Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 02:09 PM EDT

PDB ID	:	2AWI
Title	:	Structure of PrgX Y153C mutant
Authors	:	Shi, K.; Brown, C.K.; Gu, Z.Y.; Kozlowicz, B.k.; Dunny, G.M.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on	:	2005-09-01
Resolution	:	2.25 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 (i) symbol.

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

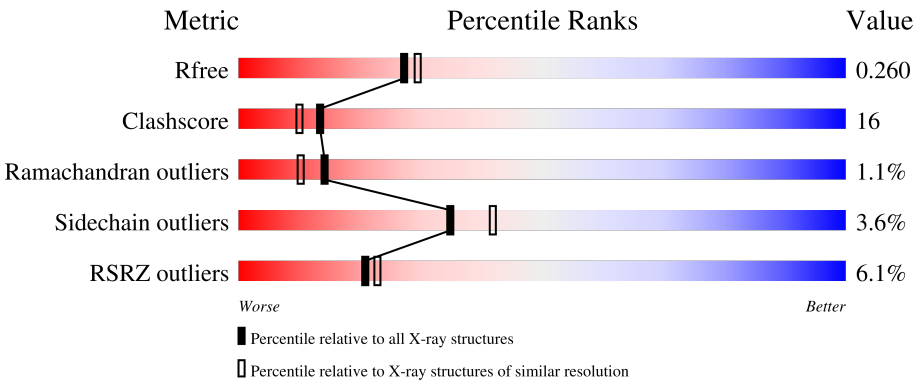
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	317	3% 68% 24% • 6%
1	B	317	4% 63% 29% • 6%
1	C	317	5% 61% 30% • 6%
1	D	317	5% 62% 31% • 6%
1	E	317	4% 67% 24% • 6%

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Mol	Chain	Length	Quality of chain
1	F	317	8% 62% 30% 6%
1	G	317	6% 65% 26% 7%
1	H	317	6% 65% 26% 7%
1	I	317	11% 57% 33% 6%
1	J	317	7% 58% 33% 7%
1	K	317	3% 66% 25% 7%
1	L	317	5% 63% 28% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 30035 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 PrgX.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	298	2461	1596	397	462	2	4	0	0	0
1	B	298	2461	1596	397	462	2	4	0	0	0
1	C	297	2450	1587	396	461	2	4	0	0	0
1	D	297	2450	1587	396	461	2	4	0	0	0
1	E	297	2450	1587	396	461	2	4	0	0	0
1	F	297	2449	1587	396	460	2	4	0	0	0
1	G	296	2441	1581	394	460	2	4	0	0	0
1	H	296	2441	1581	394	460	2	4	0	0	0
1	I	298	2461	1596	397	462	2	4	0	0	0
1	J	296	2441	1581	394	460	2	4	0	0	0
1	K	296	2441	1581	394	460	2	4	0	0	0
1	L	296	2441	1581	394	460	2	4	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MSE	MET	modified residue	UNP Q04114
A	67	MSE	MET	modified residue	UNP Q04114
A	153	CYS	TYR	engineered mutation	UNP Q04114
A	175	MSE	MET	modified residue	UNP Q04114
A	203	MSE	MET	modified residue	UNP Q04114

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	MSE	MET	modified residue	UNP Q04114
B	67	MSE	MET	modified residue	UNP Q04114
B	153	CYS	TYR	engineered mutation	UNP Q04114
B	175	MSE	MET	modified residue	UNP Q04114
B	203	MSE	MET	modified residue	UNP Q04114
C	27	MSE	MET	modified residue	UNP Q04114
C	67	MSE	MET	modified residue	UNP Q04114
C	153	CYS	TYR	engineered mutation	UNP Q04114
C	175	MSE	MET	modified residue	UNP Q04114
C	203	MSE	MET	modified residue	UNP Q04114
D	27	MSE	MET	modified residue	UNP Q04114
D	67	MSE	MET	modified residue	UNP Q04114
D	153	CYS	TYR	engineered mutation	UNP Q04114
D	175	MSE	MET	modified residue	UNP Q04114
D	203	MSE	MET	modified residue	UNP Q04114
E	27	MSE	MET	modified residue	UNP Q04114
E	67	MSE	MET	modified residue	UNP Q04114
E	153	CYS	TYR	engineered mutation	UNP Q04114
E	175	MSE	MET	modified residue	UNP Q04114
E	203	MSE	MET	modified residue	UNP Q04114
F	27	MSE	MET	modified residue	UNP Q04114
F	67	MSE	MET	modified residue	UNP Q04114
F	153	CYS	TYR	engineered mutation	UNP Q04114
F	175	MSE	MET	modified residue	UNP Q04114
F	203	MSE	MET	modified residue	UNP Q04114
G	27	MSE	MET	modified residue	UNP Q04114
G	67	MSE	MET	modified residue	UNP Q04114
G	153	CYS	TYR	engineered mutation	UNP Q04114
G	175	MSE	MET	modified residue	UNP Q04114
G	203	MSE	MET	modified residue	UNP Q04114
H	27	MSE	MET	modified residue	UNP Q04114
H	67	MSE	MET	modified residue	UNP Q04114
H	153	CYS	TYR	engineered mutation	UNP Q04114
H	175	MSE	MET	modified residue	UNP Q04114
H	203	MSE	MET	modified residue	UNP Q04114
I	27	MSE	MET	modified residue	UNP Q04114
I	67	MSE	MET	modified residue	UNP Q04114
I	153	CYS	TYR	engineered mutation	UNP Q04114
I	175	MSE	MET	modified residue	UNP Q04114
I	203	MSE	MET	modified residue	UNP Q04114
J	27	MSE	MET	modified residue	UNP Q04114
J	67	MSE	MET	modified residue	UNP Q04114

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Chain	Residue	Modelled	Actual	Comment	Reference
J	153	CYS	TYR	engineered mutation	UNP Q04114
J	175	MSE	MET	modified residue	UNP Q04114
J	203	MSE	MET	modified residue	UNP Q04114
K	27	MSE	MET	modified residue	UNP Q04114
K	67	MSE	MET	modified residue	UNP Q04114
K	153	CYS	TYR	engineered mutation	UNP Q04114
K	175	MSE	MET	modified residue	UNP Q04114
K	203	MSE	MET	modified residue	UNP Q04114
L	27	MSE	MET	modified residue	UNP Q04114
L	67	MSE	MET	modified residue	UNP Q04114
L	153	CYS	TYR	engineered mutation	UNP Q04114
L	175	MSE	MET	modified residue	UNP Q04114
L	203	MSE	MET	modified residue	UNP Q04114

- Molecule 2 is water.

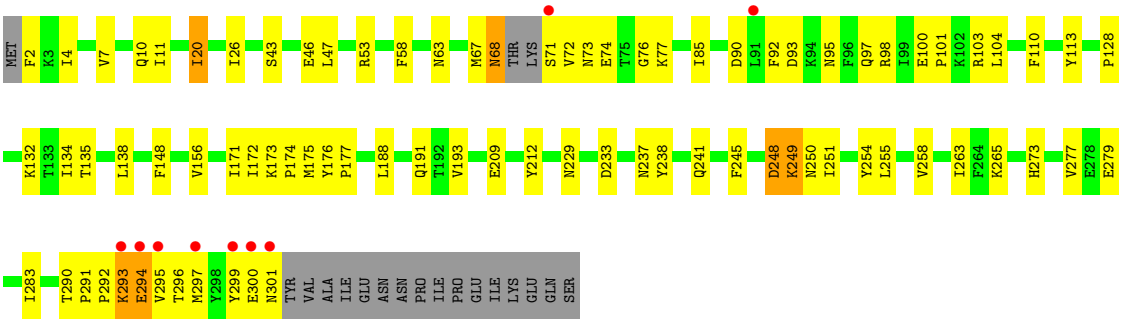
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	67	67	67	0	0
2	B	96	96	96	0	0
2	C	43	43	43	0	0
2	D	57	57	57	0	0
2	E	67	67	67	0	0
2	F	59	59	59	0	0
2	G	42	42	42	0	0
2	H	37	37	37	0	0
2	I	23	23	23	0	0
2	J	47	47	47	0	0
2	K	77	77	77	0	0
2	L	33	33	33	0	0

3 Residue-property plots (i)

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

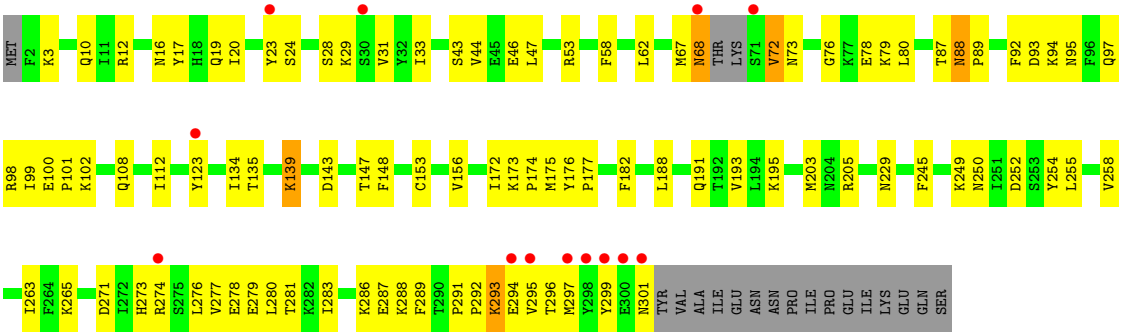
- Molecule 1: PrgX

Chain A:



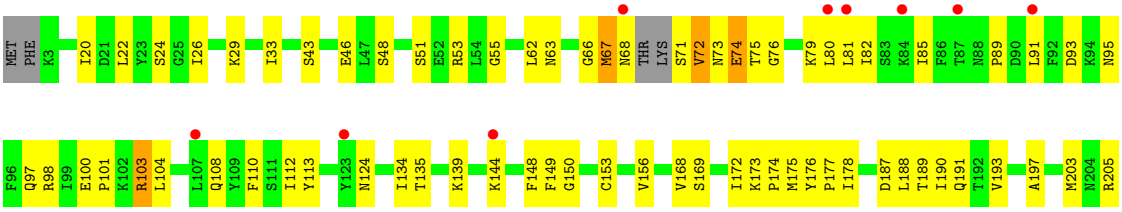
- Molecule 1: PrgX

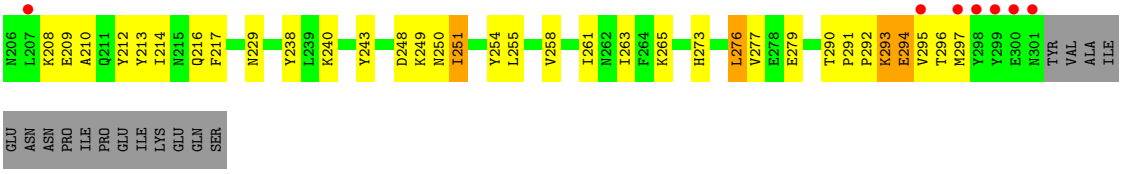
Chain B:



- Molecule 1: PrgX

Chain C:



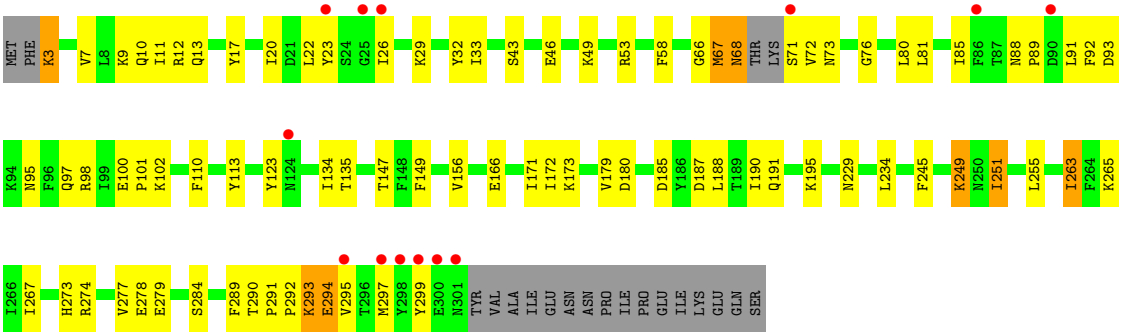


- Molecule 1: PrgX

Chain D:

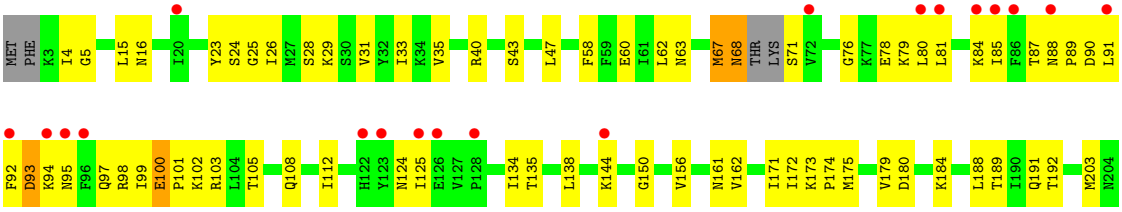
- Molecule 1: PrgX

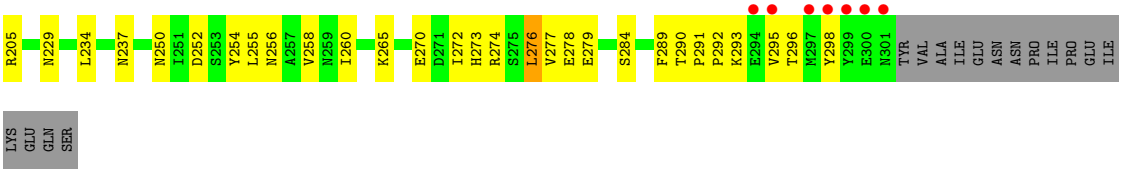
Chain E:



- Molecule 1: PrgX

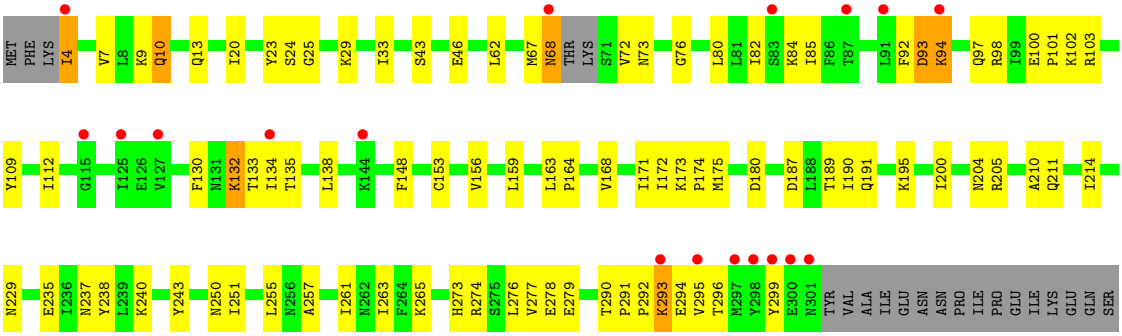
Chain F:





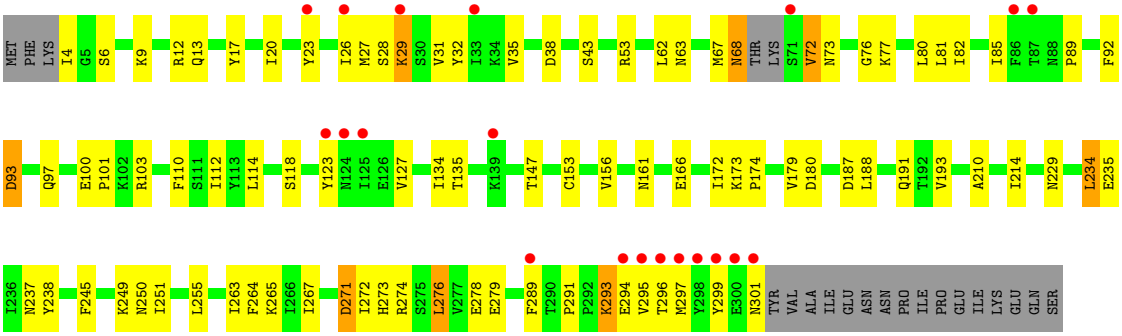
• Molecule 1: PrgX

Chain G:



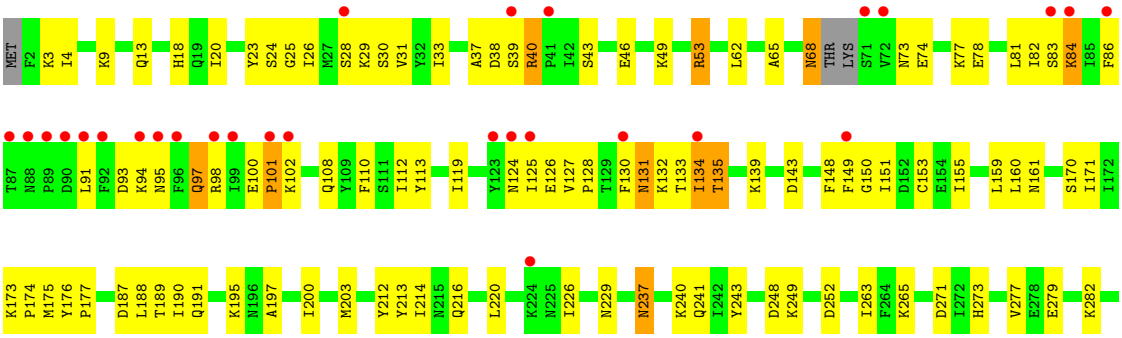
• Molecule 1: PrgX

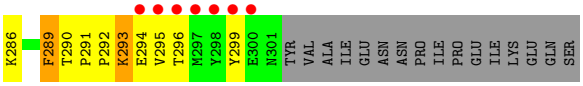
Chain H:



• Molecule 1: PrgX

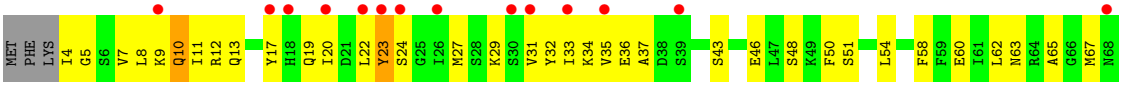
Chain I:

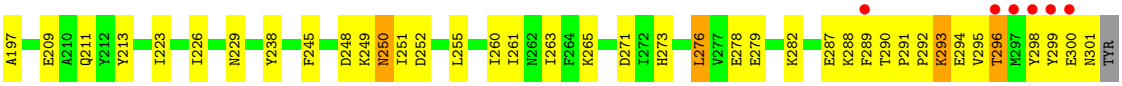




• Molecule 1: PrgX

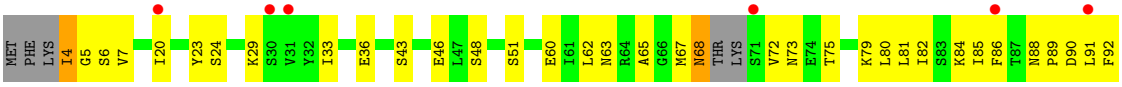
Chain J:

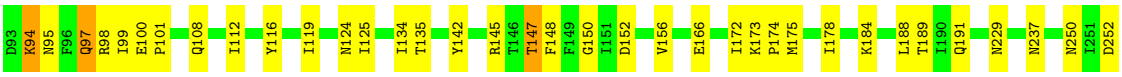


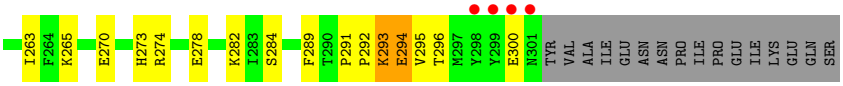


• Molecule 1: PrgX

Chain K:

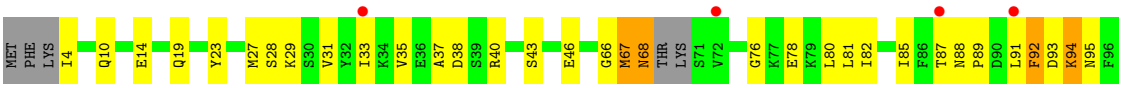


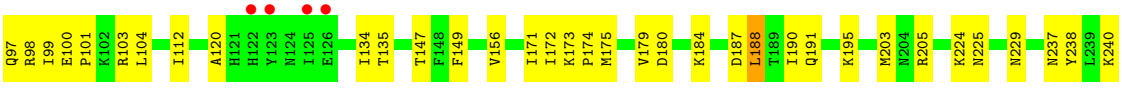


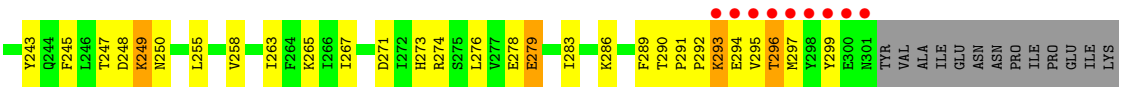


• Molecule 1: PrgX

Chain L:







GLU
GLN
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.53Å 134.37Å 195.20Å 90.00° 100.28° 90.00°	Depositor
Resolution (Å)	29.90 – 2.25 29.85 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.90-2.25) 95.4 (29.85-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.271 0.234 , 0.260	Depositor DCC
R_{free} test set	10751 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30035	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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	0.33	0/2506	0.53	0/3376
1	B	0.33	0/2506	0.54	0/3376
1	C	0.31	0/2494	0.51	0/3360
1	D	0.32	0/2494	0.52	0/3360
1	E	0.32	0/2494	0.52	0/3360
1	F	0.31	0/2493	0.52	0/3359
1	G	0.30	0/2485	0.52	0/3349
1	H	0.31	0/2485	0.52	0/3349
1	I	0.30	0/2506	0.49	0/3376
1	J	0.31	0/2485	0.51	0/3349
1	K	0.32	0/2485	0.51	0/3349
1	L	0.31	0/2485	0.52	0/3349
All	All	0.31	0/29918	0.52	0/40312

There are no bond length outliers.

There are no bond angle outliers.

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	2461	0	2493	76	0
1	B	2461	0	2493	81	0
1	C	2450	0	2484	83	0
1	D	2450	0	2484	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2450	0	2484	75	0
1	F	2449	0	2484	90	0
1	G	2441	0	2471	80	0
1	H	2441	0	2471	88	0
1	I	2461	0	2493	119	0
1	J	2441	0	2471	90	0
1	K	2441	0	2471	73	0
1	L	2441	0	2471	81	0
2	A	67	0	0	10	0
2	B	96	0	0	8	0
2	C	43	0	0	2	0
2	D	57	0	0	4	0
2	E	67	0	0	5	0
2	F	59	0	0	8	0
2	G	42	0	0	2	0
2	H	37	0	0	2	0
2	I	23	0	0	6	0
2	J	47	0	0	8	0
2	K	77	0	0	9	0
2	L	33	0	0	3	0
All	All	30035	0	29770	952	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 16.

All (952) 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:K:82:ILE:HD11	1:K:112:ILE:HG23	1.35	1.08
1:K:263:ILE:HG13	1:L:263:ILE:HG13	1.42	1.01
1:A:263:ILE:HG13	1:B:263:ILE:HG13	1.42	0.99
1:J:62:LEU:HB3	1:J:67:MSE:HG3	1.44	0.97
1:I:20:ILE:HD12	1:I:20:ILE:H	1.25	0.97
1:A:191:GLN:HE22	1:A:229:ASN:H	1.05	0.96
1:I:191:GLN:HE22	1:I:229:ASN:H	0.97	0.96
1:I:93:ASP:HB3	1:I:97:GLN:HE22	1.26	0.95
1:K:191:GLN:HE22	1:K:229:ASN:H	0.96	0.95
1:C:263:ILE:HG13	1:D:263:ILE:HG13	1.49	0.94
1:I:94:LYS:HE2	1:I:94:LYS:H	1.29	0.94
1:H:20:ILE:H	1:H:20:ILE:HD12	1.31	0.94
1:F:4:ILE:HD12	1:F:5:GLY:H	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:GLN:HE22	1:D:229:ASN:H	1.16	0.93
1:C:62:LEU:HB3	1:C:67:MSE:HG3	1.51	0.93
1:B:20:ILE:HD12	1:B:20:ILE:H	1.32	0.92
1:A:291:PRO:HB2	1:A:295:VAL:HG21	1.52	0.91
1:L:82:ILE:HD11	1:L:112:ILE:HG23	1.51	0.91
1:B:191:GLN:HE22	1:B:229:ASN:H	1.10	0.90
1:C:95:ASN:HD22	1:C:98:ARG:HH12	0.92	0.90
1:F:95:ASN:HA	1:F:98:ARG:HH12	1.36	0.89
1:J:95:ASN:HD22	1:J:98:ARG:HH22	1.15	0.89
1:A:95:ASN:HD22	1:A:98:ARG:HH12	1.14	0.89
1:E:20:ILE:HD12	1:E:20:ILE:H	1.35	0.89
1:J:191:GLN:HE22	1:J:229:ASN:H	1.21	0.89
1:F:291:PRO:HG2	1:F:296:THR:HG23	1.54	0.88
1:I:191:GLN:NE2	1:I:229:ASN:H	1.74	0.86
1:G:156:VAL:HG21	1:G:172:ILE:HG12	1.58	0.86
1:G:191:GLN:HE22	1:G:229:ASN:H	1.19	0.85
1:C:293:LYS:HD3	1:C:294:GLU:H	1.39	0.85
1:F:28:SER:HB3	1:F:31:VAL:HG23	1.56	0.85
1:F:191:GLN:HE22	1:F:229:ASN:H	1.24	0.85
1:C:95:ASN:ND2	1:C:98:ARG:HH12	1.74	0.84
1:A:68:ASN:HD22	1:A:68:ASN:H	1.22	0.84
1:C:95:ASN:HD22	1:C:98:ARG:NH1	1.74	0.84
1:G:263:ILE:HG13	1:H:263:ILE:HG13	1.61	0.83
1:G:68:ASN:H	1:G:68:ASN:HD22	1.28	0.82
1:H:82:ILE:HD11	1:H:112:ILE:HG23	1.62	0.82
1:D:95:ASN:HD22	1:D:98:ARG:HH22	1.23	0.82
1:F:291:PRO:HB2	1:F:295:VAL:HG21	1.61	0.82
1:J:50:PHE:HB3	2:J:1158:HOH:O	1.79	0.81
1:E:191:GLN:HE22	1:E:229:ASN:H	1.28	0.80
1:G:43:SER:HA	1:H:43:SER:HA	1.62	0.80
1:I:191:GLN:HE22	1:I:229:ASN:N	1.78	0.79
1:B:255:LEU:HD21	1:E:255:LEU:HD21	1.64	0.79
1:B:72:VAL:HG13	1:B:73:ASN:H	1.48	0.77
1:I:94:LYS:H	1:I:94:LYS:CE	1.97	0.77
1:I:81:LEU:HD21	1:I:95:ASN:HD22	1.50	0.77
1:J:291:PRO:HG2	1:J:296:THR:HG23	1.67	0.77
1:I:43:SER:HA	1:J:43:SER:HA	1.67	0.77
1:B:29:LYS:O	1:B:33:ILE:HG12	1.85	0.77
1:D:72:VAL:HG13	1:D:73:ASN:H	1.50	0.77
1:E:292:PRO:O	1:E:295:VAL:HG22	1.85	0.77
1:H:29:LYS:HD3	1:H:29:LYS:H	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:GLN:HE22	1:K:229:ASN:N	1.80	0.77
1:F:4:ILE:HD12	1:F:5:GLY:N	1.98	0.76
1:G:4:ILE:HD12	1:G:4:ILE:N	2.00	0.76
1:F:100:GLU:HB3	1:F:101:PRO:HD3	1.66	0.76
1:I:263:ILE:HG13	1:J:263:ILE:HG13	1.68	0.76
1:C:191:GLN:HE22	1:C:229:ASN:H	1.34	0.76
1:H:72:VAL:HG22	1:H:73:ASN:H	1.50	0.76
1:K:191:GLN:NE2	1:K:229:ASN:H	1.80	0.76
1:F:290:THR:HB	2:F:953:HOH:O	1.85	0.75
1:L:191:GLN:HE22	1:L:229:ASN:H	1.34	0.75
1:C:135:THR:O	1:C:139:LYS:HD3	1.85	0.75
1:B:283:ILE:HB	2:B:1069:HOH:O	1.87	0.75
1:F:68:ASN:HD22	1:F:68:ASN:H	1.30	0.75
1:F:234:LEU:HA	2:F:1072:HOH:O	1.85	0.75
1:L:94:LYS:NZ	1:L:94:LYS:HB3	2.02	0.75
1:K:62:LEU:HB3	1:K:67:MSE:HG3	1.66	0.75
1:H:68:ASN:HD22	1:H:68:ASN:N	1.83	0.74
1:A:100:GLU:HB3	1:A:101:PRO:HD3	1.69	0.74
1:I:43:SER:OG	1:I:46:GLU:HG3	1.87	0.73
1:C:100:GLU:HB3	1:C:101:PRO:HD3	1.70	0.73
1:D:156:VAL:HG11	1:D:172:ILE:HG12	1.69	0.73
1:I:26:ILE:HD11	1:I:53:ARG:NH1	2.03	0.73
1:I:93:ASP:HB3	1:I:97:GLN:NE2	2.02	0.73
1:B:95:ASN:HD22	1:B:98:ARG:HH22	1.35	0.73
1:F:62:LEU:HB3	1:F:67:MSE:HG3	1.71	0.73
1:K:81:LEU:O	1:K:85:ILE:HG13	1.87	0.73
1:J:179:VAL:HG23	1:J:180:ASP:OD1	1.89	0.72
1:K:147:THR:HB	2:K:932:HOH:O	1.87	0.72
1:J:95:ASN:HD22	1:J:98:ARG:NH2	1.88	0.72
1:C:208:LYS:HA	2:C:981:HOH:O	1.88	0.72
1:L:98:ARG:HH11	1:L:98:ARG:HB3	1.54	0.72
1:B:280:LEU:HD12	2:B:1069:HOH:O	1.89	0.71
1:A:250:ASN:HA	2:F:953:HOH:O	1.89	0.71
1:B:280:LEU:HA	2:B:1069:HOH:O	1.88	0.71
1:F:29:LYS:O	1:F:33:ILE:HG12	1.90	0.71
1:D:293:LYS:HD3	1:D:293:LYS:N	2.05	0.71
1:I:101:PRO:HA	2:I:1112:HOH:O	1.89	0.71
1:H:72:VAL:HG22	1:H:73:ASN:N	2.06	0.71
1:D:81:LEU:HD21	1:D:95:ASN:ND2	2.06	0.71
1:E:100:GLU:HB3	1:E:101:PRO:HD3	1.70	0.71
1:F:81:LEU:O	1:F:85:ILE:HG13	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HB3	2:B:1132:HOH:O	1.90	0.70
1:D:255:LEU:HD21	1:L:255:LEU:HD21	1.71	0.70
1:J:95:ASN:ND2	1:J:98:ARG:HH22	1.87	0.70
1:G:68:ASN:H	1:G:68:ASN:ND2	1.89	0.70
1:J:293:LYS:HD3	1:J:294:GLU:H	1.57	0.70
1:D:88:ASN:HD22	1:D:91:LEU:HG	1.55	0.69
1:H:173:LYS:HB2	1:H:174:PRO:HD3	1.74	0.69
1:E:43:SER:OG	1:E:46:GLU:HG3	1.93	0.69
1:C:293:LYS:HD3	1:C:294:GLU:N	2.08	0.69
1:K:94:LYS:HG2	2:K:650:HOH:O	1.91	0.69
1:L:94:LYS:H	1:L:94:LYS:HD2	1.55	0.69
1:C:82:ILE:HD11	1:C:112:ILE:HG23	1.72	0.69
1:G:20:ILE:HD12	1:G:20:ILE:H	1.58	0.69
1:E:67:MSE:HE1	1:F:58:PHE:CD2	2.28	0.69
1:L:104:LEU:HD21	2:L:1103:HOH:O	1.92	0.69
1:L:4:ILE:HD12	1:L:4:ILE:N	2.08	0.69
1:K:81:LEU:HG	1:K:85:ILE:HD11	1.75	0.68
1:F:68:ASN:H	1:F:68:ASN:ND2	1.91	0.68
1:J:100:GLU:HB3	1:J:101:PRO:HD3	1.75	0.68
1:B:87:THR:C	1:B:88:ASN:HD22	1.96	0.68
1:F:84:LYS:HB2	1:F:84:LYS:NZ	2.09	0.68
1:B:95:ASN:ND2	1:B:98:ARG:HH22	1.90	0.68
1:D:76:GLY:O	1:D:80:LEU:HD23	1.93	0.68
1:F:95:ASN:HA	1:F:98:ARG:NH1	2.08	0.68
1:H:251:ILE:HG21	1:I:292:PRO:HG3	1.76	0.68
1:K:43:SER:OG	1:K:46:GLU:HG3	1.94	0.68
1:I:20:ILE:H	1:I:20:ILE:CD1	2.00	0.68
1:B:20:ILE:HD12	1:B:20:ILE:N	2.08	0.67
1:H:20:ILE:H	1:H:20:ILE:CD1	2.05	0.67
1:J:81:LEU:HD21	1:J:95:ASN:ND2	2.09	0.67
1:L:98:ARG:HB3	1:L:98:ARG:NH1	2.08	0.67
1:L:100:GLU:HB3	1:L:101:PRO:HD3	1.75	0.67
1:L:265:LYS:HB2	1:L:273:HIS:CD2	2.28	0.67
1:D:179:VAL:HG22	2:D:1106:HOH:O	1.93	0.67
1:I:100:GLU:HB3	1:I:101:PRO:HD3	1.76	0.67
1:F:179:VAL:HG23	1:F:180:ASP:OD1	1.94	0.67
1:F:291:PRO:HB2	1:F:295:VAL:CG2	2.24	0.67
1:G:82:ILE:HD11	1:G:112:ILE:HG23	1.75	0.67
1:G:274:ARG:O	1:G:278:GLU:HG3	1.94	0.67
1:C:67:MSE:C	1:C:68:ASN:HD22	1.98	0.67
2:A:764:HOH:O	1:B:182:PHE:HA	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:GLY:O	1:G:80:LEU:HD23	1.95	0.67
1:B:44:VAL:HA	2:B:1132:HOH:O	1.95	0.66
1:D:93:ASP:O	1:D:97:GLN:HG3	1.95	0.66
1:G:29:LYS:O	1:G:33:ILE:HG13	1.95	0.66
1:B:20:ILE:H	1:B:20:ILE:CD1	2.05	0.66
1:E:265:LYS:HB2	1:E:273:HIS:CD2	2.31	0.66
1:G:67:MSE:HA	1:G:67:MSE:HE2	1.77	0.66
1:H:251:ILE:HG12	1:I:289:PHE:CE1	2.30	0.66
1:H:294:GLU:OE2	1:H:295:VAL:HG13	1.96	0.66
1:H:76:GLY:O	1:H:80:LEU:HD23	1.95	0.66
1:F:98:ARG:NH1	1:F:98:ARG:HB3	2.10	0.66
1:H:62:LEU:HB3	1:H:67:MSE:HG3	1.77	0.66
1:B:274:ARG:O	1:B:278:GLU:HG3	1.95	0.66
1:L:291:PRO:HG2	1:L:296:THR:HG23	1.78	0.66
1:K:148:PHE:CD2	1:K:175:MSE:HE2	2.31	0.65
1:B:43:SER:OG	1:B:46:GLU:HG3	1.95	0.65
1:B:100:GLU:HB3	1:B:101:PRO:HD3	1.76	0.65
1:G:62:LEU:HB3	1:G:67:MSE:HG3	1.76	0.65
1:A:263:ILE:CG1	1:B:263:ILE:HG13	2.22	0.65
1:L:68:ASN:N	1:L:68:ASN:HD22	1.94	0.65
1:D:29:LYS:O	1:D:33:ILE:HG12	1.96	0.65
1:K:72:VAL:HG13	1:K:73:ASN:H	1.61	0.65
1:H:68:ASN:N	1:H:68:ASN:ND2	2.45	0.64
1:I:98:ARG:NH1	1:I:98:ARG:HB3	2.12	0.64
1:K:119:ILE:HA	2:K:1123:HOH:O	1.97	0.64
1:E:95:ASN:HD22	1:E:98:ARG:HH22	1.44	0.64
1:G:293:LYS:HD3	1:G:293:LYS:N	2.13	0.64
1:G:20:ILE:HD12	1:G:20:ILE:N	2.13	0.64
1:E:20:ILE:H	1:E:20:ILE:CD1	2.09	0.63
1:L:224:LYS:NZ	1:L:225:ASN:HD21	1.96	0.63
1:B:291:PRO:HG2	1:B:296:THR:HG23	1.80	0.63
1:B:76:GLY:O	1:B:80:LEU:HD23	1.99	0.63
1:K:85:ILE:HG22	2:K:622:HOH:O	1.98	0.63
1:K:100:GLU:HB3	1:K:101:PRO:HD3	1.80	0.63
1:G:171:ILE:O	1:G:175:MSE:HE3	1.97	0.63
1:I:20:ILE:HD12	1:I:20:ILE:N	2.07	0.63
1:D:250:ASN:HA	1:L:290:THR:HB	1.80	0.63
1:F:76:GLY:O	1:F:80:LEU:HD23	1.99	0.63
1:H:191:GLN:HE22	1:H:229:ASN:H	1.44	0.63
1:D:100:GLU:HB3	1:D:101:PRO:HD3	1.79	0.63
1:A:193:VAL:HA	2:A:941:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ASN:ND2	1:E:91:LEU:HG	2.14	0.63
1:J:287:GLU:HB3	2:J:1082:HOH:O	1.99	0.63
1:J:291:PRO:HB2	1:J:295:VAL:HG21	1.81	0.63
1:A:95:ASN:ND2	1:A:98:ARG:HH12	1.92	0.62
1:D:291:PRO:HB2	1:D:296:THR:HG23	1.81	0.62
1:H:291:PRO:HG2	1:H:296:THR:HG22	1.81	0.62
1:I:132:LYS:HB2	1:I:132:LYS:NZ	2.14	0.62
1:H:291:PRO:HG2	1:H:296:THR:CG2	2.28	0.62
1:I:4:ILE:HD12	1:I:4:ILE:H	1.64	0.62
1:I:81:LEU:HD21	1:I:95:ASN:ND2	2.14	0.62
1:L:27:MSE:HE1	1:L:40:ARG:HH22	1.64	0.62
1:A:191:GLN:HE22	1:A:229:ASN:N	1.89	0.62
1:C:265:LYS:HB2	1:C:273:HIS:CD2	2.34	0.62
1:K:29:LYS:O	1:K:33:ILE:HG13	2.00	0.62
1:H:279:GLU:HB3	2:H:645:HOH:O	2.00	0.62
1:F:273:HIS:O	1:F:277:VAL:HG23	1.98	0.62
1:J:156:VAL:HG11	1:J:172:ILE:HG12	1.81	0.62
1:A:71:SER:N	1:A:76:GLY:HA3	2.14	0.62
1:B:289:PHE:CE1	1:E:251:ILE:HB	2.35	0.62
1:C:43:SER:OG	1:C:46:GLU:HG3	1.99	0.62
1:H:72:VAL:HG13	1:H:73:ASN:N	2.14	0.62
1:I:84:LYS:HD3	2:I:1035:HOH:O	2.00	0.62
1:J:72:VAL:O	1:J:77:LYS:HE3	2.00	0.62
1:B:89:PRO:HG3	1:B:123:TYR:CE2	2.34	0.62
1:A:68:ASN:H	1:A:68:ASN:ND2	1.95	0.62
1:H:20:ILE:HD12	1:H:20:ILE:N	2.09	0.62
1:B:291:PRO:HB2	1:B:295:VAL:HG21	1.81	0.61
1:E:293:LYS:HD3	1:E:294:GLU:H	1.65	0.61
1:C:74:GLU:HB3	1:D:52:GLU:OE1	2.00	0.61
1:F:234:LEU:HD12	2:F:1072:HOH:O	1.99	0.61
1:I:93:ASP:HB2	1:I:94:LYS:NZ	2.15	0.61
1:E:149:PHE:HB3	1:F:60:GLU:OE2	2.01	0.61
1:K:99:ILE:HG13	1:K:116:TYR:CZ	2.35	0.61
1:F:68:ASN:HD22	1:F:68:ASN:N	1.95	0.61
1:J:103:ARG:HG2	1:J:103:ARG:HH11	1.66	0.61
1:H:29:LYS:HD3	1:H:29:LYS:N	2.14	0.61
1:J:134:ILE:HG23	1:J:135:THR:N	2.16	0.61
1:K:4:ILE:HG22	1:K:7:VAL:HG23	1.81	0.61
1:L:187:ASP:O	1:L:191:GLN:HG3	2.01	0.61
1:E:12:ARG:HG3	1:E:17:TYR:HB2	1.83	0.61
1:A:68:ASN:HB3	2:A:764:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:8:LEU:HG	2:J:1155:HOH:O	2.01	0.60
1:K:134:ILE:HG23	1:K:135:THR:N	2.16	0.60
1:L:179:VAL:HG23	1:L:180:ASP:OD1	2.01	0.60
1:B:293:LYS:HD3	1:B:293:LYS:N	2.16	0.60
1:H:72:VAL:HG13	1:H:73:ASN:H	1.67	0.60
1:B:293:LYS:HD3	1:B:293:LYS:H	1.67	0.60
1:E:179:VAL:HG23	1:E:180:ASP:OD1	2.01	0.60
1:K:237:ASN:ND2	1:L:267:ILE:HA	2.16	0.60
1:B:271:ASP:HB2	2:B:630:HOH:O	2.02	0.60
1:L:173:LYS:HB2	1:L:174:PRO:HD3	1.83	0.60
1:F:134:ILE:HG23	1:F:135:THR:N	2.17	0.59
1:L:98:ARG:HH11	1:L:98:ARG:CB	2.14	0.59
1:B:88:ASN:HD22	1:B:88:ASN:N	2.01	0.59
1:C:240:LYS:NZ	1:C:240:LYS:HB3	2.17	0.59
1:C:156:VAL:HG11	1:C:172:ILE:HG12	1.84	0.59
1:C:251:ILE:HD13	1:C:251:ILE:O	2.03	0.59
1:G:255:LEU:HD21	1:J:255:LEU:HD21	1.85	0.59
1:H:271:ASP:HB2	2:H:655:HOH:O	2.02	0.59
1:B:252:ASP:OD2	1:E:293:LYS:HB3	2.02	0.59
1:B:102:LYS:HE2	2:B:807:HOH:O	2.03	0.59
1:D:28:SER:OG	1:D:31:VAL:HG23	2.03	0.59
1:D:26:ILE:HD11	1:D:53:ARG:NH1	2.17	0.59
1:G:265:LYS:HB2	1:G:273:HIS:CD2	2.38	0.59
1:K:68:ASN:N	1:K:68:ASN:HD22	2.00	0.59
1:C:79:LYS:HD2	1:C:112:ILE:HG12	1.84	0.59
1:L:88:ASN:ND2	1:L:91:LEU:HG	2.17	0.59
1:B:139:LYS:HD3	1:B:143:ASP:OD1	2.03	0.58
1:D:265:LYS:HB2	1:D:273:HIS:CD2	2.38	0.58
1:I:265:LYS:HB2	1:I:273:HIS:CD2	2.38	0.58
1:L:293:LYS:HD3	1:L:294:GLU:H	1.68	0.58
1:B:95:ASN:HD22	1:B:98:ARG:NH2	2.00	0.58
1:B:273:HIS:O	1:B:277:VAL:HG23	2.02	0.58
1:C:144:LYS:NZ	1:C:144:LYS:HB2	2.18	0.58
1:I:26:ILE:HD11	1:I:53:ARG:HH12	1.68	0.58
1:I:139:LYS:O	1:I:143:ASP:HB2	2.03	0.58
1:J:58:PHE:CE2	1:J:62:LEU:HD11	2.38	0.58
1:J:173:LYS:HB2	1:J:174:PRO:HD3	1.85	0.58
1:B:291:PRO:HG2	1:B:296:THR:CG2	2.32	0.58
1:F:161:ASN:HD22	1:F:162:VAL:HG13	1.69	0.58
1:G:156:VAL:CG2	1:G:172:ILE:HG12	2.33	0.58
1:J:43:SER:OG	1:J:46:GLU:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:PRO:HB2	1:B:295:VAL:CG2	2.34	0.58
1:E:68:ASN:N	1:E:68:ASN:HD22	2.00	0.58
1:K:43:SER:HA	1:L:43:SER:HA	1.85	0.58
1:A:291:PRO:HB2	1:A:295:VAL:CG2	2.30	0.58
1:E:20:ILE:HG13	1:E:23:TYR:OH	2.03	0.58
1:G:173:LYS:HB2	1:G:174:PRO:HD3	1.85	0.58
1:A:2:PHE:CE2	1:A:67:MSE:HG2	2.39	0.58
1:A:138:LEU:HD13	1:A:171:ILE:CD1	2.34	0.58
1:G:94:LYS:HE3	1:G:94:LYS:N	2.18	0.58
1:C:240:LYS:O	1:C:243:TYR:HB3	2.03	0.58
1:E:29:LYS:O	1:E:33:ILE:HG12	2.04	0.58
1:A:26:ILE:HD11	1:A:53:ARG:NH1	2.19	0.58
1:G:251:ILE:HG12	1:J:290:THR:O	2.04	0.58
1:H:20:ILE:HA	1:H:23:TYR:CE1	2.39	0.58
1:C:293:LYS:HB3	1:K:252:ASP:OD2	2.04	0.57
1:E:274:ARG:HG3	2:E:966:HOH:O	2.02	0.57
1:C:66:GLY:C	1:C:68:ASN:H	2.07	0.57
1:E:88:ASN:HD22	1:E:91:LEU:HG	1.69	0.57
1:F:81:LEU:HG	1:F:85:ILE:HD11	1.87	0.57
1:G:68:ASN:HD22	1:G:68:ASN:N	1.92	0.57
1:L:81:LEU:O	1:L:85:ILE:HG13	2.04	0.57
1:A:293:LYS:HD3	1:A:293:LYS:N	2.19	0.57
1:K:95:ASN:HA	1:K:98:ARG:HH12	1.69	0.57
1:L:93:ASP:O	1:L:97:GLN:HG3	2.04	0.57
1:A:254:TYR:O	1:A:258:VAL:HG23	2.05	0.57
1:D:3:LYS:HD2	1:D:65:ALA:O	2.04	0.57
1:I:86:PHE:HD1	1:I:119:ILE:HG12	1.70	0.57
1:E:93:ASP:O	1:E:97:GLN:HG3	2.04	0.57
1:H:278:GLU:HA	1:H:299:TYR:CD2	2.40	0.57
1:K:60:GLU:OE2	1:L:149:PHE:HB3	2.04	0.57
1:I:171:ILE:O	1:I:175:MSE:HE3	2.03	0.57
1:F:87:THR:O	1:F:89:PRO:HD3	2.05	0.57
1:A:93:ASP:O	1:A:97:GLN:HG3	2.04	0.56
1:I:277:VAL:CG1	1:I:299:TYR:HB2	2.35	0.56
1:A:73:ASN:O	1:A:77:LYS:HG3	2.05	0.56
1:H:210:ALA:O	1:H:214:ILE:HG13	2.05	0.56
1:H:293:LYS:HB3	1:I:252:ASP:OD2	2.04	0.56
1:L:240:LYS:O	1:L:243:TYR:HB3	2.05	0.56
1:D:4:ILE:HG23	1:D:5:GLY:N	2.19	0.56
1:F:98:ARG:HB3	1:F:98:ARG:HH11	1.71	0.56
1:I:82:ILE:HG23	1:I:83:SER:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:ARG:O	1:I:101:PRO:HD2	2.05	0.56
1:L:68:ASN:N	1:L:68:ASN:ND2	2.54	0.56
1:C:43:SER:HA	1:D:43:SER:HA	1.86	0.56
1:D:103:ARG:HH11	1:D:103:ARG:HG2	1.71	0.56
1:E:23:TYR:HB3	1:E:32:TYR:CD2	2.39	0.56
1:I:212:TYR:O	1:I:216:GLN:HG2	2.04	0.56
1:E:251:ILE:HG22	2:E:1185:HOH:O	2.04	0.56
1:F:81:LEU:HG	1:F:85:ILE:HG13	1.87	0.56
1:H:291:PRO:HB2	1:H:295:VAL:HG21	1.87	0.56
1:F:63:ASN:HA	1:F:67:MSE:HB2	1.88	0.56
1:J:271:ASP:HB2	2:J:960:HOH:O	2.05	0.56
1:L:134:ILE:HG23	1:L:135:THR:N	2.21	0.56
1:A:296:THR:HG21	2:A:1242:HOH:O	2.05	0.56
1:B:254:TYR:O	1:B:258:VAL:HG23	2.06	0.56
1:C:254:TYR:O	1:C:258:VAL:HG23	2.06	0.56
1:I:74:GLU:HA	1:I:77:LYS:HD2	1.88	0.56
1:L:94:LYS:HB3	1:L:94:LYS:HZ3	1.70	0.56
1:E:71:SER:HB2	2:E:1026:HOH:O	2.05	0.56
1:G:296:THR:HG21	2:G:965:HOH:O	2.06	0.56
1:B:265:LYS:HB2	1:B:273:HIS:CD2	2.41	0.55
1:L:43:SER:OG	1:L:46:GLU:HG3	2.05	0.55
1:A:43:SER:OG	1:A:46:GLU:HG3	2.06	0.55
1:G:210:ALA:O	1:G:214:ILE:HG13	2.06	0.55
1:D:295:VAL:HG23	1:D:296:THR:N	2.21	0.55
1:F:150:GLY:O	1:F:189:THR:HG21	2.05	0.55
1:L:28:SER:OG	1:L:31:VAL:HG23	2.07	0.55
1:F:79:LYS:NZ	1:F:108:GLN:HE22	2.04	0.55
1:K:263:ILE:HG13	1:L:263:ILE:CG1	2.27	0.55
1:B:134:ILE:HG23	1:B:135:THR:N	2.22	0.55
1:C:169:SER:O	1:C:173:LYS:HG2	2.06	0.55
1:D:9:LYS:HA	1:D:36:GLU:OE2	2.07	0.55
1:A:134:ILE:HG23	1:A:135:THR:N	2.22	0.55
1:D:178:ILE:HG13	1:D:190:ILE:HD12	1.89	0.55
1:I:98:ARG:HB3	1:I:98:ARG:CZ	2.36	0.55
1:I:170:SER:OG	1:I:171:ILE:HD12	2.06	0.55
1:L:247:THR:HG22	1:L:248:ASP:OD1	2.07	0.55
1:E:134:ILE:HG23	1:E:135:THR:N	2.21	0.55
1:F:88:ASN:OD1	1:F:90:ASP:HB2	2.07	0.55
1:C:295:VAL:HG23	1:C:296:THR:N	2.21	0.54
1:F:156:VAL:HG11	1:F:172:ILE:HG12	1.89	0.54
1:I:40:ARG:HH21	1:I:40:ARG:HG3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:86:PHE:C	1:K:88:ASN:H	2.11	0.54
1:B:93:ASP:O	1:B:97:GLN:HG3	2.07	0.54
1:D:74:GLU:HA	1:D:77:LYS:HE2	1.88	0.54
1:B:72:VAL:HG13	1:B:73:ASN:N	2.19	0.54
1:C:108:GLN:O	1:C:112:ILE:HG13	2.07	0.54
1:K:173:LYS:HB2	1:K:174:PRO:HD3	1.89	0.54
1:B:250:ASN:HA	1:E:290:THR:HB	1.87	0.54
1:H:29:LYS:H	1:H:29:LYS:CD	2.19	0.54
1:J:156:VAL:CG1	1:J:172:ILE:HG12	2.37	0.54
1:D:156:VAL:CG1	1:D:172:ILE:HG12	2.35	0.54
1:D:205:ARG:HG2	1:D:205:ARG:HH11	1.72	0.54
1:D:254:TYR:O	1:D:258:VAL:HG23	2.08	0.54
1:J:12:ARG:HG3	1:J:22:LEU:HD21	1.90	0.54
1:A:292:PRO:O	1:A:295:VAL:HG22	2.07	0.54
1:B:289:PHE:HE1	1:E:251:ILE:HB	1.70	0.54
1:D:147:THR:HG23	2:J:1111:HOH:O	2.06	0.54
1:I:173:LYS:HB2	1:I:174:PRO:HD3	1.90	0.54
1:I:271:ASP:HB2	2:I:790:HOH:O	2.07	0.54
1:L:278:GLU:HA	1:L:299:TYR:CE2	2.43	0.54
1:A:251:ILE:HB	1:F:289:PHE:CZ	2.42	0.54
1:E:251:ILE:HD13	1:E:251:ILE:O	2.07	0.54
1:I:214:ILE:HD13	1:I:240:LYS:HG3	1.90	0.54
1:D:292:PRO:HG2	1:D:295:VAL:HG22	1.90	0.54
1:I:73:ASN:O	1:I:77:LYS:HG3	2.08	0.54
1:L:205:ARG:HH11	1:L:205:ARG:HG2	1.72	0.54
1:A:296:THR:O	1:A:300:GLU:HB2	2.08	0.54
1:G:20:ILE:H	1:G:20:ILE:CD1	2.21	0.54
1:A:251:ILE:HG21	1:F:292:PRO:HD3	1.90	0.53
1:F:98:ARG:HH11	1:F:98:ARG:CB	2.21	0.53
1:A:191:GLN:NE2	1:A:229:ASN:H	1.88	0.53
1:A:248:ASP:O	1:A:250:ASN:N	2.41	0.53
1:D:72:VAL:HG13	1:D:73:ASN:N	2.22	0.53
1:K:178:ILE:HG23	2:K:1152:HOH:O	2.08	0.53
1:L:29:LYS:O	1:L:33:ILE:HG13	2.08	0.53
1:L:291:PRO:HG2	1:L:296:THR:CG2	2.38	0.53
1:F:81:LEU:HG	1:F:85:ILE:CG1	2.38	0.53
1:J:197:ALA:HB1	1:J:213:TYR:CZ	2.44	0.53
1:A:20:ILE:HG12	2:A:1050:HOH:O	2.08	0.53
1:D:12:ARG:O	1:D:17:TYR:HB2	2.08	0.53
1:D:89:PRO:HB3	1:D:123:TYR:CD2	2.43	0.53
1:E:278:GLU:HG2	1:E:299:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:187:ASP:O	1:I:190:ILE:HG12	2.08	0.53
1:J:4:ILE:N	1:J:4:ILE:HD12	2.23	0.53
1:J:293:LYS:HD3	1:J:294:GLU:N	2.22	0.53
1:B:3:LYS:HA	2:B:1125:HOH:O	2.08	0.53
1:B:293:LYS:H	1:B:293:LYS:CD	2.21	0.53
1:F:81:LEU:HG	1:F:85:ILE:CD1	2.39	0.53
1:H:28:SER:OG	1:H:31:VAL:HG23	2.08	0.53
1:H:153:CYS:HB3	1:H:193:VAL:HG21	1.89	0.53
1:J:31:VAL:O	1:J:35:VAL:HG23	2.08	0.53
1:J:265:LYS:HB2	1:J:273:HIS:CD2	2.44	0.53
1:D:255:LEU:HD12	2:D:1232:HOH:O	2.07	0.53
1:A:93:ASP:HB2	2:A:1184:HOH:O	2.07	0.53
1:B:156:VAL:HG11	1:B:172:ILE:HG12	1.91	0.53
1:C:55:GLY:O	1:D:108:GLN:HG2	2.08	0.53
1:I:20:ILE:HA	1:I:23:TYR:CE1	2.44	0.53
1:I:127:VAL:N	1:I:128:PRO:HD3	2.24	0.53
1:I:293:LYS:HD3	1:I:294:GLU:H	1.74	0.53
1:C:76:GLY:O	1:C:80:LEU:HD23	2.09	0.53
1:H:93:ASP:O	1:H:97:GLN:HG3	2.09	0.53
1:E:49:LYS:O	1:E:53:ARG:HG2	2.10	0.52
1:J:12:ARG:O	1:J:17:TYR:HB2	2.08	0.52
1:J:245:PHE:O	1:J:249:LYS:HD3	2.08	0.52
1:G:293:LYS:HD3	1:G:294:GLU:H	1.74	0.52
1:H:272:ILE:HG22	1:H:276:LEU:HD22	1.90	0.52
1:E:68:ASN:N	1:E:68:ASN:ND2	2.57	0.52
1:K:274:ARG:O	1:K:278:GLU:HG3	2.09	0.52
1:L:274:ARG:O	1:L:278:GLU:HG3	2.09	0.52
1:E:58:PHE:HE2	1:F:62:LEU:HD13	1.75	0.52
1:G:293:LYS:H	1:G:293:LYS:CD	2.22	0.52
1:J:22:LEU:HG	1:J:32:TYR:OH	2.09	0.52
1:C:104:LEU:HB2	2:C:1037:HOH:O	2.09	0.52
1:F:256:ASN:O	1:F:260:ILE:HG13	2.09	0.52
1:J:238:TYR:HB2	1:J:260:ILE:HG21	1.90	0.52
1:C:291:PRO:HB2	1:C:296:THR:HG23	1.91	0.52
1:E:20:ILE:HA	1:E:23:TYR:CZ	2.45	0.52
1:G:156:VAL:HA	1:G:159:LEU:HD12	1.91	0.52
1:K:68:ASN:N	1:K:68:ASN:ND2	2.57	0.52
1:K:292:PRO:HG2	1:K:295:VAL:HG13	1.90	0.52
1:C:75:THR:HG21	1:C:108:GLN:HB3	1.92	0.52
1:C:148:PHE:CG	1:C:175:MSE:HG2	2.45	0.52
1:D:48:SER:O	1:D:51:SER:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:SER:HB3	1:F:289:PHE:O	2.10	0.52
1:G:200:ILE:HG22	1:G:204:ASN:ND2	2.25	0.52
1:G:293:LYS:HD3	1:G:293:LYS:H	1.74	0.52
1:L:76:GLY:O	1:L:80:LEU:HD23	2.10	0.52
1:A:26:ILE:HD11	1:A:53:ARG:HH12	1.74	0.52
1:C:210:ALA:O	1:C:214:ILE:HG13	2.10	0.52
1:D:293:LYS:HD3	1:D:293:LYS:H	1.75	0.52
1:K:142:TYR:HA	1:K:145:ARG:HG2	1.92	0.52
1:G:277:VAL:CG1	1:G:299:TYR:HB2	2.40	0.51
1:J:19:GLN:HE22	1:J:33:ILE:HD13	1.75	0.51
1:J:34:LYS:HA	1:J:37:ALA:HB3	1.92	0.51
1:C:68:ASN:HD22	1:C:68:ASN:N	2.07	0.51
1:C:156:VAL:CG1	1:C:172:ILE:HG12	2.39	0.51
1:A:148:PHE:CG	1:A:175:MSE:HG2	2.45	0.51
1:A:293:LYS:HD3	1:A:294:GLU:H	1.76	0.51
1:E:23:TYR:CZ	1:E:29:LYS:HB2	2.45	0.51
1:I:95:ASN:HA	1:I:98:ARG:HH22	1.75	0.51
1:I:296:THR:HG21	2:I:1159:HOH:O	2.11	0.51
1:L:103:ARG:HG2	1:L:103:ARG:HH11	1.76	0.51
1:H:72:VAL:CG2	1:H:73:ASN:H	2.18	0.51
1:A:249:LYS:HE3	2:A:1157:HOH:O	2.10	0.51
1:D:34:LYS:HB3	1:D:40:ARG:HB2	1.90	0.51
1:G:293:LYS:CD	1:G:294:GLU:H	2.24	0.51
1:H:289:PHE:CE1	1:I:289:PHE:HE2	2.29	0.51
1:L:81:LEU:HD21	1:L:95:ASN:ND2	2.26	0.51
1:A:291:PRO:HG2	1:A:296:THR:HG23	1.93	0.51
1:F:71:SER:HB3	2:F:1099:HOH:O	2.10	0.51
1:J:299:TYR:C	1:J:301:ASN:H	2.12	0.51
1:K:63:ASN:HA	1:K:67:MSE:HB2	1.93	0.51
1:L:271:ASP:HB2	2:L:667:HOH:O	2.10	0.51
1:E:187:ASP:O	1:E:190:ILE:HG12	2.11	0.51
1:F:173:LYS:HB2	1:F:174:PRO:HD3	1.92	0.51
1:B:153:CYS:HB3	1:B:193:VAL:HG21	1.93	0.51
1:A:72:VAL:HG13	1:A:73:ASN:N	2.25	0.51
1:D:295:VAL:HG23	1:D:296:THR:H	1.76	0.51
1:E:89:PRO:HG3	1:E:123:TYR:CE2	2.46	0.51
1:G:4:ILE:N	1:G:7:VAL:HG23	2.26	0.51
1:I:9:LYS:O	1:I:13:GLN:HG3	2.11	0.51
1:E:277:VAL:HG12	1:E:299:TYR:HB2	1.92	0.50
1:D:4:ILE:HG23	1:D:5:GLY:H	1.76	0.50
1:F:291:PRO:HG2	1:F:296:THR:CG2	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:VAL:HG11	1:H:172:ILE:HG12	1.93	0.50
1:J:138:LEU:HD13	1:J:171:ILE:HD11	1.93	0.50
1:E:251:ILE:HD13	1:E:255:LEU:HG	1.93	0.50
1:F:84:LYS:HB2	1:F:84:LYS:HZ3	1.76	0.50
1:G:293:LYS:HD2	1:J:252:ASP:OD1	2.11	0.50
1:H:250:ASN:HA	1:I:290:THR:HB	1.93	0.50
1:J:83:SER:O	1:J:87:THR:HG23	2.11	0.50
1:K:284:SER:HB3	1:K:289:PHE:O	2.12	0.50
1:L:224:LYS:HZ3	1:L:225:ASN:HD21	1.59	0.50
1:B:297:MET:HE3	1:B:297:MET:HA	1.93	0.50
1:E:3:LYS:HD2	1:E:3:LYS:N	2.26	0.50
1:G:205:ARG:HH11	1:G:205:ARG:HG2	1.77	0.50
1:G:153:CYS:HA	1:G:156:VAL:HG12	1.93	0.50
1:I:148:PHE:CG	1:I:175:MSE:HG2	2.46	0.50
1:C:176:TYR:HB3	1:C:177:PRO:HA	1.94	0.50
1:E:81:LEU:HD21	1:E:95:ASN:ND2	2.26	0.50
1:E:102:LYS:NZ	1:E:102:LYS:HB3	2.27	0.50
1:F:78:GLU:OE2	1:F:99:ILE:HD11	2.12	0.50
1:G:293:LYS:HG2	1:G:294:GLU:N	2.26	0.50
1:I:28:SER:OG	1:I:31:VAL:HG23	2.12	0.50
1:J:7:VAL:HG21	1:J:65:ALA:HA	1.94	0.50
1:J:32:TYR:HE1	1:J:36:GLU:CD	2.15	0.50
1:B:68:ASN:N	1:B:68:ASN:HD22	2.08	0.49
1:F:274:ARG:O	1:F:278:GLU:HG3	2.12	0.49
1:G:23:TYR:O	1:G:25:GLY:N	2.44	0.49
1:H:297:MET:CE	1:H:301:ASN:HD21	2.25	0.49
1:I:98:ARG:NH1	1:I:98:ARG:CB	2.75	0.49
1:J:291:PRO:HB2	1:J:295:VAL:CG2	2.41	0.49
1:D:74:GLU:HA	1:D:77:LYS:CE	2.41	0.49
1:G:148:PHE:CG	1:G:175:MSE:HG2	2.47	0.49
1:K:75:THR:O	1:K:79:LYS:HG3	2.12	0.49
1:L:295:VAL:HG23	1:L:296:THR:N	2.27	0.49
1:G:102:LYS:HE3	1:G:109:TYR:CE1	2.47	0.49
1:B:12:ARG:HG3	1:B:17:TYR:HB2	1.93	0.49
1:F:47:LEU:HG	1:F:58:PHE:CE1	2.47	0.49
1:H:100:GLU:HB3	1:H:101:PRO:HD3	1.94	0.49
1:I:18:HIS:HB3	1:I:20:ILE:HD13	1.95	0.49
1:I:132:LYS:HB2	1:I:132:LYS:HZ2	1.76	0.49
1:K:84:LYS:O	1:K:88:ASN:HB3	2.13	0.49
1:C:63:ASN:HA	1:C:67:MSE:HB2	1.94	0.49
1:C:248:ASP:O	1:C:250:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:PHE:O	1:H:249:LYS:HD3	2.12	0.49
1:H:251:ILE:O	1:H:255:LEU:HG	2.13	0.49
1:K:75:THR:HG21	1:K:108:GLN:HB3	1.95	0.49
1:C:291:PRO:HB3	1:C:295:VAL:HG21	1.94	0.49
1:K:5:GLY:HA3	1:K:36:GLU:HA	1.95	0.49
1:G:163:LEU:HD12	1:G:164:PRO:HD2	1.93	0.49
1:G:237:ASN:ND2	1:H:267:ILE:HA	2.27	0.49
1:G:138:LEU:HD13	1:G:171:ILE:HD11	1.95	0.49
1:G:291:PRO:HB2	1:G:296:THR:HG23	1.93	0.49
1:H:293:LYS:HD3	1:H:294:GLU:H	1.78	0.49
1:J:27:MSE:SE	1:J:35:VAL:HG21	2.63	0.49
1:K:94:LYS:HB2	1:K:94:LYS:NZ	2.28	0.49
1:A:4:ILE:HD11	1:B:44:VAL:HG11	1.93	0.49
1:A:248:ASP:O	1:A:249:LYS:C	2.50	0.49
1:B:297:MET:CE	1:B:301:ASN:HD21	2.25	0.49
1:F:23:TYR:O	1:F:25:GLY:N	2.46	0.49
1:G:100:GLU:HB3	1:G:101:PRO:HD3	1.93	0.49
1:I:277:VAL:HG12	1:I:299:TYR:HB2	1.95	0.49
1:J:299:TYR:O	1:J:301:ASN:N	2.39	0.49
1:C:292:PRO:O	1:C:295:VAL:HG22	2.13	0.48
1:G:250:ASN:HA	1:J:290:THR:HB	1.95	0.48
1:G:292:PRO:HD2	1:G:295:VAL:HG21	1.93	0.48
1:G:293:LYS:CG	1:G:294:GLU:N	2.76	0.48
1:H:127:VAL:HG23	1:H:127:VAL:O	2.13	0.48
1:A:104:LEU:HB2	2:A:1059:HOH:O	2.13	0.48
1:I:98:ARG:C	1:I:101:PRO:HD2	2.33	0.48
1:K:119:ILE:HG21	2:K:622:HOH:O	2.11	0.48
1:E:185:ASP:OD2	1:F:184:LYS:HD2	2.13	0.48
1:K:142:TYR:HA	1:K:145:ARG:CG	2.43	0.48
1:B:281:THR:HG21	1:B:299:TYR:CE1	2.48	0.48
1:F:102:LYS:HB2	1:F:105:THR:OG1	2.13	0.48
1:I:237:ASN:O	1:I:241:GLN:HG2	2.12	0.48
1:C:139:LYS:HD2	1:C:139:LYS:N	2.27	0.48
1:C:205:ARG:HG2	1:C:205:ARG:HH11	1.78	0.48
1:C:261:ILE:HG12	1:C:276:LEU:HB3	1.94	0.48
1:I:68:ASN:N	1:I:68:ASN:HD22	2.10	0.48
1:B:295:VAL:HG23	1:B:296:THR:N	2.26	0.48
1:C:103:ARG:HG2	1:C:103:ARG:HH11	1.78	0.48
1:D:153:CYS:HB3	1:D:193:VAL:HG21	1.96	0.48
1:G:153:CYS:HB2	1:G:189:THR:HG22	1.95	0.48
1:I:20:ILE:HA	1:I:23:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:62:LEU:O	1:I:65:ALA:HB3	2.14	0.48
1:J:265:LYS:HE3	1:J:298:TYR:OH	2.14	0.48
1:L:248:ASP:O	1:L:250:ASN:N	2.46	0.48
1:A:295:VAL:HG23	1:A:296:THR:N	2.29	0.48
1:E:67:MSE:HE1	1:F:58:PHE:CG	2.49	0.48
1:F:23:TYR:O	1:F:26:ILE:N	2.47	0.48
1:G:9:LYS:O	1:G:13:GLN:HG3	2.14	0.48
1:J:62:LEU:CB	1:J:67:MSE:HG3	2.32	0.48
1:D:245:PHE:O	1:D:249:LYS:HA	2.14	0.48
1:I:203:MSE:CE	1:I:286:LYS:HE2	2.43	0.48
1:K:94:LYS:HE3	2:K:1096:HOH:O	2.12	0.48
1:L:37:ALA:O	1:L:38:ASP:HB2	2.12	0.48
1:D:148:PHE:CG	1:D:175:MSE:HG2	2.49	0.48
1:H:272:ILE:CG2	1:H:276:LEU:HD22	2.44	0.48
1:I:82:ILE:CG2	1:I:83:SER:N	2.76	0.48
1:C:24:SER:O	1:C:53:ARG:NH2	2.47	0.48
1:G:43:SER:OG	1:G:46:GLU:HG3	2.14	0.48
1:I:134:ILE:HG23	1:I:135:THR:N	2.29	0.48
1:I:151:ILE:O	1:I:155:ILE:HG13	2.13	0.48
1:C:22:LEU:O	1:C:26:ILE:HD12	2.14	0.47
1:C:173:LYS:HB2	1:C:174:PRO:HD3	1.95	0.47
1:E:284:SER:CB	1:E:291:PRO:HG3	2.44	0.47
1:K:156:VAL:HG11	1:K:172:ILE:HG12	1.96	0.47
1:C:153:CYS:HB3	1:C:193:VAL:HG21	1.97	0.47
1:D:293:LYS:HG2	1:D:294:GLU:N	2.29	0.47
1:F:272:ILE:HG22	1:F:276:LEU:HD22	1.95	0.47
1:G:293:LYS:N	1:G:293:LYS:CD	2.77	0.47
1:I:160:LEU:HB3	1:I:200:ILE:CD1	2.44	0.47
1:K:265:LYS:HB2	1:K:273:HIS:CD2	2.50	0.47
1:C:26:ILE:HD11	1:C:53:ARG:NH1	2.30	0.47
1:D:293:LYS:N	1:D:293:LYS:CD	2.75	0.47
1:E:20:ILE:HD12	1:E:20:ILE:N	2.14	0.47
1:B:20:ILE:O	1:B:24:SER:HB3	2.14	0.47
1:B:28:SER:OG	1:B:31:VAL:HG23	2.15	0.47
1:B:292:PRO:N	1:E:251:ILE:HG21	2.29	0.47
1:C:29:LYS:O	1:C:33:ILE:HG13	2.15	0.47
1:I:149:PHE:HB3	1:J:60:GLU:OE2	2.15	0.47
1:K:48:SER:O	1:K:51:SER:HB3	2.15	0.47
1:L:23:TYR:HB2	1:L:27:MSE:HG3	1.97	0.47
1:C:66:GLY:O	1:C:68:ASN:N	2.46	0.47
1:I:91:LEU:HA	1:I:94:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:282:LYS:O	1:I:286:LYS:HG3	2.15	0.47
1:J:8:LEU:HD22	2:J:1158:HOH:O	2.15	0.47
1:B:68:ASN:N	1:B:68:ASN:ND2	2.62	0.47
1:C:68:ASN:N	1:C:68:ASN:ND2	2.62	0.47
1:H:156:VAL:CG1	1:H:172:ILE:HG12	2.45	0.47
1:G:130:PHE:O	1:G:134:ILE:HG22	2.14	0.47
1:G:180:ASP:HB2	2:G:1036:HOH:O	2.13	0.47
1:G:240:LYS:O	1:G:243:TYR:HB3	2.15	0.47
1:G:293:LYS:CG	1:G:294:GLU:H	2.28	0.47
1:I:153:CYS:HB2	1:I:189:THR:HG22	1.97	0.47
1:K:291:PRO:HB2	1:K:296:THR:HG23	1.97	0.47
1:L:171:ILE:O	1:L:175:MSE:HE3	2.15	0.47
1:H:89:PRO:HG3	1:H:123:TYR:CE2	2.49	0.47
1:I:4:ILE:HD12	1:I:4:ILE:N	2.28	0.47
1:L:66:GLY:C	1:L:68:ASN:H	2.18	0.47
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.81	0.47
1:C:273:HIS:O	1:C:277:VAL:HG23	2.14	0.47
1:E:7:VAL:O	1:E:11:ILE:HG13	2.14	0.47
1:E:171:ILE:N	1:E:171:ILE:HD12	2.30	0.47
1:E:293:LYS:CD	1:E:294:GLU:H	2.28	0.47
1:F:28:SER:HB3	1:F:31:VAL:CG2	2.37	0.47
1:K:134:ILE:HG23	1:K:135:THR:H	1.76	0.47
1:J:11:ILE:CG2	1:J:54:LEU:HD13	2.45	0.46
1:A:293:LYS:HG2	1:A:294:GLU:N	2.29	0.46
1:A:173:LYS:N	1:A:174:PRO:HD2	2.31	0.46
1:B:245:PHE:O	1:B:249:LYS:HA	2.15	0.46
1:C:93:ASP:O	1:C:97:GLN:HG3	2.15	0.46
1:C:176:TYR:HB3	1:C:216:GLN:OE1	2.16	0.46
1:D:134:ILE:HG23	1:D:135:THR:N	2.30	0.46
1:D:294:GLU:O	1:D:297:MET:HB3	2.15	0.46
1:H:73:ASN:O	1:H:77:LYS:HG3	2.15	0.46
1:I:100:GLU:CB	1:I:101:PRO:HD3	2.45	0.46
1:J:134:ILE:HG23	1:J:135:THR:H	1.78	0.46
1:L:248:ASP:O	1:L:249:LYS:C	2.54	0.46
1:F:171:ILE:HD12	1:F:171:ILE:N	2.30	0.46
1:I:93:ASP:HB2	1:I:94:LYS:HZ3	1.80	0.46
1:A:251:ILE:HB	1:F:289:PHE:CE1	2.51	0.46
1:D:3:LYS:O	1:D:7:VAL:HG23	2.16	0.46
1:H:4:ILE:HG22	1:H:6:SER:N	2.31	0.46
1:H:4:ILE:HG22	1:H:6:SER:H	1.79	0.46
1:J:103:ARG:HG2	1:J:103:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:MET:HA	1:C:297:MET:CE	2.45	0.46
1:H:187:ASP:O	1:H:191:GLN:HG3	2.15	0.46
1:I:171:ILE:HD12	1:I:171:ILE:N	2.30	0.46
1:I:291:PRO:HB2	1:I:296:THR:HG23	1.98	0.46
1:J:261:ILE:HG12	1:J:276:LEU:HB3	1.98	0.46
1:B:24:SER:O	1:B:53:ARG:NH2	2.43	0.46
1:C:251:ILE:HB	1:K:289:PHE:CE1	2.51	0.46
1:G:187:ASP:O	1:G:190:ILE:HG12	2.15	0.46
1:G:257:ALA:O	1:G:261:ILE:HG13	2.16	0.46
1:L:27:MSE:CE	1:L:40:ARG:HH22	2.28	0.46
1:L:279:GLU:O	1:L:283:ILE:HG12	2.16	0.46
1:L:297:MET:HE2	1:L:297:MET:HA	1.98	0.46
1:A:237:ASN:O	1:A:241:GLN:HG2	2.15	0.46
1:B:87:THR:C	1:B:89:PRO:HD3	2.36	0.46
1:G:93:ASP:O	1:G:97:GLN:HG3	2.16	0.46
1:I:293:LYS:HG2	1:I:294:GLU:N	2.31	0.46
2:K:932:HOH:O	1:L:14:GLU:HG2	2.16	0.46
1:C:110:PHE:O	1:C:113:TYR:HB3	2.15	0.46
1:H:68:ASN:HD22	1:H:68:ASN:H	1.62	0.46
1:H:274:ARG:O	1:H:278:GLU:HG3	2.15	0.46
1:K:72:VAL:HG13	1:K:73:ASN:N	2.30	0.46
1:B:156:VAL:CG1	1:B:172:ILE:HG12	2.46	0.45
1:D:173:LYS:HB2	1:D:174:PRO:HD3	1.98	0.45
1:F:88:ASN:HB3	1:F:91:LEU:HD12	1.97	0.45
1:I:23:TYR:O	1:I:26:ILE:N	2.36	0.45
1:J:250:ASN:HD22	1:J:251:ILE:N	2.13	0.45
1:A:85:ILE:HD11	1:A:95:ASN:OD1	2.16	0.45
1:E:43:SER:HA	1:F:43:SER:HA	1.98	0.45
1:F:103:ARG:HG2	1:F:103:ARG:HH11	1.81	0.45
1:F:108:GLN:O	1:F:112:ILE:HG13	2.16	0.45
1:G:72:VAL:HG13	1:G:73:ASN:N	2.31	0.45
1:I:37:ALA:O	1:I:38:ASP:HB2	2.16	0.45
1:J:165:TYR:OH	1:J:209:GLU:OE1	2.29	0.45
1:C:72:VAL:HG13	1:C:73:ASN:N	2.31	0.45
1:F:134:ILE:O	1:F:138:LEU:HG	2.16	0.45
1:C:134:ILE:HG23	1:C:135:THR:N	2.31	0.45
1:E:297:MET:HE2	1:E:297:MET:O	2.17	0.45
1:A:293:LYS:N	1:F:252:ASP:OD2	2.46	0.45
1:H:81:LEU:O	1:H:85:ILE:HG13	2.17	0.45
1:L:19:GLN:HG3	2:L:769:HOH:O	2.15	0.45
1:C:293:LYS:CD	1:C:294:GLU:N	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:LYS:HG2	1:H:294:GLU:N	2.30	0.45
1:K:296:THR:O	1:K:300:GLU:HB2	2.17	0.45
1:L:35:VAL:HG22	1:L:40:ARG:HD3	1.99	0.45
1:L:94:LYS:HB3	1:L:94:LYS:HZ2	1.80	0.45
1:A:68:ASN:HD22	1:A:68:ASN:N	1.91	0.45
1:D:226:ILE:HG13	1:D:227:SER:N	2.32	0.45
1:I:220:LEU:O	1:I:226:ILE:HG21	2.17	0.45
1:J:58:PHE:HE2	1:J:62:LEU:HD11	1.81	0.45
1:J:278:GLU:O	1:J:282:LYS:HG3	2.17	0.45
1:K:152:ASP:HB3	1:K:175:MSE:HE1	1.99	0.45
1:J:287:GLU:O	1:J:288:LYS:HB2	2.17	0.45
1:L:171:ILE:HG22	1:L:175:MSE:HE3	1.99	0.45
1:A:279:GLU:O	1:A:283:ILE:HG12	2.17	0.45
1:C:209:GLU:O	1:C:212:TYR:HB3	2.17	0.45
1:H:82:ILE:CD1	1:H:112:ILE:HG23	2.40	0.45
1:J:48:SER:O	1:J:51:SER:HB3	2.17	0.45
1:A:128:PRO:O	1:A:132:LYS:HD2	2.17	0.45
1:A:176:TYR:HB3	1:A:177:PRO:HA	1.98	0.45
1:D:293:LYS:H	1:D:293:LYS:CD	2.30	0.45
1:H:103:ARG:HG2	1:H:103:ARG:HH11	1.81	0.45
1:I:130:PHE:O	1:I:134:ILE:HG22	2.17	0.45
1:A:7:VAL:O	1:A:11:ILE:HG13	2.17	0.44
1:D:78:GLU:OE1	1:D:99:ILE:HD11	2.16	0.44
1:J:11:ILE:HG21	1:J:54:LEU:HD13	1.98	0.44
1:K:97:GLN:HE21	1:K:97:GLN:HB2	1.56	0.44
1:L:245:PHE:O	1:L:249:LYS:HD3	2.17	0.44
1:D:245:PHE:O	1:D:249:LYS:HD3	2.17	0.44
1:E:22:LEU:HB3	1:E:32:TYR:CE2	2.51	0.44
1:E:156:VAL:HG11	1:E:172:ILE:HG12	1.98	0.44
1:F:156:VAL:HG21	1:F:175:MSE:SE	2.68	0.44
1:H:63:ASN:HA	1:H:67:MSE:HB2	1.99	0.44
1:A:43:SER:HA	1:B:43:SER:HA	1.99	0.44
1:B:293:LYS:HD3	1:B:294:GLU:H	1.83	0.44
1:K:88:ASN:C	1:K:90:ASP:H	2.21	0.44
1:L:87:THR:O	1:L:89:PRO:HD3	2.17	0.44
1:E:72:VAL:HG13	1:E:73:ASN:N	2.32	0.44
1:J:32:TYR:CE1	1:J:36:GLU:CD	2.91	0.44
1:J:82:ILE:HD11	1:J:112:ILE:HG23	1.98	0.44
1:H:278:GLU:HG2	1:H:299:TYR:CD2	2.52	0.44
1:L:78:GLU:CD	1:L:99:ILE:HD11	2.37	0.44
1:L:88:ASN:HD22	1:L:91:LEU:HG	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HG13	1:A:73:ASN:H	1.83	0.44
1:I:30:SER:HB2	2:I:690:HOH:O	2.17	0.44
1:J:211:GLN:HB3	2:J:700:HOH:O	2.17	0.44
1:A:156:VAL:CG1	1:A:172:ILE:HG12	2.47	0.44
1:A:265:LYS:HB2	1:A:273:HIS:CD2	2.53	0.44
1:H:291:PRO:HB2	1:H:295:VAL:CG2	2.47	0.44
1:L:278:GLU:HA	1:L:299:TYR:HE2	1.82	0.44
1:F:192:THR:HB	2:F:978:HOH:O	2.17	0.44
1:J:5:GLY:HA2	2:J:1155:HOH:O	2.18	0.44
1:J:63:ASN:HA	1:J:67:MSE:HB2	2.00	0.44
1:L:134:ILE:HG23	1:L:135:THR:H	1.83	0.44
1:E:81:LEU:O	1:E:85:ILE:HG13	2.18	0.44
1:E:293:LYS:HG2	1:E:294:GLU:N	2.33	0.44
1:G:263:ILE:HG13	1:H:263:ILE:CG1	2.39	0.44
1:H:32:TYR:O	1:H:35:VAL:HB	2.18	0.44
1:H:234:LEU:HB3	1:H:264:PHE:CZ	2.53	0.44
1:J:91:LEU:O	1:J:92:PHE:C	2.55	0.44
1:L:68:ASN:HD22	1:L:68:ASN:H	1.61	0.44
1:L:258:VAL:HG21	1:L:292:PRO:HG3	2.00	0.44
1:A:293:LYS:CG	1:A:294:GLU:N	2.81	0.43
1:B:78:GLU:CD	1:B:99:ILE:HD11	2.38	0.43
1:D:273:HIS:O	1:D:277:VAL:HG23	2.18	0.43
1:G:195:LYS:HD3	1:G:235:GLU:OE2	2.18	0.43
1:I:176:TYR:HB3	1:I:177:PRO:HA	1.99	0.43
1:K:20:ILE:HA	1:K:23:TYR:CZ	2.53	0.43
1:A:277:VAL:HG12	1:A:299:TYR:HB2	1.99	0.43
1:B:23:TYR:OH	1:B:29:LYS:HE3	2.18	0.43
1:C:150:GLY:O	1:C:189:THR:HG21	2.18	0.43
1:D:11:ILE:HG22	1:D:54:LEU:HD22	1.99	0.43
1:D:23:TYR:HB2	1:D:27:MSE:HG3	1.99	0.43
1:I:292:PRO:HD2	1:I:295:VAL:HG21	2.00	0.43
1:J:23:TYR:CE1	1:J:29:LYS:HA	2.53	0.43
1:K:86:PHE:HD2	2:K:942:HOH:O	2.00	0.43
1:L:293:LYS:HD3	1:L:293:LYS:H	1.83	0.43
1:C:91:LEU:O	1:C:95:ASN:HB2	2.18	0.43
1:D:103:ARG:HG2	1:D:103:ARG:NH1	2.33	0.43
1:F:92:PHE:CE2	1:F:125:ILE:HG21	2.53	0.43
1:I:293:LYS:HD3	1:I:293:LYS:N	2.33	0.43
1:K:293:LYS:HG2	1:K:294:GLU:N	2.33	0.43
1:E:66:GLY:O	1:E:68:ASN:N	2.49	0.43
1:E:110:PHE:O	1:E:113:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:TYR:O	1:F:258:VAL:HG23	2.18	0.43
1:H:23:TYR:CZ	1:H:29:LYS:HB3	2.53	0.43
1:I:291:PRO:HD3	2:I:794:HOH:O	2.17	0.43
1:C:251:ILE:HD13	1:C:255:LEU:HG	2.01	0.43
1:G:100:GLU:HB3	1:G:101:PRO:CD	2.48	0.43
1:G:168:VAL:O	1:G:172:ILE:HG13	2.18	0.43
1:G:274:ARG:HG3	1:G:274:ARG:HH11	1.83	0.43
1:H:278:GLU:HA	1:H:299:TYR:CE2	2.53	0.43
1:J:10:GLN:HE21	1:J:10:GLN:HB3	1.57	0.43
1:A:74:GLU:HA	1:A:77:LYS:HD2	2.01	0.43
1:C:79:LYS:CD	1:C:112:ILE:HG12	2.49	0.43
1:C:187:ASP:O	1:C:190:ILE:HG12	2.18	0.43
1:F:100:GLU:HB3	1:F:101:PRO:CD	2.43	0.43
1:G:134:ILE:HG23	1:G:135:THR:N	2.34	0.43
1:H:118:SER:CB	1:H:161:ASN:HD21	2.32	0.43
1:I:4:ILE:H	1:I:4:ILE:CD1	2.29	0.43
1:E:9:LYS:O	1:E:13:GLN:HB2	2.18	0.43
1:G:132:LYS:NZ	1:G:132:LYS:HB3	2.34	0.43
1:J:295:VAL:HG23	1:J:296:THR:N	2.33	0.43
1:B:293:LYS:N	1:B:293:LYS:CD	2.81	0.43
1:C:81:LEU:O	1:C:85:ILE:HG13	2.19	0.43
1:I:3:LYS:O	1:I:3:LYS:HG3	2.17	0.43
1:K:91:LEU:HD23	1:K:94:LYS:HD3	2.01	0.43
1:L:187:ASP:O	1:L:190:ILE:HG12	2.18	0.43
1:C:71:SER:O	1:C:72:VAL:HB	2.19	0.43
1:H:23:TYR:HB2	1:H:27:MSE:HG3	2.01	0.43
1:H:289:PHE:CE1	1:I:289:PHE:CE2	3.06	0.43
1:I:148:PHE:CD1	1:I:175:MSE:HG2	2.53	0.43
1:J:176:TYR:HB3	1:J:177:PRO:HA	2.00	0.43
1:K:4:ILE:HG22	1:K:4:ILE:O	2.19	0.43
1:F:274:ARG:HE	1:F:274:ARG:HB2	1.43	0.43
1:H:4:ILE:CG2	1:H:6:SER:HB3	2.49	0.43
1:K:92:PHE:CE2	1:K:125:ILE:HG21	2.53	0.43
1:B:295:VAL:CG2	1:B:296:THR:N	2.82	0.42
1:B:297:MET:HE3	1:B:301:ASN:HD21	1.84	0.42
1:F:92:PHE:O	1:F:93:ASP:C	2.57	0.42
1:I:240:LYS:O	1:I:243:TYR:HB3	2.18	0.42
1:A:63:ASN:HB3	2:A:764:HOH:O	2.19	0.42
1:B:19:GLN:OE1	1:B:33:ILE:HD13	2.19	0.42
1:B:176:TYR:HB3	1:B:177:PRO:HA	2.00	0.42
1:B:203:MSE:CE	1:B:286:LYS:HD3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LEU:HD23	1:D:264:PHE:CZ	2.54	0.42
1:E:76:GLY:O	1:E:80:LEU:HD23	2.19	0.42
1:G:4:ILE:N	1:G:4:ILE:CD1	2.71	0.42
1:G:10:GLN:HE21	1:G:10:GLN:HB3	1.58	0.42
1:G:85:ILE:HG22	1:G:85:ILE:O	2.19	0.42
1:H:179:VAL:HG23	1:H:180:ASP:OD1	2.18	0.42
1:H:276:LEU:HD12	1:H:276:LEU:HA	1.79	0.42
1:H:4:ILE:HG23	1:H:38:ASP:OD2	2.18	0.42
1:I:159:LEU:C	1:I:161:ASN:H	2.22	0.42
1:K:278:GLU:O	1:K:282:LYS:HG3	2.18	0.42
1:L:4:ILE:N	1:L:4:ILE:CD1	2.79	0.42
1:A:47:LEU:HG	1:A:58:PHE:CE1	2.54	0.42
1:D:23:TYR:HB3	1:D:32:TYR:CD2	2.55	0.42
1:E:95:ASN:HA	1:E:98:ARG:HH12	1.84	0.42
1:I:29:LYS:O	1:I:33:ILE:HG12	2.19	0.42
1:I:98:ARG:CB	1:I:98:ARG:HH11	2.32	0.42
1:L:156:VAL:HG11	1:L:172:ILE:HG12	2.01	0.42
1:C:295:VAL:CG2	1:C:296:THR:N	2.83	0.42
1:I:295:VAL:HG23	1:I:296:THR:N	2.34	0.42
1:J:23:TYR:HD2	1:J:23:TYR:C	2.23	0.42
1:B:62:LEU:HB3	1:B:67:MSE:HG3	2.00	0.42
1:B:205:ARG:HH11	1:B:205:ARG:HG2	1.84	0.42
1:F:31:VAL:O	1:F:35:VAL:HG23	2.20	0.42
1:F:40:ARG:HG2	1:F:40:ARG:HH21	1.84	0.42
1:F:237:ASN:HB3	2:F:1072:HOH:O	2.20	0.42
1:G:94:LYS:HE3	1:G:94:LYS:CA	2.50	0.42
1:I:93:ASP:HB2	1:I:94:LYS:HZ1	1.84	0.42
1:I:110:PHE:O	1:I:113:TYR:HB3	2.19	0.42
1:I:133:THR:O	1:I:135:THR:N	2.52	0.42
1:K:134:ILE:CG2	1:K:135:THR:N	2.82	0.42
1:K:184:LYS:HB3	1:L:184:LYS:HD3	2.02	0.42
1:A:233:ASP:O	1:A:237:ASN:HB2	2.20	0.42
1:B:283:ILE:O	1:B:287:GLU:HG2	2.18	0.42
1:E:291:PRO:HB3	1:E:295:VAL:HG21	2.02	0.42
1:G:163:LEU:HA	1:G:164:PRO:HD3	1.94	0.42
1:J:288:LYS:O	1:J:289:PHE:HD2	2.03	0.42
1:A:110:PHE:O	1:A:113:TYR:HB3	2.19	0.42
1:C:197:ALA:HB1	1:C:213:TYR:CZ	2.55	0.42
1:D:235:GLU:O	1:D:238:TYR:HB3	2.20	0.42
1:F:134:ILE:CG2	1:F:135:THR:N	2.81	0.42
1:H:12:ARG:HG3	1:H:17:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:293:LYS:CG	1:I:294:GLU:N	2.83	0.42
1:J:139:LYS:O	1:J:143:ASP:HB2	2.20	0.42
1:K:265:LYS:HE2	1:K:265:LYS:HB3	1.93	0.42
1:A:255:LEU:HD21	1:F:255:LEU:HD21	2.01	0.42
1:F:203:MSE:HA	1:F:203:MSE:HE3	2.01	0.42
1:I:125:ILE:CG2	1:I:126:GLU:N	2.82	0.42
1:J:171:ILE:O	1:J:174:PRO:HD2	2.19	0.42
1:K:184:LYS:HE2	1:L:188:LEU:HD12	2.02	0.42
1:A:209:GLU:O	1:A:212:TYR:HB3	2.20	0.41
1:C:66:GLY:C	1:C:68:ASN:N	2.73	0.41
1:E:234:LEU:HD21	1:E:263:ILE:HG21	2.01	0.41
1:E:245:PHE:O	1:E:249:LYS:HD3	2.20	0.41
1:E:293:LYS:CG	1:E:294:GLU:N	2.82	0.41
1:H:72:VAL:CG1	1:H:73:ASN:N	2.80	0.41
1:H:134:ILE:HG23	1:H:135:THR:N	2.35	0.41
1:H:265:LYS:HB2	1:H:273:HIS:CD2	2.53	0.41
1:I:23:TYR:O	1:I:25:GLY:N	2.52	0.41
1:I:49:LYS:O	1:I:53:ARG:HG2	2.20	0.41
1:J:23:TYR:C	1:J:23:TYR:CD2	2.93	0.41
1:L:92:PHE:CZ	1:L:120:ALA:HB2	2.55	0.41
1:A:53:ARG:NE	2:A:924:HOH:O	2.52	0.41
1:C:168:VAL:O	1:C:172:ILE:HG13	2.19	0.41
1:C:191:GLN:HE21	1:C:217:PHE:HE1	1.68	0.41
1:L:205:ARG:HG2	1:L:205:ARG:NH1	2.34	0.41
1:C:148:PHE:CD1	1:C:148:PHE:N	2.89	0.41
1:D:22:LEU:HD11	1:D:54:LEU:HG	2.03	0.41
1:G:295:VAL:HG23	1:G:296:THR:N	2.35	0.41
1:I:68:ASN:N	1:I:68:ASN:ND2	2.69	0.41
1:I:263:ILE:HG13	1:J:263:ILE:CG1	2.45	0.41
1:J:9:LYS:O	1:J:13:GLN:HG3	2.21	0.41
1:K:4:ILE:HB	1:K:65:ALA:HB1	2.02	0.41
1:A:291:PRO:HG2	1:A:296:THR:CG2	2.49	0.41
1:E:195:LYS:HB3	1:E:195:LYS:HE3	1.91	0.41
1:C:144:LYS:HB2	1:C:144:LYS:HZ2	1.84	0.41
1:C:178:ILE:HG13	1:C:190:ILE:HD12	2.01	0.41
1:D:81:LEU:O	1:D:85:ILE:HG13	2.20	0.41
1:H:166:GLU:HA	1:H:166:GLU:OE2	2.21	0.41
1:I:39:SER:O	1:I:40:ARG:CB	2.69	0.41
1:I:171:ILE:HD12	1:I:171:ILE:H	1.84	0.41
1:D:291:PRO:HB2	1:D:295:VAL:HG23	2.01	0.41
1:F:265:LYS:CD	1:F:298:TYR:OH	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:VAL:CG1	1:H:73:ASN:H	2.29	0.41
1:H:251:ILE:CG2	1:I:292:PRO:HG3	2.48	0.41
1:J:223:ILE:HB	1:J:226:ILE:HB	2.03	0.41
1:L:203:MSE:O	1:L:286:LYS:NZ	2.51	0.41
1:L:263:ILE:HD13	1:L:263:ILE:HA	1.88	0.41
1:C:48:SER:O	1:C:51:SER:HB3	2.21	0.41
1:C:203:MSE:SE	1:C:279:GLU:HG3	2.70	0.41
1:D:171:ILE:O	1:D:174:PRO:HD2	2.21	0.41
1:E:267:ILE:CG2	2:F:1072:HOH:O	2.69	0.41
1:H:26:ILE:HD11	1:H:53:ARG:HE	1.86	0.41
1:I:108:GLN:O	1:I:112:ILE:HG13	2.21	0.41
1:I:148:PHE:CD1	1:I:148:PHE:N	2.88	0.41
1:J:134:ILE:CG2	1:J:135:THR:N	2.83	0.41
1:K:4:ILE:CG2	1:K:6:SER:HB3	2.51	0.41
1:K:20:ILE:H	1:K:20:ILE:HG13	1.62	0.41
1:K:20:ILE:O	1:K:24:SER:HB3	2.20	0.41
1:A:138:LEU:HD13	1:A:171:ILE:HD11	2.03	0.41
1:B:173:LYS:HB2	1:B:174:PRO:HD3	2.03	0.41
1:E:80:LEU:HD21	2:E:1026:HOH:O	2.21	0.41
1:H:9:LYS:O	1:H:13:GLN:HG3	2.20	0.41
1:H:110:PHE:O	1:H:114:LEU:HG	2.21	0.41
1:J:20:ILE:HA	1:J:23:TYR:CE2	2.55	0.41
1:J:88:ASN:HD22	1:J:91:LEU:HG	1.86	0.41
1:K:150:GLY:O	1:K:189:THR:HG21	2.21	0.41
1:A:297:MET:CE	1:A:301:ASN:HD21	2.34	0.41
1:B:108:GLN:O	1:B:112:ILE:HG13	2.21	0.41
1:D:3:LYS:N	1:D:38:ASP:OD2	2.54	0.41
1:E:22:LEU:O	1:E:26:ILE:HD12	2.21	0.41
1:F:270:GLU:OE1	1:F:270:GLU:HA	2.21	0.41
1:G:98:ARG:NH1	1:G:98:ARG:HB3	2.36	0.41
1:G:103:ARG:HH21	1:G:133:THR:HB	1.86	0.41
1:H:72:VAL:CG2	1:H:73:ASN:N	2.74	0.41
1:I:134:ILE:HG23	1:I:135:THR:H	1.86	0.41
1:I:150:GLY:O	1:I:189:THR:HG21	2.21	0.41
1:J:292:PRO:O	1:J:295:VAL:HG22	2.20	0.41
1:K:173:LYS:HD3	1:K:173:LYS:HA	1.89	0.41
1:L:103:ARG:HG2	1:L:103:ARG:NH1	2.35	0.41
1:A:293:LYS:CD	1:A:294:GLU:H	2.33	0.41
1:D:62:LEU:HB3	1:D:67:MSE:HG3	2.03	0.41
1:D:234:LEU:HB3	1:D:264:PHE:CZ	2.56	0.41
1:F:98:ARG:NH1	1:F:98:ARG:CB	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:290:THR:HA	1:I:291:PRO:HD3	1.94	0.41
1:L:224:LYS:HZ2	1:L:225:ASN:HD21	1.65	0.41
1:A:245:PHE:O	1:A:249:LYS:HD3	2.20	0.40
1:B:203:MSE:O	1:B:286:LYS:NZ	2.54	0.40
1:D:271:ASP:HB2	2:D:797:HOH:O	2.20	0.40
1:E:173:LYS:HA	1:E:173:LYS:HD3	1.80	0.40
1:F:15:LEU:O	1:F:16:ASN:HB2	2.21	0.40
1:G:290:THR:HB	1:J:250:ASN:HA	2.03	0.40
1:I:78:GLU:HA	1:I:78:GLU:OE1	2.21	0.40
1:B:148:PHE:CG	1:B:175:MSE:HG2	2.56	0.40
1:E:267:ILE:HA	1:F:237:ASN:ND2	2.36	0.40
1:H:297:MET:HE2	1:H:297:MET:HA	2.03	0.40
1:I:131:ASN:HD22	1:I:131:ASN:HA	1.67	0.40
1:J:293:LYS:HA	1:J:296:THR:OG1	2.21	0.40
1:A:67:MSE:HE1	1:B:58:PHE:CG	2.56	0.40
1:C:290:THR:HB	1:K:250:ASN:HA	2.03	0.40
1:D:20:ILE:O	1:D:24:SER:HB3	2.21	0.40
1:E:173:LYS:HD2	2:E:863:HOH:O	2.20	0.40
1:F:94:LYS:O	1:F:97:GLN:HG2	2.22	0.40
1:G:235:GLU:O	1:G:238:TYR:HB3	2.20	0.40
1:I:94:LYS:CE	1:I:94:LYS:N	2.77	0.40
1:I:197:ALA:HB1	1:I:213:TYR:CZ	2.56	0.40
1:I:293:LYS:CD	1:I:294:GLU:H	2.35	0.40
1:D:95:ASN:HD22	1:D:98:ARG:NH2	2.05	0.40
1:F:40:ARG:HG2	1:F:40:ARG:NH2	2.36	0.40
1:I:248:ASP:O	1:I:249:LYS:C	2.58	0.40
1:J:62:LEU:O	1:J:67:MSE:HG2	2.21	0.40
1:A:290:THR:HB	1:F:250:ASN:HA	2.02	0.40
1:D:135:THR:HG22	1:D:139:LYS:HE2	2.03	0.40
1:D:252:ASP:HA	2:D:1232:HOH:O	2.21	0.40
1:E:166:GLU:OE2	1:E:166:GLU:HA	2.21	0.40
1:F:4:ILE:H	1:F:4:ILE:HG13	1.60	0.40
1:F:205:ARG:HG2	1:F:205:ARG:HH11	1.87	0.40
1:G:84:LYS:HB3	1:G:84:LYS:HE2	1.91	0.40
1:H:235:GLU:O	1:H:238:TYR:HB3	2.21	0.40
1:H:297:MET:HE1	1:H:301:ASN:HD21	1.85	0.40
1:J:110:PHE:O	1:J:113:TYR:HB3	2.21	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	294/317 (93%)	281 (96%)	10 (3%)	3 (1%)	15	13
1	B	294/317 (93%)	281 (96%)	11 (4%)	2 (1%)	22	21
1	C	293/317 (92%)	276 (94%)	10 (3%)	7 (2%)	6	3
1	D	293/317 (92%)	274 (94%)	17 (6%)	2 (1%)	22	21
1	E	293/317 (92%)	277 (94%)	13 (4%)	3 (1%)	15	13
1	F	293/317 (92%)	269 (92%)	21 (7%)	3 (1%)	15	13
1	G	292/317 (92%)	273 (94%)	16 (6%)	3 (1%)	15	13
1	H	292/317 (92%)	278 (95%)	11 (4%)	3 (1%)	15	13
1	I	294/317 (93%)	262 (89%)	27 (9%)	5 (2%)	9	4
1	J	292/317 (92%)	271 (93%)	18 (6%)	3 (1%)	15	13
1	K	292/317 (92%)	267 (91%)	22 (8%)	3 (1%)	15	13
1	L	292/317 (92%)	272 (93%)	17 (6%)	3 (1%)	15	13
All	All	3514/3804 (92%)	3281 (93%)	193 (6%)	40 (1%)	14	10

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LYS
1	C	72	VAL
1	C	249	LYS
1	E	92	PHE
1	F	24	SER
1	H	72	VAL
1	H	92	PHE
1	I	24	SER
1	I	40	ARG
1	I	134	ILE
1	L	92	PHE
1	L	249	LYS

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Mol	Chain	Res	Type
1	A	92	PHE
1	B	92	PHE
1	C	294	GLU
1	D	103	ARG
1	E	249	LYS
1	F	93	ASP
1	F	124	ASN
1	G	24	SER
1	G	92	PHE
1	C	67	MSE
1	C	103	ARG
1	J	92	PHE
1	J	300	GLU
1	K	124	ASN
1	C	74	GLU
1	E	67	MSE
1	H	93	ASP
1	K	294	GLU
1	A	294	GLU
1	D	72	VAL
1	G	93	ASP
1	I	101	PRO
1	I	124	ASN
1	J	24	SER
1	K	89	PRO
1	L	67	MSE
1	B	72	VAL
1	C	89	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	281/295 (95%)	273 (97%)	8 (3%)	43	52
1	B	281/295 (95%)	267 (95%)	14 (5%)	24	26
1	C	280/295 (95%)	272 (97%)	8 (3%)	42	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	280/295 (95%)	273 (98%)	7 (2%)	47	56
1	E	280/295 (95%)	269 (96%)	11 (4%)	32	38
1	F	280/295 (95%)	272 (97%)	8 (3%)	42	51
1	G	279/295 (95%)	270 (97%)	9 (3%)	39	47
1	H	279/295 (95%)	270 (97%)	9 (3%)	39	47
1	I	281/295 (95%)	268 (95%)	13 (5%)	27	30
1	J	279/295 (95%)	268 (96%)	11 (4%)	32	38
1	K	279/295 (95%)	269 (96%)	10 (4%)	35	42
1	L	279/295 (95%)	265 (95%)	14 (5%)	24	26
All	All	3358/3540 (95%)	3236 (96%)	122 (4%)	35	42

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	20	ILE
1	A	68	ASN
1	A	90	ASP
1	A	188	LEU
1	A	238	TYR
1	A	248	ASP
1	A	293	LYS
1	B	10	GLN
1	B	16	ASN
1	B	68	ASN
1	B	79	LYS
1	B	88	ASN
1	B	94	LYS
1	B	139	LYS
1	B	147	THR
1	B	188	LEU
1	B	195	LYS
1	B	276	LEU
1	B	279	GLU
1	B	288	LYS
1	B	293	LYS
1	C	20	ILE
1	C	124	ASN
1	C	149	PHE

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Mol	Chain	Res	Type
1	C	188	LEU
1	C	238	TYR
1	C	251	ILE
1	C	276	LEU
1	C	293	LYS
1	D	67	MSE
1	D	147	THR
1	D	188	LEU
1	D	276	LEU
1	D	279	GLU
1	D	293	LYS
1	D	301	ASN
1	E	3	LYS
1	E	10	GLN
1	E	68	ASN
1	E	147	THR
1	E	188	LEU
1	E	251	ILE
1	E	263	ILE
1	E	279	GLU
1	E	289	PHE
1	E	293	LYS
1	E	294	GLU
1	F	67	MSE
1	F	68	ASN
1	F	100	GLU
1	F	144	LYS
1	F	188	LEU
1	F	276	LEU
1	F	279	GLU
1	F	293	LYS
1	G	4	ILE
1	G	10	GLN
1	G	68	ASN
1	G	94	LYS
1	G	132	LYS
1	G	211	GLN
1	G	276	LEU
1	G	279	GLU
1	G	293	LYS
1	H	29	LYS
1	H	68	ASN

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Mol	Chain	Res	Type
1	H	147	THR
1	H	188	LEU
1	H	234	LEU
1	H	237	ASN
1	H	271	ASP
1	H	276	LEU
1	H	293	LYS
1	I	53	ARG
1	I	68	ASN
1	I	84	LYS
1	I	97	GLN
1	I	102	LYS
1	I	131	ASN
1	I	135	THR
1	I	188	LEU
1	I	195	LYS
1	I	237	ASN
1	I	279	GLU
1	I	289	PHE
1	I	293	LYS
1	J	10	GLN
1	J	23	TYR
1	J	93	ASP
1	J	97	GLN
1	J	188	LEU
1	J	248	ASP
1	J	250	ASN
1	J	276	LEU
1	J	279	GLU
1	J	293	LYS
1	J	296	THR
1	K	4	ILE
1	K	68	ASN
1	K	80	LEU
1	K	94	LYS
1	K	97	GLN
1	K	147	THR
1	K	166	GLU
1	K	188	LEU
1	K	270	GLU
1	K	293	LYS
1	L	10	GLN

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Mol	Chain	Res	Type
1	L	67	MSE
1	L	68	ASN
1	L	94	LYS
1	L	147	THR
1	L	188	LEU
1	L	195	LYS
1	L	237	ASN
1	L	238	TYR
1	L	276	LEU
1	L	279	GLU
1	L	289	PHE
1	L	293	LYS
1	L	296	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	68	ASN
1	A	88	ASN
1	A	95	ASN
1	A	97	GLN
1	A	108	GLN
1	A	131	ASN
1	A	161	ASN
1	A	191	GLN
1	A	211	GLN
1	A	215	ASN
1	A	225	ASN
1	A	237	ASN
1	A	244	GLN
1	A	273	HIS
1	A	301	ASN
1	B	10	GLN
1	B	16	ASN
1	B	68	ASN
1	B	88	ASN
1	B	95	ASN
1	B	97	GLN
1	B	108	GLN
1	B	122	HIS
1	B	161	ASN

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Mol	Chain	Res	Type
1	B	191	GLN
1	B	215	ASN
1	B	237	ASN
1	B	244	GLN
1	B	262	ASN
1	B	273	HIS
1	B	301	ASN
1	C	10	GLN
1	C	63	ASN
1	C	68	ASN
1	C	88	ASN
1	C	95	ASN
1	C	97	GLN
1	C	108	GLN
1	C	124	ASN
1	C	131	ASN
1	C	191	GLN
1	C	215	ASN
1	C	273	HIS
1	C	301	ASN
1	D	10	GLN
1	D	63	ASN
1	D	68	ASN
1	D	88	ASN
1	D	95	ASN
1	D	97	GLN
1	D	108	GLN
1	D	131	ASN
1	D	158	ASN
1	D	161	ASN
1	D	191	GLN
1	D	215	ASN
1	D	225	ASN
1	D	244	GLN
1	D	273	HIS
1	E	10	GLN
1	E	16	ASN
1	E	68	ASN
1	E	88	ASN
1	E	95	ASN
1	E	97	GLN
1	E	108	GLN

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Mol	Chain	Res	Type
1	E	131	ASN
1	E	161	ASN
1	E	191	GLN
1	E	211	GLN
1	E	215	ASN
1	E	225	ASN
1	E	273	HIS
1	E	301	ASN
1	F	10	GLN
1	F	68	ASN
1	F	97	GLN
1	F	108	GLN
1	F	131	ASN
1	F	158	ASN
1	F	161	ASN
1	F	191	GLN
1	F	211	GLN
1	F	215	ASN
1	F	259	ASN
1	F	273	HIS
1	G	10	GLN
1	G	68	ASN
1	G	97	GLN
1	G	108	GLN
1	G	131	ASN
1	G	158	ASN
1	G	161	ASN
1	G	191	GLN
1	G	204	ASN
1	G	215	ASN
1	G	237	ASN
1	G	244	GLN
1	G	250	ASN
1	G	259	ASN
1	H	68	ASN
1	H	97	GLN
1	H	108	GLN
1	H	131	ASN
1	H	158	ASN
1	H	161	ASN
1	H	191	GLN
1	H	215	ASN

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Mol	Chain	Res	Type
1	H	225	ASN
1	H	237	ASN
1	H	244	GLN
1	H	262	ASN
1	H	273	HIS
1	H	301	ASN
1	I	68	ASN
1	I	95	ASN
1	I	97	GLN
1	I	108	GLN
1	I	121	HIS
1	I	131	ASN
1	I	158	ASN
1	I	161	ASN
1	I	191	GLN
1	I	211	GLN
1	I	215	ASN
1	I	225	ASN
1	I	237	ASN
1	I	244	GLN
1	J	10	GLN
1	J	19	GLN
1	J	88	ASN
1	J	95	ASN
1	J	108	GLN
1	J	131	ASN
1	J	161	ASN
1	J	191	GLN
1	J	211	GLN
1	J	215	ASN
1	J	225	ASN
1	J	244	GLN
1	J	250	ASN
1	J	273	HIS
1	K	68	ASN
1	K	97	GLN
1	K	108	GLN
1	K	131	ASN
1	K	158	ASN
1	K	191	GLN
1	K	211	GLN
1	K	215	ASN

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Mol	Chain	Res	Type
1	K	237	ASN
1	K	244	GLN
1	K	273	HIS
1	L	16	ASN
1	L	68	ASN
1	L	88	ASN
1	L	97	GLN
1	L	108	GLN
1	L	131	ASN
1	L	191	GLN
1	L	211	GLN
1	L	215	ASN
1	L	225	ASN
1	L	244	GLN
1	L	259	ASN
1	L	273	HIS
1	L	301	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	294/317 (92%)	0.11	9 (3%) 49 52	17, 40, 79, 114	0
1	B	294/317 (92%)	0.15	13 (4%) 34 37	12, 39, 75, 117	0
1	C	293/317 (92%)	0.41	16 (5%) 25 27	25, 52, 93, 113	0
1	D	293/317 (92%)	0.32	16 (5%) 25 27	20, 46, 88, 119	0
1	E	293/317 (92%)	0.22	13 (4%) 34 37	22, 45, 86, 114	0
1	F	293/317 (92%)	0.45	26 (8%) 9 10	24, 52, 98, 118	0
1	G	292/317 (92%)	0.42	18 (6%) 20 22	27, 56, 95, 112	0
1	H	292/317 (92%)	0.45	20 (6%) 17 18	25, 52, 95, 130	0
1	I	294/317 (92%)	0.61	35 (11%) 4 3	29, 64, 110, 124	0
1	J	292/317 (92%)	0.30	23 (7%) 12 14	23, 49, 98, 114	0
1	K	292/317 (92%)	0.36	10 (3%) 45 47	22, 47, 95, 112	0
1	L	292/317 (92%)	0.33	17 (5%) 23 25	23, 49, 89, 126	0
All	All	3514/3804 (92%)	0.34	216 (6%) 21 23	12, 49, 96, 130	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	299	TYR	9.1
1	H	301	ASN	8.3
1	I	91	LEU	8.3
1	H	300	GLU	7.6
1	H	297	MET	7.1
1	L	301	ASN	6.8
1	L	297	MET	6.5
1	I	92	PHE	6.5
1	D	297	MET	6.4
1	L	299	TYR	6.1
1	D	299	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	296	THR	5.9
1	H	296	THR	5.8
1	H	298	TYR	5.7
1	L	300	GLU	5.6
1	D	300	GLU	5.4
1	B	297	MET	5.4
1	B	299	TYR	5.3
1	I	102	LYS	5.2
1	I	297	MET	5.2
1	C	297	MET	5.2
1	J	297	MET	5.0
1	A	301	ASN	4.9
1	I	88	ASN	4.9
1	C	299	TYR	4.8
1	H	295	VAL	4.8
1	I	86	PHE	4.8
1	E	297	MET	4.7
1	D	301	ASN	4.7
1	G	91	LEU	4.6
1	B	301	ASN	4.6
1	I	90	ASP	4.6
1	K	71	SER	4.5
1	E	299	TYR	4.4
1	E	26	ILE	4.4
1	C	300	GLU	4.4
1	F	300	GLU	4.4
1	J	31	VAL	4.3
1	C	301	ASN	4.2
1	D	298	TYR	4.2
1	I	123	TYR	4.2
1	B	300	GLU	4.2
1	F	91	LEU	4.2
1	K	298	TYR	4.1
1	H	289	PHE	4.1
1	F	86	PHE	3.9
1	I	87	THR	3.9
1	L	296	THR	3.8
1	G	300	GLU	3.8
1	C	87	THR	3.8
1	F	123	TYR	3.7
1	I	125	ILE	3.7
1	F	301	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	293	LYS	3.6
1	G	87	THR	3.6
1	J	22	LEU	3.5
1	G	298	TYR	3.5
1	I	84	LYS	3.5
1	L	294	GLU	3.5
1	C	80	LEU	3.5
1	G	295	VAL	3.5
1	B	298	TYR	3.5
1	H	71	SER	3.5
1	J	300	GLU	3.4
1	K	299	TYR	3.4
1	C	144	LYS	3.4
1	I	299	TYR	3.4
1	A	297	MET	3.4
1	E	300	GLU	3.4
1	F	298	TYR	3.4
1	I	296	THR	3.4
1	G	297	MET	3.4
1	A	299	TYR	3.3
1	J	20	ILE	3.3
1	F	299	TYR	3.3
1	K	91	LEU	3.3
1	J	298	TYR	3.3
1	I	295	VAL	3.3
1	I	124	ASN	3.3
1	L	298	TYR	3.3
1	E	90	ASP	3.3
1	C	68	ASN	3.2
1	D	39	SER	3.2
1	G	299	TYR	3.2
1	I	98	ARG	3.2
1	D	71	SER	3.1
1	J	17	TYR	3.1
1	J	24	SER	3.1
1	J	299	TYR	3.1
1	I	94	LYS	3.1
1	E	295	VAL	3.1
1	F	95	ASN	3.1
1	C	91	LEU	3.1
1	I	300	GLU	3.1
1	I	298	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	107	LEU	3.0
1	I	71	SER	3.0
1	I	95	ASN	3.0
1	F	94	LYS	2.9
1	I	89	PRO	2.9
1	D	294	GLU	2.9
1	G	83	SER	2.9
1	I	101	PRO	2.9
1	H	86	PHE	2.9
1	I	96	PHE	2.9
1	F	72	VAL	2.9
1	K	86	PHE	2.8
1	K	31	VAL	2.8
1	F	85	ILE	2.8
1	F	125	ILE	2.8
1	E	301	ASN	2.8
1	F	84	LYS	2.8
1	G	301	ASN	2.8
1	H	124	ASN	2.8
1	F	92	PHE	2.8
1	J	289	PHE	2.8
1	B	68	ASN	2.8
1	C	207	LEU	2.8
1	K	301	ASN	2.8
1	H	29	LYS	2.8
1	F	295	VAL	2.8
1	G	68	ASN	2.8
1	C	84	LYS	2.8
1	F	20	ILE	2.8
1	E	124	ASN	2.8
1	J	68	ASN	2.8
1	L	126	GLU	2.8
1	F	144	LYS	2.7
1	C	298	TYR	2.7
1	D	23	TYR	2.7
1	I	83	SER	2.7
1	E	298	TYR	2.7
1	H	123	TYR	2.6
1	B	123	TYR	2.6
1	H	294	GLU	2.6
1	I	224	LYS	2.6
1	E	25	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	26	ILE	2.6
1	J	33	ILE	2.6
1	E	71	SER	2.6
1	A	300	GLU	2.6
1	J	30	SER	2.5
1	D	295	VAL	2.5
1	E	86	PHE	2.5
1	J	296	THR	2.5
1	D	34	LYS	2.5
1	J	26	ILE	2.5
1	L	295	VAL	2.5
1	F	96	PHE	2.4
1	G	293	LYS	2.4
1	J	23	TYR	2.4
1	C	81	LEU	2.4
1	I	99	ILE	2.4
1	C	123	TYR	2.4
1	L	87	THR	2.4
1	A	294	GLU	2.4
1	A	293	LYS	2.3
1	I	39	SER	2.4
1	J	39	SER	2.4
1	H	33	ILE	2.3
1	H	23	TYR	2.3
1	J	9	LYS	2.3
1	B	274	ARG	2.3
1	J	71	SER	2.3
1	I	72	VAL	2.3
1	I	130	PHE	2.3
1	J	72	VAL	2.3
1	I	134	ILE	2.3
1	I	149	PHE	2.3
1	B	294	GLU	2.3
1	F	81	LEU	2.3
1	F	122	HIS	2.3
1	F	128	PRO	2.3
1	F	297	MET	2.3
1	B	295	VAL	2.3
1	L	72	VAL	2.3
1	F	88	ASN	2.3
1	H	87	THR	2.2
1	J	18	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	295	VAL	2.2
1	F	126	GLU	2.2
1	K	30	SER	2.2
1	G	134	ILE	2.2
1	A	295	VAL	2.2
1	J	35	VAL	2.2
1	F	294	GLU	2.2
1	B	30	SER	2.2
1	D	289	PHE	2.2
1	D	37	ALA	2.2
1	D	293	LYS	2.2
1	I	294	GLU	2.2
1	I	41	PRO	2.2
1	G	144	LYS	2.1
1	E	23	TYR	2.1
1	I	28	SER	2.1
1	G	4	ILE	2.1
1	K	20	ILE	2.1
1	L	33	ILE	2.1
1	G	115	GLY	2.1
1	G	125	ILE	2.1
1	J	81	LEU	2.1
1	L	91	LEU	2.1
1	L	123	TYR	2.1
1	G	94	LYS	2.1
1	G	127	VAL	2.1
1	H	139	LYS	2.1
1	F	80	LEU	2.1
1	K	300	GLU	2.0
1	L	122	HIS	2.0
1	D	286	LYS	2.0
1	A	91	LEU	2.0
1	H	125	ILE	2.0
1	B	71	SER	2.0
1	B	23	TYR	2.0
1	L	125	ILE	2.0
1	A	71	SER	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.