU:HD22	1.99	0.44
1:F:241:GLU:HG2	1:F:249:ARG:HD3	1.98	0.44
1:D:231:ALA:CB	1:D:415:VAL:HG13	2.48	0.44
1:B:147:ILE:HG12	1:B:399:PHE:CE2	2.52	0.44
1:B:243:ILE:CG2	1:B:249:ARG:HG2	2.48	0.43
1:A:178:ILE:HB	1:A:277:CYS:SG	2.58	0.43
1:F:262:LEU:HD12	1:F:263:LEU:C	2.38	0.43
1:B:430:ILE:HA	1:B:430:ILE:HD13	1.66	0.43
1:B:283:LYS:HB3	1:B:284:PRO:HA	2.00	0.43
1:A:265:GLN:HB2	1:B:265:GLN:NE2	2.34	0.43
1:E:420:MET:HE3	1:E:420:MET:HB2	1.82	0.43
1:F:160:ARG:NH1	1:F:353:TYR:CE1	2.86	0.43
1:C:197:ILE:HG12	1:C:198:TYR:CE1	2.53	0.43
1:E:178:ILE:HD11	1:E:218:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:TRP:HE1	1:F:209:THR:HA	1.84	0.43
1:E:147:ILE:HG12	1:E:399:PHE:CE2	2.53	0.43
1:F:50:THR:HG21	1:F:86:THR:O	2.18	0.43
1:B:245:GLU:HA	1:B:245:GLU:OE1	2.18	0.43
1:B:58:GLU:HG3	1:B:58:GLU:H	1.48	0.43
1:A:76:PRO:HD2	1:A:80:SER:OG	2.19	0.43
1:A:155:SER:HA	1:A:364:ASN:ND2	2.33	0.43
1:E:115:ASN:HD22	1:E:115:ASN:HA	1.52	0.43
1:C:417:LYS:O	1:C:421:MET:HG3	2.17	0.43
1:C:217:ILE:HG12	1:C:217:ILE:H	1.46	0.43
1:E:60:SER:HB3	1:E:74:ALA:CB	2.48	0.43
1:F:243:ILE:HD12	1:F:243:ILE:O	2.18	0.43
1:C:430:ILE:HD13	1:C:430:ILE:HA	1.64	0.43
1:F:314:ILE:HB	1:F:361:ILE:HG13	2.00	0.43
1:D:178:ILE:CD1	1:D:218:LEU:HD22	2.47	0.43
1:B:145:GLN:NE2	1:B:389:PHE:H	2.17	0.43
1:A:110:SER:HB2	1:A:116:LEU:HD22	1.99	0.43
1:D:79:GLU:HG3	1:D:109:PHE:CD2	2.54	0.43
1:D:243:ILE:CG2	1:D:249:ARG:HG2	2.49	0.43
1:E:96:VAL:HG11	1:E:124:ALA:HB1	1.99	0.43
1:F:356:ARG:O	1:F:357:ASN:HB2	2.19	0.43
1:B:89:MET:HB2	1:B:118:TYR:HB2	2.00	0.43
1:B:178:ILE:HB	1:B:277:CYS:SG	2.59	0.43
1:D:214:THR:O	1:D:217:ILE:HG13	2.19	0.43
1:E:241:GLU:HG2	1:E:249:ARG:HD3	2.01	0.43
1:F:232:MET:HB2	1:F:263:LEU:HB2	2.00	0.43
1:E:21:GLY:N	1:E:87:ILE:HG23	2.34	0.43
1:A:178:ILE:CD1	1:A:218:LEU:HD22	2.47	0.43
1:E:169:TYR:CE2	1:E:322:SER:O	2.71	0.43
1:F:397:GLU:H	1:F:397:GLU:CD	2.21	0.43
1:F:262:LEU:HD11	1:F:264:PHE:HB2	2.00	0.42
1:D:430:ILE:HA	1:D:430:ILE:HD13	1.68	0.42
1:C:190:PRO:HA	1:C:243:ILE:O	2.19	0.42
1:A:146:THR:C	1:A:147:ILE:HG13	2.40	0.42
1:C:197:ILE:HG12	1:C:198:TYR:CD1	2.54	0.42
1:F:153:ARG:O	1:F:154:LYS:HD3	2.18	0.42
1:E:353:TYR:C	1:E:353:TYR:CD2	2.92	0.42
1:D:147:ILE:HG12	1:D:399:PHE:CE2	2.54	0.42
1:A:207:VAL:O	1:A:211:PHE:HB3	2.19	0.42
1:E:75:PHE:HA	1:E:76:PRO:HD3	1.71	0.42
1:C:75:PHE:HA	1:C:76:PRO:HD3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:HA	1:A:245:GLU:OE1	2.18	0.42
1:A:417:LYS:HZ3	1:C:417:LYS:HZ3	1.66	0.42
1:E:174:ASN:ND2	1:F:187:TYR:HE1	2.15	0.42
1:C:16:ALA:N	1:C:17:PRO:HD3	2.34	0.42
1:D:347:LYS:HE2	1:D:347:LYS:HB2	1.92	0.42
1:F:160:ARG:NH1	1:F:353:TYR:HE1	2.17	0.42
1:C:243:ILE:CG2	1:C:249:ARG:HG2	2.49	0.42
1:C:285:THR:HB	1:C:291:ASN:ND2	2.29	0.42
1:E:397:GLU:H	1:E:397:GLU:CD	2.22	0.42
1:C:245:GLU:HA	1:C:245:GLU:OE1	2.18	0.42
1:A:314:ILE:O	1:A:314:ILE:HD12	2.19	0.42
1:D:245:GLU:HA	1:D:245:GLU:OE1	2.19	0.42
1:E:29:LYS:HB3	1:E:30:GLY:H	1.72	0.42
1:D:325:ARG:HG3	1:D:348:GLU:HB3	2.01	0.42
1:F:180:GLY:HA3	1:F:279:PHE:CE2	2.55	0.42
1:C:89:MET:HB2	1:C:118:TYR:HB2	2.02	0.42
1:C:189:ARG:HA	1:C:190:PRO:HD3	1.92	0.42
1:C:227:SER:HB3	1:C:267:THR:OG1	2.20	0.42
1:E:158:ILE:HD12	1:E:158:ILE:N	2.34	0.42
1:E:265:GLN:OE1	1:F:265:GLN:OE1	2.37	0.42
1:A:243:ILE:CG2	1:A:249:ARG:HG2	2.50	0.42
1:E:318:VAL:HG22	1:E:354:HIS:CG	2.55	0.42
1:A:181:ASN:OD1	1:A:282:GLY:HA2	2.20	0.42
1:B:107:LEU:HD13	1:B:107:LEU:HA	1.83	0.42
1:B:129:LEU:HA	1:B:129:LEU:HD23	1.83	0.42
1:E:264:PHE:CD2	1:E:265:GLN:N	2.88	0.42
1:A:417:LYS:HD2	1:C:417:LYS:HD2	2.02	0.42
1:F:85:SER:HA	1:F:113:ASN:OD1	2.20	0.42
1:F:115:ASN:HA	1:F:115:ASN:HD22	1.51	0.42
1:E:172:ASP:O	1:E:299:THR:HG23	2.19	0.42
1:F:197:ILE:HG13	1:F:198:TYR:CD1	2.55	0.42
1:E:207:VAL:HB	1:E:416:TYR:OH	2.20	0.41
1:C:297:HIS:CE1	1:D:286:LYS:HG2	2.54	0.41
1:F:303:LEU:HD23	1:F:303:LEU:C	2.41	0.41
1:F:95:GLN:HG2	1:F:196:TYR:OH	2.20	0.41
1:E:123:TRP:HE1	1:E:209:THR:HA	1.86	0.41
1:D:197:ILE:HG13	1:D:197:ILE:O	2.19	0.41
1:F:214:THR:O	1:F:217:ILE:CG1	2.67	0.41
1:A:231:ALA:CB	1:A:415:VAL:HG13	2.50	0.41
1:E:262:LEU:O	1:E:262:LEU:HG	2.20	0.41
1:E:288:PHE:CD2	1:F:320:TYR:HB3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:HA	1:A:243:ILE:O	2.20	0.41
1:D:89:MET:HB2	1:D:118:TYR:HB2	2.02	0.41
1:F:302:ASP:HB3	1:F:303:LEU:H	1.65	0.41
1:D:314:ILE:O	1:D:314:ILE:HD12	2.20	0.41
1:E:284:PRO:HB3	1:F:325:ARG:HH22	1.86	0.41
1:C:194:PRO:HB2	1:C:196:TYR:CD2	2.55	0.41
1:C:147:ILE:HG12	1:C:399:PHE:CE2	2.55	0.41
1:D:123:TRP:CD1	1:D:124:ALA:N	2.88	0.41
1:F:290:LYS:HG3	1:F:306:GLU:HB3	2.01	0.41
1:B:313:GLU:HG2	1:B:314:ILE:HG23	2.02	0.41
1:C:214:THR:O	1:C:217:ILE:HG13	2.20	0.41
1:C:214:THR:HA	1:C:217:ILE:HG13	2.02	0.41
1:A:432:HIS:HB2	1:A:433:TYR:H	1.47	0.41
1:F:169:TYR:CE2	1:F:323:GLY:HA3	2.55	0.41
1:D:67:LEU:H	1:D:67:LEU:HG	1.61	0.41
1:D:178:ILE:HB	1:D:277:CYS:SG	2.60	0.41
1:E:389:PHE:CE1	1:E:401:THR:HG21	2.56	0.41
1:D:210:THR:HG1	1:D:311:PHE:HE1	1.68	0.41
1:C:376:HIS:HD2	1:C:377:PHE:CE1	2.38	0.41
1:A:145:GLN:NE2	1:A:388:GLN:HG3	2.36	0.41
1:A:420:MET:SD	1:C:433:TYR:CE1	3.14	0.41
1:A:210:THR:HG1	1:A:311:PHE:HE1	1.68	0.41
1:B:148:ILE:HG22	1:B:400:PRO:HB2	2.03	0.41
1:B:190:PRO:HA	1:B:243:ILE:O	2.20	0.41
1:A:417:LYS:CG	1:C:417:LYS:HZ3	2.28	0.41
1:F:153:ARG:CD	1:F:400:PRO:HG3	2.47	0.41
1:D:214:THR:HA	1:D:217:ILE:HG13	2.03	0.41
1:F:388:GLN:O	1:F:389:PHE:HB3	2.20	0.41
1:D:110:SER:HB2	1:D:116:LEU:HD22	2.03	0.41
1:A:180:GLY:HA3	1:A:279:PHE:CE2	2.55	0.41
1:F:424:THR:HG22	1:F:425:LEU:N	2.36	0.41
1:A:230:ASN:ND2	1:B:230:ASN:ND2	2.69	0.41
1:D:75:PHE:HA	1:D:76:PRO:HD3	1.77	0.41
1:E:43:LEU:HD11	1:E:366:HIS:NE2	2.36	0.41
1:A:256:LYS:HE2	1:A:258:VAL:O	2.20	0.41
1:A:227:SER:HB3	1:A:267:THR:OG1	2.21	0.41
1:B:194:PRO:HB2	1:B:196:TYR:CD2	2.56	0.41
1:E:89:MET:HB2	1:E:118:TYR:HB2	2.03	0.41
1:E:262:LEU:HD12	1:E:263:LEU:C	2.42	0.40
1:E:389:PHE:HE1	1:E:401:THR:HG21	1.85	0.40
1:D:317:LEU:O	1:D:354:HIS:CD2	2.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:THR:O	1:C:38:PRO:HD2	2.21	0.40
1:F:200:ILE:HB	1:F:257:THR:O	2.21	0.40
1:D:180:GLY:HA3	1:D:279:PHE:CE2	2.56	0.40
1:E:408:LEU:HD23	1:E:408:LEU:HA	1.82	0.40
1:D:435:LEU:HD13	1:D:435:LEU:HA	1.87	0.40
1:B:314:ILE:HD12	1:B:314:ILE:O	2.21	0.40
1:C:113:ASN:HA	1:C:114:PRO:HD3	1.93	0.40
1:C:297:HIS:CE1	1:D:286:LYS:CD	3.03	0.40
1:D:376:HIS:C	1:D:378:ASN:H	2.24	0.40
1:C:286:LYS:HD3	1:D:297:HIS:NE2	2.36	0.40
1:E:50:THR:HG21	1:E:86:THR:O	2.21	0.40
1:E:214:THR:O	1:E:217:ILE:CG1	2.69	0.40
1:F:159:LEU:HA	1:F:159:LEU:HD23	1.98	0.40
1:E:258:VAL:HA	1:E:259:PRO:HD3	1.89	0.40
1:B:155:SER:HA	1:B:364:ASN:ND2	2.37	0.40
1:C:258:VAL:HG22	1:C:259:PRO:HD3	2.03	0.40
1:F:41:LEU:C	1:F:43:LEU:H	2.24	0.40
1:B:432:HIS:O	1:B:433:TYR:C	2.60	0.40
1:E:19:ARG:O	1:E:88:ASP:HB2	2.22	0.40
1:A:297:HIS:CE1	1:B:286:LYS:CD	3.04	0.40
1:B:264:PHE:CG	1:B:265:GLN:N	2.90	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	386/438 (88%)	356 (92%)	24 (6%)	6 (2%)	12	36
1	B	383/438 (87%)	353 (92%)	26 (7%)	4 (1%)	19	49
1	C	382/438 (87%)	350 (92%)	25 (6%)	7 (2%)	11	33
1	D	386/438 (88%)	352 (91%)	27 (7%)	7 (2%)	11	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	381/438 (87%)	304 (80%)	65 (17%)	12 (3%)	5 18
1	F	381/438 (87%)	298 (78%)	67 (18%)	16 (4%)	3 11
All	All	2299/2628 (88%)	2013 (88%)	234 (10%)	52 (2%)	8 26

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	TYR
1	C	349	ILE
1	C	378	ASN
1	C	433	TYR
1	D	124	ALA
1	E	378	ASN
1	F	378	ASN
1	D	324	THR
1	E	66	ARG
1	E	76	PRO
1	E	183	GLY
1	E	310	GLY
1	F	66	ARG
1	F	76	PRO
1	F	321	TYR
1	F	324	THR
1	A	388	GLN
1	C	388	GLN
1	E	28	ALA
1	E	309	ALA
1	F	28	ALA
1	F	302	ASP
1	A	28	ALA
1	B	52	LEU
1	B	76	PRO
1	C	28	ALA
1	D	28	ALA
1	D	388	GLN
1	E	265	GLN
1	E	321	TYR
1	F	265	GLN
1	F	303	LEU
1	F	309	ALA
1	A	76	PRO

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Mol	Chain	Res	Type
1	B	28	ALA
1	C	52	LEU
1	C	76	PRO
1	D	52	LEU
1	D	76	PRO
1	D	433	TYR
1	E	149	SER
1	E	415	VAL
1	F	149	SER
1	A	434	SER
1	F	296	ILE
1	E	296	ILE
1	F	17	PRO
1	A	430	ILE
1	F	352	VAL
1	B	430	ILE
1	F	314	ILE
1	F	55	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	338/375 (90%)	309 (91%)	29 (9%)	13	34
1	B	335/375 (89%)	305 (91%)	30 (9%)	12	31
1	C	335/375 (89%)	307 (92%)	28 (8%)	14	35
1	D	338/375 (90%)	309 (91%)	29 (9%)	13	34
1	E	333/375 (89%)	308 (92%)	25 (8%)	17	41
1	F	333/375 (89%)	311 (93%)	22 (7%)	21	48
All	All	2012/2250 (89%)	1849 (92%)	163 (8%)	15	37

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	58	GLU
1	A	65	GLN
1	A	67	LEU
1	A	83	SER
1	A	84	SER
1	A	107	LEU
1	A	120	PHE
1	A	129	LEU
1	A	151	GLN
1	A	191	VAL
1	A	193	SER
1	A	197	ILE
1	A	217	ILE
1	A	229	ILE
1	A	250	LEU
1	A	252	GLN
1	A	258	VAL
1	A	263	LEU
1	A	347	LYS
1	A	349	ILE
1	A	367	ARG
1	A	379	THR
1	A	390	VAL
1	A	408	LEU
1	A	417	LYS
1	A	427	VAL
1	A	428	SER
1	A	430	ILE
1	B	22	PHE
1	B	58	GLU
1	B	65	GLN
1	B	67	LEU
1	B	83	SER
1	B	84	SER
1	B	107	LEU
1	B	120	PHE
1	B	129	LEU
1	B	151	GLN
1	B	191	VAL
1	B	193	SER
1	B	197	ILE
1	B	217	ILE

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Mol	Chain	Res	Type
1	B	229	ILE
1	B	250	LEU
1	B	252	GLN
1	B	258	VAL
1	B	263	LEU
1	B	347	LYS
1	B	348	GLU
1	B	349	ILE
1	B	367	ARG
1	B	387	SER
1	B	390	VAL
1	B	408	LEU
1	B	417	LYS
1	B	427	VAL
1	B	428	SER
1	B	430	ILE
1	C	22	PHE
1	C	58	GLU
1	C	65	GLN
1	C	67	LEU
1	C	83	SER
1	C	84	SER
1	C	107	LEU
1	C	120	PHE
1	C	129	LEU
1	C	151	GLN
1	C	191	VAL
1	C	193	SER
1	C	197	ILE
1	C	217	ILE
1	C	229	ILE
1	C	250	LEU
1	C	252	GLN
1	C	258	VAL
1	C	263	LEU
1	C	347	LYS
1	C	349	ILE
1	C	367	ARG
1	C	390	VAL
1	C	408	LEU
1	C	417	LYS
1	C	427	VAL

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Mol	Chain	Res	Type
1	C	428	SER
1	C	430	ILE
1	D	22	PHE
1	D	58	GLU
1	D	65	GLN
1	D	67	LEU
1	D	83	SER
1	D	84	SER
1	D	107	LEU
1	D	120	PHE
1	D	129	LEU
1	D	151	GLN
1	D	191	VAL
1	D	193	SER
1	D	197	ILE
1	D	217	ILE
1	D	229	ILE
1	D	250	LEU
1	D	252	GLN
1	D	258	VAL
1	D	263	LEU
1	D	325	ARG
1	D	347	LYS
1	D	367	ARG
1	D	390	VAL
1	D	408	LEU
1	D	417	LYS
1	D	427	VAL
1	D	428	SER
1	D	430	ILE
1	D	435	LEU
1	E	34	LYS
1	E	58	GLU
1	E	67	LEU
1	E	107	LEU
1	E	115	ASN
1	E	120	PHE
1	E	129	LEU
1	E	151	GLN
1	E	217	ILE
1	E	254	VAL
1	E	262	LEU

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Mol	Chain	Res	Type
1	E	285	THR
1	E	322	SER
1	E	325	ARG
1	E	348	GLU
1	E	355	LEU
1	E	367	ARG
1	E	379	THR
1	E	408	LEU
1	E	414	SER
1	E	417	LYS
1	E	420	MET
1	E	421	MET
1	E	427	VAL
1	E	431	SER
1	F	34	LYS
1	F	58	GLU
1	F	67	LEU
1	F	70	SER
1	F	107	LEU
1	F	115	ASN
1	F	120	PHE
1	F	129	LEU
1	F	157	TYR
1	F	184	TRP
1	F	193	SER
1	F	217	ILE
1	F	254	VAL
1	F	262	LEU
1	F	285	THR
1	F	325	ARG
1	F	348	GLU
1	F	367	ARG
1	F	388	GLN
1	F	408	LEU
1	F	417	LYS
1	F	421	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	112	ASN

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Mol	Chain	Res	Type
1	A	115	ASN
1	A	145	GLN
1	A	202	ASN
1	A	219	GLN
1	A	236	ASN
1	A	252	GLN
1	A	265	GLN
1	A	272	ASN
1	A	354	HIS
1	A	357	ASN
1	A	364	ASN
1	B	65	GLN
1	B	112	ASN
1	B	115	ASN
1	B	145	GLN
1	B	202	ASN
1	B	219	GLN
1	B	230	ASN
1	B	236	ASN
1	B	252	GLN
1	B	265	GLN
1	B	272	ASN
1	B	354	HIS
1	B	364	ASN
1	B	378	ASN
1	C	65	GLN
1	C	112	ASN
1	C	115	ASN
1	C	145	GLN
1	C	202	ASN
1	C	219	GLN
1	C	236	ASN
1	C	252	GLN
1	C	265	GLN
1	C	272	ASN
1	C	354	HIS
1	C	357	ASN
1	C	364	ASN
1	D	65	GLN
1	D	112	ASN
1	D	115	ASN
1	D	145	GLN

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Mol	Chain	Res	Type
1	D	202	ASN
1	D	219	GLN
1	D	230	ASN
1	D	236	ASN
1	D	252	GLN
1	D	265	GLN
1	D	272	ASN
1	D	354	HIS
1	D	364	ASN
1	E	65	GLN
1	E	99	HIS
1	E	112	ASN
1	E	115	ASN
1	E	145	GLN
1	E	151	GLN
1	E	174	ASN
1	E	202	ASN
1	E	236	ASN
1	E	252	GLN
1	E	261	HIS
1	E	265	GLN
1	E	272	ASN
1	E	354	HIS
1	E	357	ASN
1	E	364	ASN
1	E	376	HIS
1	F	65	GLN
1	F	99	HIS
1	F	112	ASN
1	F	115	ASN
1	F	145	GLN
1	F	202	ASN
1	F	213	HIS
1	F	219	GLN
1	F	236	ASN
1	F	252	GLN
1	F	261	HIS
1	F	272	ASN
1	F	297	HIS
1	F	357	ASN
1	F	364	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	392/438 (89%)	0.43	23 (5%) 26 19	51, 88, 138, 216	0
1	B	389/438 (88%)	0.29	13 (3%) 50 43	53, 89, 131, 169	0
1	C	388/438 (88%)	0.54	28 (7%) 18 12	54, 93, 163, 296	0
1	D	392/438 (89%)	0.21	10 (2%) 59 54	20, 86, 131, 183	0
1	E	387/438 (88%)	1.06	59 (15%) 3 2	80, 129, 203, 281	0
1	F	387/438 (88%)	1.38	90 (23%) 1 0	74, 136, 215, 350	0
All	All	2335/2628 (88%)	0.65	223 (9%) 10 6	20, 102, 181, 350	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	27	ALA	9.2
1	C	57	ILE	8.1
1	C	76	PRO	7.6
1	F	29	LYS	7.0
1	E	325	ARG	6.7
1	F	48	GLN	6.5
1	F	47	PHE	6.4
1	C	49	ILE	6.4
1	F	30	GLY	6.0
1	F	325	ARG	5.5
1	F	118	TYR	5.4
1	C	116	LEU	5.3
1	F	72	ALA	5.3
1	A	30	GLY	5.2
1	F	28	ALA	5.2
1	E	68	LYS	5.1
1	F	365	ILE	5.0
1	F	25	LEU	4.8
1	B	433	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	29	LYS	4.7
1	E	82	ALA	4.6
1	E	42	GLN	4.6
1	E	321	TYR	4.6
1	E	69	LEU	4.6
1	C	144	VAL	4.6
1	E	36	HIS	4.6
1	E	277	CYS	4.5
1	E	67	LEU	4.4
1	F	37	TYR	4.4
1	F	41	LEU	4.4
1	C	30	GLY	4.3
1	F	119	LEU	4.2
1	E	52	LEU	4.2
1	F	36	HIS	4.2
1	E	25	LEU	4.1
1	E	358	TYR	4.1
1	E	324	THR	4.0
1	A	72	ALA	4.0
1	E	125	LEU	4.0
1	F	74	ALA	4.0
1	D	27	ALA	4.0
1	A	252	GLN	4.0
1	E	18	ILE	4.0
1	E	278	SER	3.9
1	C	58	GLU	3.9
1	E	24	GLY	3.8
1	F	49	ILE	3.8
1	D	325	ARG	3.8
1	F	194	PRO	3.7
1	F	61	ILE	3.7
1	F	23	VAL	3.7
1	C	61	ILE	3.6
1	E	16	ALA	3.6
1	C	369	TYR	3.6
1	F	55	PRO	3.6
1	F	369	TYR	3.6
1	C	72	ALA	3.6
1	E	309	ALA	3.5
1	E	365	ILE	3.5
1	F	319	LEU	3.5
1	F	151	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	369	TYR	3.5
1	E	72	ALA	3.5
1	F	277	CYS	3.5
1	F	375	PHE	3.5
1	F	116	LEU	3.4
1	C	376	HIS	3.4
1	F	125	LEU	3.4
1	C	29	LYS	3.4
1	B	31	TRP	3.4
1	F	90	ILE	3.4
1	C	48	GLN	3.4
1	E	319	LEU	3.4
1	A	31	TRP	3.3
1	B	380	LYS	3.3
1	A	58	GLU	3.3
1	B	245	GLU	3.3
1	F	276	SER	3.3
1	F	257	THR	3.3
1	F	53	TYR	3.3
1	F	67	LEU	3.2
1	C	252	GLN	3.2
1	E	93	ALA	3.2
1	E	399	PHE	3.2
1	E	30	GLY	3.1
1	E	89	MET	3.1
1	F	64	ILE	3.1
1	A	52	LEU	3.1
1	F	33	ILE	3.1
1	E	31	TRP	3.1
1	C	377	PHE	3.0
1	D	22	PHE	3.0
1	D	31	TRP	3.0
1	F	402	LEU	3.0
1	B	27	ALA	3.0
1	F	250	LEU	3.0
1	F	76	PRO	3.0
1	E	43	LEU	3.0
1	F	153	ARG	3.0
1	F	58	GLU	2.9
1	E	276	SER	2.9
1	B	420	MET	2.9
1	F	71	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	118	TYR	2.9
1	F	65	GLN	2.9
1	F	73	THR	2.9
1	F	150	LEU	2.9
1	F	18	ILE	2.8
1	C	321	TYR	2.8
1	D	246	ARG	2.8
1	F	24	GLY	2.8
1	F	399	PHE	2.8
1	F	35	THR	2.8
1	F	278	SER	2.8
1	C	399	PHE	2.8
1	E	156	PRO	2.8
1	F	84	SER	2.7
1	C	322	SER	2.7
1	B	94	ILE	2.7
1	B	169	TYR	2.7
1	A	56	LYS	2.7
1	F	115	ASN	2.7
1	F	292	LEU	2.7
1	F	379	THR	2.7
1	E	378	ASN	2.6
1	C	31	TRP	2.6
1	C	389	PHE	2.6
1	E	22	PHE	2.6
1	A	42	GLN	2.6
1	A	145	GLN	2.6
1	E	49	ILE	2.6
1	F	372	ILE	2.6
1	A	65	GLN	2.6
1	B	184	TRP	2.6
1	E	194	PRO	2.6
1	F	265	GLN	2.6
1	E	372	ILE	2.6
1	E	320	TYR	2.6
1	A	325	ARG	2.6
1	F	235	ASN	2.5
1	D	144	VAL	2.5
1	F	68	LYS	2.5
1	F	123	TRP	2.5
1	E	368	LEU	2.5
1	F	361	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	22	PHE	2.5
1	E	304	LYS	2.5
1	C	146	THR	2.5
1	E	29	LYS	2.5
1	E	279	PHE	2.5
1	F	295	ASP	2.5
1	F	204	VAL	2.5
1	B	423	SER	2.4
1	F	170	ILE	2.4
1	F	228	ARG	2.4
1	E	88	ASP	2.4
1	A	246	ARG	2.4
1	E	78	LEU	2.4
1	E	47	PHE	2.4
1	F	242	LEU	2.4
1	B	196	TYR	2.4
1	D	435	LEU	2.4
1	F	56	LYS	2.4
1	F	291	ASN	2.3
1	A	22	PHE	2.3
1	F	299	THR	2.3
1	E	300	LYS	2.3
1	C	107	LEU	2.3
1	F	179	ALA	2.3
1	E	294	ILE	2.3
1	D	245	GLU	2.3
1	E	74	ALA	2.3
1	F	57	ILE	2.3
1	F	89	MET	2.3
1	E	175	SER	2.3
1	F	261	HIS	2.3
1	F	307	GLY	2.3
1	F	16	ALA	2.2
1	F	31	TRP	2.2
1	E	205	ASP	2.2
1	C	118	TYR	2.2
1	C	373	SER	2.2
1	E	127	CYS	2.2
1	E	296	ILE	2.2
1	A	49	ILE	2.2
1	D	118	TYR	2.2
1	F	353	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	47	PHE	2.2
1	E	349	ILE	2.2
1	F	94	ILE	2.2
1	D	399	PHE	2.2
1	F	289	THR	2.2
1	E	62	ALA	2.2
1	F	316	ASN	2.2
1	F	376	HIS	2.2
1	A	120	PHE	2.1
1	F	244	ASP	2.1
1	A	393	GLY	2.1
1	F	263	LEU	2.1
1	E	287	LYS	2.1
1	F	294	ILE	2.1
1	B	101	GLU	2.1
1	F	122	GLU	2.1
1	F	366	HIS	2.1
1	E	177	GLU	2.1
1	E	73	THR	2.1
1	E	17	PRO	2.1
1	A	67	LEU	2.1
1	C	16	ALA	2.1
1	F	203	GLY	2.1
1	A	57	ILE	2.1
1	A	387	SER	2.1
1	C	23	VAL	2.1
1	F	169	TYR	2.0
1	C	228	ARG	2.0
1	A	55	PRO	2.0
1	A	59	THR	2.0
1	A	392	GLN	2.0
1	B	321	TYR	2.0
1	E	160	ARG	2.0
1	F	357	ASN	2.0
1	F	180	GLY	2.0
1	F	370	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.