Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:29 AM GMT

PDB ID	:	3M4W
Title	:	Structural basis for the negative regulation of bacterial stress response by RseB
Authors	:	Kim, D.Y.; Kwon, E.; Choi, J.K.; Hwang, H.-Y.; Kim, K.K.
Deposited on	:	2010-03-12
Resolution	:	2.30 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 ⓘ symbol.

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

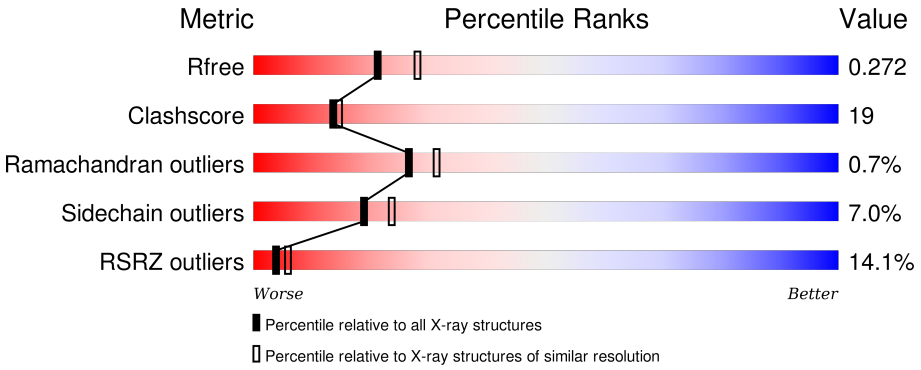
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	295	11% 63% 31%
1	B	295	8% 72% 22%
1	C	295	13% 60% 29% 6%
1	D	295	14% 55% 31% 9%
2	E	96	7% 26% 10% 7% 56%

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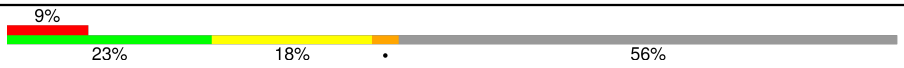
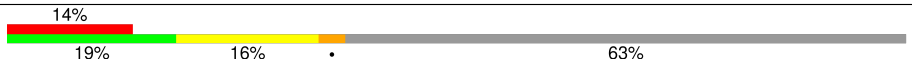
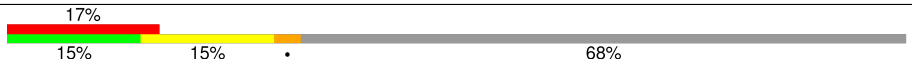
Mol	Chain	Length	Quality of chain
2	F	96	
2	G	96	
2	H	96	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10535 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 Sigma-E factor regulatory protein rseB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2263	1424	401	430	8			
1	B	284	Total	C	N	O	S	0	0	0
			2263	1424	401	430	8			
1	C	276	Total	C	N	O	S	0	0	0
			2206	1387	392	420	7			
1	D	269	Total	C	N	O	S	0	0	0
			2147	1349	378	413	7			

- Molecule 2 is a protein called Sigma-E factor negative regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	42	Total	C	N	O	S	0	0	0
			341	210	66	62	3			
2	F	42	Total	C	N	O	S	0	0	0
			341	210	66	62	3			
2	G	36	Total	C	N	O	S	0	0	0
			300	185	60	52	3			
2	H	31	Total	C	N	O	S	0	0	0
			247	157	44	43	3			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	F	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

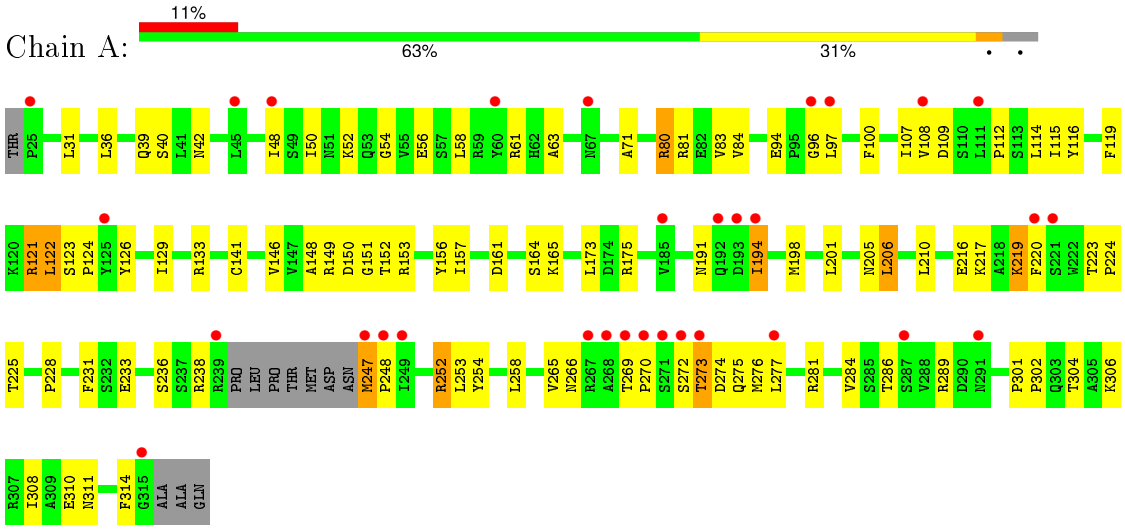
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	112	Total O 112 112	0	0
4	B	103	Total O 103 103	0	0
4	C	77	Total O 77 77	0	0
4	D	91	Total O 91 91	0	0
4	E	11	Total O 11 11	0	0
4	F	12	Total O 12 12	0	0
4	G	9	Total O 9 9	0	0
4	H	6	Total O 6 6	0	0

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.

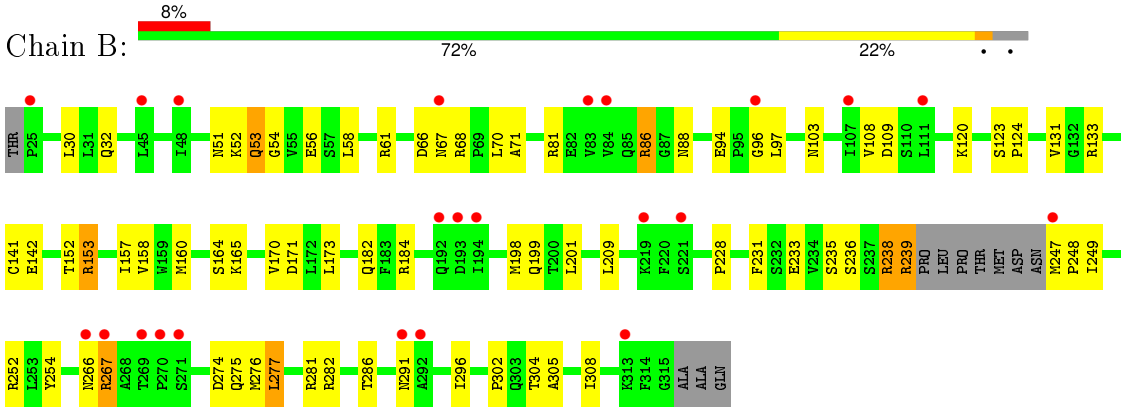
- Molecule 1: Sigma-E factor regulatory protein rseB

Chain A:



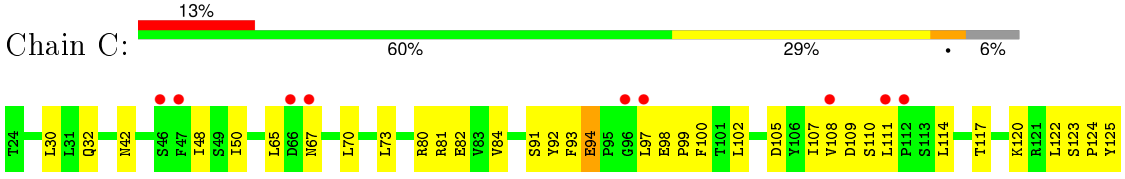
- Molecule 1: Sigma-E factor regulatory protein rseB

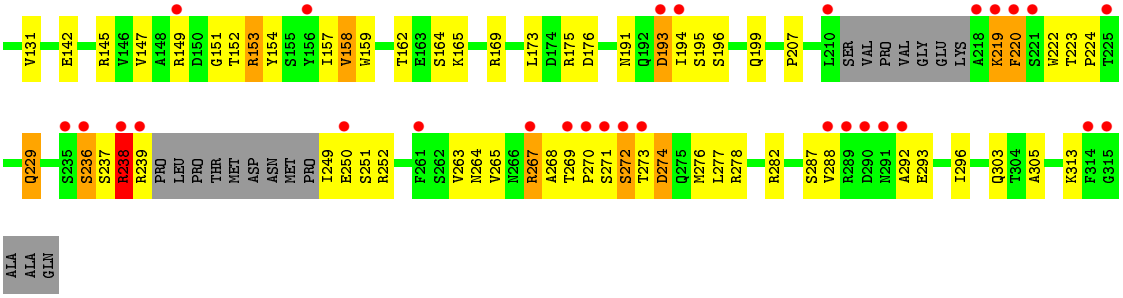
Chain B:



- Molecule 1: Sigma-E factor regulatory protein rseB

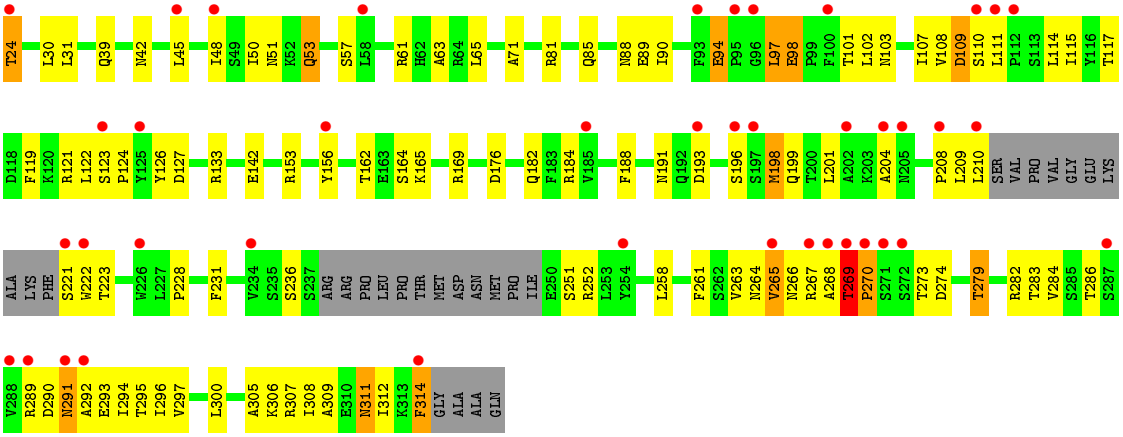
Chain C:





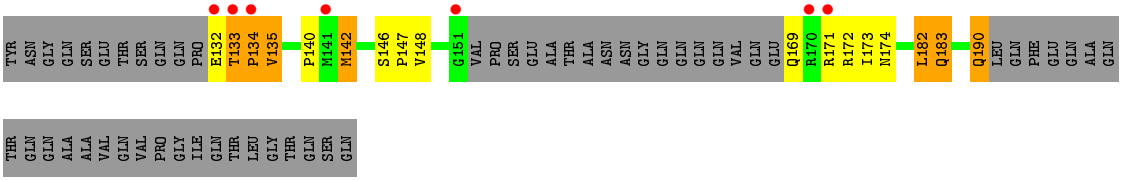
• Molecule 1: Sigma-E factor regulatory protein rseB

Chain D:



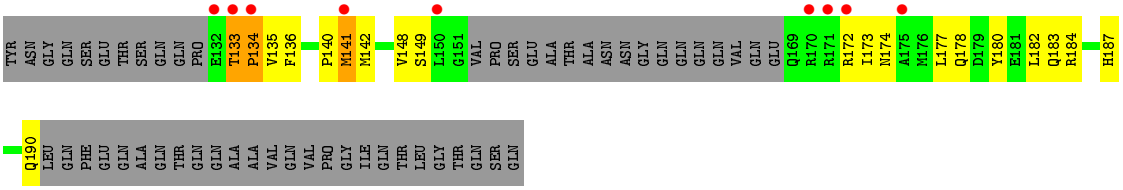
• Molecule 2: Sigma-E factor negative regulatory protein

Chain E:



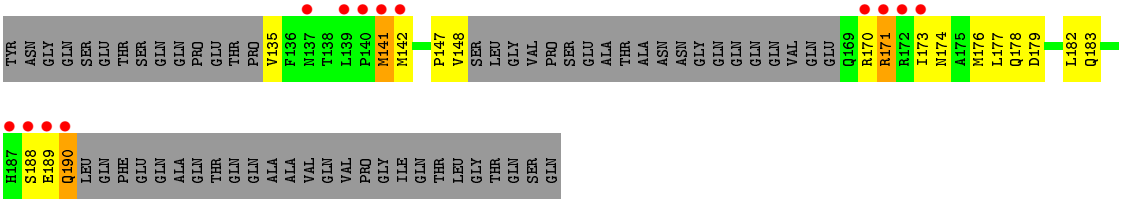
• Molecule 2: Sigma-E factor negative regulatory protein

Chain F:



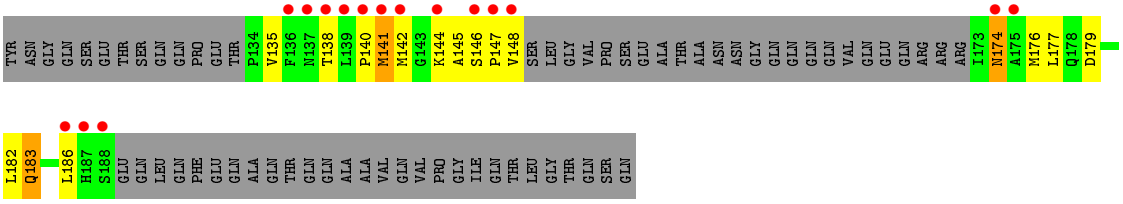
• Molecule 2: Sigma-E factor negative regulatory protein

Chain G:



- Molecule 2: Sigma-E factor negative regulatory protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.10Å 119.51Å 150.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 29.39 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.98-2.30) 92.6 (29.39-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.272 0.240 , 0.272	Depositor DCC
R_{free} test set	3325 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Outliers	4 of 66650 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10535	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.53 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6066e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.39	0/2307	0.67	0/3125
1	B	0.38	0/2307	0.71	0/3125
1	C	0.39	0/2247	0.70	2/3043 (0.1%)
1	D	0.40	0/2187	0.71	0/2965
2	E	0.32	0/345	0.71	1/461 (0.2%)
2	F	0.34	0/345	0.64	0/461
2	G	0.36	0/303	0.56	0/403
2	H	0.35	0/251	0.59	0/336
All	All	0.39	0/10292	0.69	3/13919 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	133	THR	N-CA-C	-6.90	92.38	111.00
1	C	238	ARG	N-CA-CB	-5.60	100.52	110.60
1	C	158	VAL	CB-CA-C	-5.18	101.56	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2263	0	2262	95	0
1	B	2263	0	2262	52	0
1	C	2206	0	2199	92	0
1	D	2147	0	2132	93	0
2	E	341	0	344	25	0
2	F	341	0	344	19	0
2	G	300	0	305	20	0
2	H	247	0	252	24	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	112	0	0	4	0
4	B	103	0	0	3	0
4	C	77	0	0	7	0
4	D	91	0	0	5	0
4	E	11	0	0	0	0
4	F	12	0	0	0	0
4	G	9	0	0	0	0
4	H	6	0	0	0	0
All	All	10535	0	10100	376	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 (376) 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:A:219:LYS:HD3	1:A:219:LYS:H	1.11	1.07
1:D:209:LEU:HD23	1:D:210:LEU:H	1.27	0.97
1:D:81:ARG:HD3	2:H:146:SER:HA	1.49	0.94
1:D:209:LEU:HD23	1:D:210:LEU:N	1.82	0.94
1:C:267:ARG:HH11	1:C:267:ARG:HG3	1.34	0.93
2:E:171:ARG:HA	2:E:174:ASN:HD22	1.34	0.93
1:D:286:THR:HG23	1:D:295:THR:HG22	1.53	0.89
1:B:267:ARG:HH11	1:B:267:ARG:HB3	1.35	0.88
1:B:30:LEU:HD13	1:B:142:GLU:HG2	1.56	0.88
1:A:219:LYS:HD3	1:A:219:LYS:N	1.90	0.85
2:E:133:THR:HG22	2:E:135:VAL:HG23	1.59	0.85
2:H:174:ASN:HB2	2:H:177:LEU:HD13	1.61	0.82
2:G:173:ILE:HG13	2:G:174:ASN:N	1.92	0.82
2:G:189:GLU:O	2:G:190:GLN:HB2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:TRP:CE2	1:D:265:VAL:HG21	2.15	0.81
1:B:266:ASN:HD21	2:F:172:ARG:HH12	1.25	0.81
1:C:222:TRP:NE1	1:C:265:VAL:HG11	1.95	0.80
1:A:194:ILE:H	1:A:194:ILE:HD13	1.44	0.79
1:C:114:LEU:HD21	1:C:158:VAL:HG22	1.65	0.79
1:D:294:ILE:HD13	1:D:312:ILE:HD12	1.63	0.79
1:C:267:ARG:CG	1:C:267:ARG:HH11	1.97	0.78
1:A:112:PRO:HD2	1:A:115:ILE:HD12	1.66	0.77
1:A:252:ARG:HG2	1:A:254:TYR:CE1	2.20	0.77
1:C:267:ARG:HG3	1:C:267:ARG:NH1	1.97	0.77
1:A:39:GLN:HE22	2:E:190:GLN:HE22	1.31	0.76
1:D:24:THR:O	1:D:24:THR:HG23	1.84	0.76
1:D:63:ALA:HB3	1:D:198:MET:HG2	1.68	0.75
2:G:173:ILE:HG13	2:G:174:ASN:H	1.47	0.75
1:D:264:ASN:HB2	1:D:295:THR:OG1	1.85	0.75
1:B:171:ASP:OD1	1:B:182:GLN:HG3	1.87	0.75
1:D:201:LEU:HA	1:D:204:ALA:HB2	1.69	0.74
1:C:114:LEU:O	1:C:117:THR:HG22	1.87	0.73
1:C:238:ARG:O	1:C:239:ARG:HB2	1.88	0.73
1:C:282:ARG:HE	2:G:177:LEU:HD22	1.54	0.73
1:B:233:GLU:OE2	1:B:236:SER:HB3	1.88	0.72
2:F:141:MET:H	2:F:141:MET:HE3	1.55	0.71
1:A:175:ARG:HD2	1:A:301:PRO:CG	2.20	0.71
1:B:96:GLY:O	1:B:97:LEU:HD23	1.90	0.71
1:C:100:PHE:CE1	1:C:102:LEU:HD11	2.24	0.71
1:A:228:PRO:HG2	1:A:231:PHE:CD1	2.27	0.69
1:A:233:GLU:OE2	1:A:236:SER:HB2	1.93	0.69
1:D:307:ARG:O	1:D:311:ASN:HB2	1.92	0.69
1:A:81:ARG:HG2	1:A:94:GLU:HG3	1.75	0.69
2:F:135:VAL:HG13	2:H:135:VAL:HG23	1.73	0.69
1:A:157:ILE:HD11	1:A:173:LEU:HD11	1.74	0.68
1:C:42:ASN:HB2	1:C:191:ASN:O	1.93	0.68
1:C:114:LEU:HD21	1:C:158:VAL:CG2	2.24	0.68
1:C:100:PHE:HE1	1:C:102:LEU:HD11	1.58	0.68
1:B:157:ILE:CD1	1:B:173:LEU:HD11	2.25	0.67
1:A:116:TYR:O	2:E:190:GLN:HG3	1.94	0.67
1:D:114:LEU:O	1:D:117:THR:HG22	1.94	0.67
1:D:101:THR:O	1:D:102:LEU:HD23	1.93	0.67
1:C:274:ASP:OD2	1:C:287:SER:HA	1.95	0.67
1:A:112:PRO:HD2	1:A:115:ILE:CD1	2.25	0.66
1:C:94:GLU:HG3	2:G:147:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ALA:CB	1:D:198:MET:HG2	2.26	0.66
1:B:51:ASN:OD1	1:B:53:GLN:HG2	1.95	0.66
1:D:209:LEU:O	1:D:210:LEU:HB2	1.95	0.66
1:A:54:GLY:HA2	2:E:134:PRO:O	1.95	0.66
1:B:266:ASN:ND2	2:F:172:ARG:HH12	1.94	0.66
1:B:275:GLN:HG2	1:B:286:THR:HB	1.77	0.66
2:G:141:MET:O	2:G:142:MET:HB3	1.95	0.66
1:B:157:ILE:HD11	1:B:173:LEU:HD11	1.78	0.65
2:E:169:GLN:O	2:E:172:ARG:HG2	1.97	0.65
1:B:123:SER:OG	1:B:124:PRO:HD3	1.96	0.65
1:A:157:ILE:CD1	1:A:173:LEU:HD11	2.27	0.65
2:H:141:MET:CE	2:H:141:MET:H	2.09	0.65
1:A:39:GLN:HE22	2:E:190:GLN:NE2	1.95	0.65
1:D:153:ARG:HD3	1:D:231:PHE:CZ	2.31	0.65
1:C:114:LEU:CD2	1:C:158:VAL:HG22	2.27	0.65
1:C:98:GLU:HB2	4:C:369:HOH:O	1.96	0.64
1:C:81:ARG:HG2	1:C:94:GLU:HG2	1.80	0.64
1:B:32:GLN:OE1	1:B:120:LYS:HG3	1.97	0.64
1:B:184:ARG:NH1	2:H:138:THR:HG22	2.13	0.64
1:B:238:ARG:HA	1:B:249:ILE:O	1.98	0.64
1:C:269:THR:HG22	1:C:269:THR:O	1.97	0.64
1:A:194:ILE:HD13	1:A:194:ILE:N	2.13	0.63
1:C:269:THR:HG23	1:C:272:SER:HB3	1.79	0.63
1:C:220:PHE:HB2	1:C:252:ARG:HH21	1.63	0.63
1:D:268:ALA:HB2	1:D:293:GLU:HB2	1.79	0.63
2:H:182:LEU:HD11	2:H:186:LEU:CD1	2.29	0.63
1:D:24:THR:O	1:D:24:THR:CG2	2.47	0.63
1:C:219:LYS:NZ	1:C:219:LYS:HB2	2.13	0.63
1:D:267:ARG:O	1:D:269:THR:HG22	1.98	0.62
1:C:249:ILE:HD12	1:C:264:ASN:HB3	1.78	0.62
1:D:111:LEU:HD13	1:D:115:ILE:HG21	1.80	0.62
1:A:219:LYS:CD	1:A:219:LYS:H	1.97	0.61
1:A:175:ARG:HD2	1:A:301:PRO:HG2	1.82	0.61
2:E:142:MET:HE2	2:E:142:MET:HA	1.81	0.61
1:C:175:ARG:HH12	1:C:303:GLN:NE2	1.99	0.61
1:D:209:LEU:CD2	1:D:210:LEU:H	2.06	0.61
2:F:141:MET:H	2:F:141:MET:CE	2.13	0.61
1:B:247:MET:N	1:B:248:PRO:CD	2.64	0.60
1:A:225:THR:HB	1:A:311:ASN:O	2.01	0.60
2:G:179:ASP:O	2:G:183:GLN:HG2	2.02	0.60
1:A:269:THR:HB	1:A:270:PRO:CD	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:OE2	1:A:252:ARG:HD3	2.00	0.60
1:A:150:ASP:O	1:A:152:THR:HG23	2.02	0.60
1:D:292:ALA:HB3	1:D:314:PHE:HE1	1.66	0.59
1:A:191:ASN:HB3	4:A:321:HOH:O	2.02	0.59
1:A:252:ARG:HG2	1:A:254:TYR:CZ	2.37	0.59
1:A:253:LEU:HD22	2:E:183:GLN:HG2	1.83	0.59
2:H:141:MET:HE3	2:H:141:MET:H	1.67	0.59
1:D:31:LEU:HB3	1:D:119:PHE:CE2	2.37	0.59
1:D:236:SER:OG	1:D:252:ARG:HG2	2.02	0.59
1:B:199:GLN:HG2	4:B:383:HOH:O	2.02	0.59
1:A:84:VAL:CG1	1:A:201:LEU:HD21	2.32	0.59
1:A:277:LEU:HD11	4:A:377:HOH:O	2.01	0.59
1:A:269:THR:HB	1:A:270:PRO:HD2	1.85	0.57
2:G:174:ASN:O	2:G:178:GLN:HG3	2.04	0.57
1:B:54:GLY:HA2	2:F:134:PRO:O	2.04	0.57
1:B:131:VAL:HG12	1:B:131:VAL:O	2.05	0.57
1:B:68:ARG:NH1	1:B:86:ARG:HD2	2.19	0.57
1:C:282:ARG:HH11	1:C:282:ARG:HB2	1.70	0.57
1:C:32:GLN:OE1	1:C:120:LYS:HG3	2.05	0.57
1:D:85:GLN:HG3	1:D:90:ILE:HD11	1.86	0.56
1:D:286:THR:HA	1:D:294:ILE:O	2.04	0.56
1:B:30:LEU:CD1	1:B:142:GLU:HG2	2.33	0.56
1:D:153:ARG:HD3	1:D:231:PHE:CE1	2.40	0.56
1:A:31:LEU:HB3	1:A:119:PHE:CD2	2.40	0.56
1:D:48:ILE:HD12	1:D:50:ILE:HD11	1.88	0.56
1:B:277:LEU:HA	4:B:409:HOH:O	2.04	0.56
1:A:306:LYS:O	1:A:310:GLU:HG2	2.05	0.56
2:F:148:VAL:HG13	2:F:148:VAL:O	2.06	0.56
2:E:142:MET:CE	2:E:142:MET:HA	2.36	0.56
1:B:228:PRO:HG2	1:B:231:PHE:CD1	2.41	0.56
2:G:142:MET:O	2:G:142:MET:HG3	2.05	0.55
1:C:250:GLU:HB2	1:C:265:VAL:HG12	1.88	0.55
1:D:296:ILE:CD1	1:D:309:ALA:HB2	2.37	0.55
1:D:269:THR:HG23	1:D:270:PRO:CD	2.37	0.55
2:F:133:THR:HG23	2:F:136:PHE:CD2	2.41	0.55
1:D:42:ASN:HB2	1:D:191:ASN:O	2.07	0.55
1:C:263:VAL:O	1:C:263:VAL:HG13	2.07	0.55
1:D:81:ARG:HG2	2:H:145:ALA:O	2.07	0.55
1:A:216:GLU:O	1:A:217:LYS:HD2	2.07	0.55
2:H:141:MET:O	2:H:142:MET:HB2	2.05	0.55
1:C:84:VAL:HG22	1:C:91:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:THR:HG23	1:D:295:THR:CG2	2.31	0.54
2:G:148:VAL:HG13	2:G:148:VAL:O	2.06	0.54
1:C:73:LEU:HD22	1:C:110:SER:HA	1.89	0.54
1:A:275:GLN:NE2	2:E:169:GLN:OE1	2.39	0.54
1:C:67:ASN:HA	4:C:16:HOH:O	2.07	0.54
2:H:177:LEU:HD12	2:H:177:LEU:N	2.22	0.54
1:D:269:THR:HG23	1:D:270:PRO:HD3	1.90	0.54
1:A:56:GLU:HB2	2:E:140:PRO:HG3	1.89	0.54
1:A:52:LYS:O	2:E:134:PRO:HB3	2.09	0.53
1:C:220:PHE:CB	1:C:252:ARG:HH21	2.19	0.53
1:C:250:GLU:HB2	1:C:265:VAL:CG1	2.38	0.53
1:B:267:ARG:NH1	1:B:267:ARG:HB3	2.14	0.53
2:F:148:VAL:HG21	2:F:182:LEU:HA	1.90	0.53
2:E:132:GLU:O	2:E:132:GLU:HG2	2.08	0.53
1:D:222:TRP:CZ2	1:D:265:VAL:HG21	2.43	0.53
1:D:108:VAL:O	1:D:109:ASP:HB2	2.08	0.53
1:D:266:ASN:O	1:D:292:ALA:HA	2.09	0.53
1:D:85:GLN:HG3	1:D:90:ILE:CD1	2.38	0.53
1:A:153:ARG:HD3	1:A:231:PHE:CE1	2.44	0.53
1:B:108:VAL:O	1:B:109:ASP:HB2	2.09	0.53
2:H:182:LEU:O	2:H:182:LEU:HD12	2.09	0.52
1:A:96:GLY:O	1:A:97:LEU:HD23	2.09	0.52
1:D:45:LEU:HD23	1:D:188:PHE:HB2	1.89	0.52
1:C:194:ILE:HG22	1:C:195:SER:O	2.09	0.52
1:C:142:GLU:HG2	1:C:162:THR:HG22	1.92	0.52
2:H:179:ASP:O	2:H:183:GLN:HB2	2.10	0.52
1:D:196:SER:HB3	4:D:396:HOH:O	2.09	0.52
1:C:222:TRP:CE2	1:C:265:VAL:HG11	2.45	0.52
1:D:296:ILE:HD11	1:D:309:ALA:HB2	1.90	0.51
1:A:108:VAL:O	1:A:109:ASP:HB2	2.08	0.51
1:C:152:THR:OG1	1:C:153:ARG:HD2	2.10	0.51
1:C:100:PHE:HZ	2:G:148:VAL:HG12	1.76	0.51
1:D:89:GLU:C	1:D:90:ILE:HD12	2.29	0.51
1:B:282:ARG:NH2	2:F:177:LEU:HG	2.26	0.51
1:B:158:VAL:HG23	1:B:170:VAL:HG22	1.92	0.51
1:A:50:ILE:CG2	2:G:135:VAL:HG22	2.40	0.51
1:D:264:ASN:HB3	2:H:176:MET:CE	2.41	0.51
1:A:228:PRO:HG2	1:A:231:PHE:CE1	2.44	0.51
1:A:194:ILE:CD1	1:A:194:ILE:H	2.06	0.51
1:A:224:PRO:HG2	1:A:254:TYR:OH	2.11	0.51
1:D:264:ASN:HB3	2:H:176:MET:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:THR:HG23	2:F:136:PHE:HD2	1.75	0.50
1:A:216:GLU:C	1:A:217:LYS:HD2	2.32	0.50
1:D:251:SER:HB3	1:D:264:ASN:OD1	2.11	0.50
1:A:252:ARG:HD2	1:A:254:TYR:OH	2.11	0.50
1:C:191:ASN:HB3	1:C:193:ASP:OD1	2.11	0.50
1:C:145:ARG:HG2	1:C:147:VAL:HG23	1.94	0.50
1:C:123:SER:N	1:C:124:PRO:CD	2.75	0.50
2:G:148:VAL:HG21	2:G:182:LEU:HA	1.93	0.50
1:D:50:ILE:CG2	2:F:135:VAL:HG12	2.41	0.50
1:D:81:ARG:CD	2:H:146:SER:HA	2.32	0.49
2:H:174:ASN:HB2	2:H:177:LEU:CD1	2.39	0.49
1:D:222:TRP:CH2	1:D:252:ARG:HG3	2.47	0.49
1:D:296:ILE:HD12	1:D:305:ALA:O	2.12	0.49
1:A:272:SER:O	1:A:273:THR:HG23	2.12	0.49
1:D:261:PHE:CD2	1:D:300:LEU:HD11	2.47	0.49
1:C:110:SER:O	1:C:111:LEU:HD23	2.13	0.49
1:D:142:GLU:HG2	1:D:162:THR:HG22	1.95	0.49
1:A:153:ARG:HD3	1:A:231:PHE:HE1	1.78	0.49
1:D:169:ARG:HH21	1:D:182:GLN:HE21	1.61	0.49
1:A:233:GLU:CD	1:A:252:ARG:HD3	2.32	0.49
1:C:99:PRO:HB2	1:C:207:PRO:HB3	1.94	0.49
1:B:164:SER:O	1:B:165:LYS:HB2	2.12	0.49
1:B:133:ARG:HA	1:B:141:CYS:O	2.12	0.49
1:A:198:MET:HE2	1:A:201:LEU:HD12	1.93	0.48
1:C:151:GLY:HA2	4:C:355:HOH:O	2.13	0.48
1:C:65:LEU:HD12	1:C:70:LEU:HD21	1.96	0.48
1:A:31:LEU:HB3	1:A:119:PHE:CE2	2.48	0.48
1:C:65:LEU:HD12	1:C:70:LEU:CD2	2.44	0.48
1:A:100:PHE:HB2	1:A:210:LEU:HD13	1.96	0.48
1:C:265:VAL:O	1:C:265:VAL:HG13	2.13	0.48
1:A:266:ASN:ND2	2:E:172:ARG:HH12	2.11	0.48
1:B:56:GLU:HG2	1:B:58:LEU:HG	1.95	0.48
1:B:252:ARG:HD3	1:B:254:TYR:OH	2.14	0.48
1:B:239:ARG:HD2	4:B:328:HOH:O	2.14	0.48
1:C:268:ALA:N	4:C:320:HOH:O	2.47	0.47
2:H:183:GLN:CA	2:H:183:GLN:HE21	2.26	0.47
1:B:296:ILE:HD12	1:B:305:ALA:O	2.13	0.47
1:D:123:SER:OG	1:D:124:PRO:HD3	2.14	0.47
1:A:80:ARG:HG2	1:A:80:ARG:O	2.14	0.47
1:B:81:ARG:HG2	1:B:94:GLU:HG3	1.95	0.47
1:B:53:GLN:HB2	2:F:141:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:GLN:HG2	2:E:169:GLN:O	2.15	0.47
1:C:100:PHE:CZ	2:G:148:VAL:HG12	2.50	0.47
1:B:302:PRO:HD2	1:C:176:ASP:HB3	1.97	0.47
1:A:274:ASP:HA	1:A:286:THR:O	2.14	0.47
1:A:94:GLU:HB2	2:E:147:PRO:HG2	1.96	0.47
1:A:48:ILE:HD12	1:A:50:ILE:HD11	1.96	0.47
1:A:50:ILE:HG23	2:G:135:VAL:HG22	1.96	0.47
1:A:304:THR:O	1:A:308:ILE:HG13	2.14	0.47
2:G:171:ARG:C	2:G:171:ARG:HE	2.18	0.47
1:A:121:ARG:O	1:A:124:PRO:HD2	2.14	0.47
1:A:39:GLN:NE2	2:E:190:GLN:OE1	2.48	0.47
2:E:148:VAL:O	2:E:148:VAL:HG13	2.15	0.47
1:A:164:SER:O	1:A:165:LYS:HB2	2.15	0.47
1:A:220:PHE:HB2	1:A:252:ARG:HH22	1.79	0.46
1:A:220:PHE:HB2	1:A:252:ARG:NH2	2.30	0.46
1:A:175:ARG:HD2	1:A:301:PRO:CB	2.44	0.46
2:F:135:VAL:HG13	2:H:135:VAL:CG2	2.43	0.46
1:D:61:ARG:O	1:D:71:ALA:HA	2.15	0.46
1:D:209:LEU:HD23	1:D:210:LEU:CA	2.43	0.46
2:H:174:ASN:N	2:H:174:ASN:HD22	2.12	0.46
1:C:153:ARG:HB3	4:C:10:HOH:O	2.15	0.46
1:C:124:PRO:C	1:C:149:ARG:HH12	2.19	0.46
2:G:170:ARG:CZ	2:G:170:ARG:HB3	2.45	0.46
1:C:97:LEU:HG	1:C:98:GLU:H	1.80	0.46
1:C:175:ARG:HH12	1:C:303:GLN:HE22	1.63	0.46
1:A:133:ARG:HA	1:A:141:CYS:O	2.15	0.46
1:C:32:GLN:HE21	1:C:32:GLN:HA	1.79	0.46
1:A:114:LEU:HD11	1:A:146:VAL:HG21	1.98	0.46
1:B:304:THR:O	1:B:308:ILE:HG13	2.16	0.46
1:D:228:PRO:HD3	1:D:308:ILE:HD11	1.97	0.46
1:D:88:ASN:O	1:D:103:ASN:HA	2.15	0.46
2:F:180:TYR:CZ	2:F:184:ARG:HD3	2.51	0.46
1:C:157:ILE:CD1	1:C:173:LEU:HD11	2.47	0.45
1:C:282:ARG:NH1	1:C:282:ARG:HB2	2.30	0.45
1:C:80:ARG:HB2	4:C:343:HOH:O	2.15	0.45
1:B:152:THR:OG1	1:B:153:ARG:HD2	2.17	0.45
1:C:222:TRP:NE1	1:C:265:VAL:CG1	2.73	0.45
1:C:249:ILE:CD1	2:G:176:MET:HE2	2.46	0.45
1:D:221:SER:OG	1:D:222:TRP:N	2.49	0.45
1:B:233:GLU:OE2	1:B:252:ARG:HG2	2.17	0.45
1:C:157:ILE:HD11	1:C:173:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:HG11	2:E:173:ILE:CG2	2.46	0.45
1:A:247:MET:SD	1:A:247:MET:N	2.90	0.45
1:A:161:ASP:O	1:A:165:LYS:HA	2.16	0.45
1:A:219:LYS:N	1:A:219:LYS:CD	2.61	0.45
2:E:133:THR:O	2:E:134:PRO:C	2.54	0.45
1:D:156:TYR:CE2	1:D:258:LEU:HD11	2.52	0.45
1:A:223:THR:HA	1:A:224:PRO:HD3	1.80	0.45
1:C:84:VAL:CG2	1:C:91:SER:HB2	2.46	0.45
2:G:171:ARG:HG2	2:G:171:ARG:O	2.17	0.45
1:C:108:VAL:O	1:C:109:ASP:HB2	2.16	0.45
1:D:267:ARG:HG2	1:D:291:ASN:ND2	2.31	0.44
1:A:198:MET:HE2	1:A:198:MET:HA	1.99	0.44
1:A:112:PRO:HA	4:A:422:HOH:O	2.17	0.44
1:C:219:LYS:HB2	1:C:219:LYS:HZ3	1.82	0.44
1:C:196:SER:O	1:C:199:GLN:HB2	2.16	0.44
1:D:164:SER:O	1:D:165:LYS:HB2	2.17	0.44
1:D:121:ARG:O	1:D:124:PRO:HD2	2.16	0.44
1:A:83:VAL:HG11	1:A:107:ILE:HG23	1.99	0.44
1:D:222:TRP:HH2	1:D:252:ARG:HG3	1.83	0.44
1:A:201:LEU:HD23	1:A:201:LEU:O	2.17	0.44
1:D:97:LEU:HD13	1:D:98:GLU:H	1.82	0.44
1:D:208:PRO:HA	4:D:407:HOH:O	2.16	0.44
1:C:269:THR:HA	1:C:272:SER:HB3	2.00	0.44
1:A:84:VAL:HG11	1:A:201:LEU:HD21	2.00	0.44
1:A:81:ARG:HD2	2:E:146:SER:HA	1.99	0.44
1:C:251:SER:HB2	1:C:264:ASN:OD1	2.18	0.44
2:H:182:LEU:HD11	2:H:186:LEU:HD11	2.00	0.44
1:C:73:LEU:HD22	1:C:110:SER:CB	2.48	0.44
1:D:30:LEU:HD13	1:D:142:GLU:HG3	2.00	0.44
1:D:53:GLN:HB3	2:H:140:PRO:HB3	1.99	0.44
1:D:31:LEU:HB3	1:D:119:PHE:CD2	2.53	0.44
1:D:109:ASP:O	2:H:144:LYS:HB3	2.17	0.44
1:B:276:MET:SD	1:B:302:PRO:HB3	2.58	0.44
1:D:222:TRP:CZ2	1:D:265:VAL:CG2	3.01	0.43
1:C:92:TYR:CE2	1:C:102:LEU:HD13	2.53	0.43
1:A:122:LEU:HG	1:A:126:TYR:CD1	2.53	0.43
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.86	0.43
1:D:122:LEU:HG	1:D:126:TYR:CD1	2.53	0.43
1:C:164:SER:O	1:C:165:LYS:HB2	2.16	0.43
1:D:97:LEU:HD13	1:D:98:GLU:N	2.33	0.43
1:C:94:GLU:HG3	2:G:147:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:SER:O	1:C:237:SER:HB3	2.19	0.43
1:D:283:THR:O	1:D:297:VAL:HA	2.18	0.43
1:D:153:ARG:HD3	1:D:231:PHE:HZ	1.78	0.43
2:H:147:PRO:O	2:H:148:VAL:C	2.56	0.43
1:C:267:ARG:HG2	1:C:292:ALA:HA	2.01	0.43
1:B:247:MET:N	1:B:248:PRO:HD3	2.33	0.43
1:A:123:SER:OG	1:A:124:PRO:HD3	2.19	0.43
1:A:276:MET:SD	1:A:302:PRO:HB3	2.59	0.43
1:D:223:THR:HG21	4:D:352:HOH:O	2.17	0.43
1:B:201:LEU:HD12	1:B:201:LEU:O	2.18	0.43
1:C:98:GLU:O	1:C:98:GLU:HG3	2.18	0.43
1:A:61:ARG:O	1:A:71:ALA:HA	2.19	0.43
1:B:30:LEU:HD22	1:B:160:MET:CE	2.49	0.42
1:D:296:ILE:HD11	1:D:309:ALA:N	2.33	0.42
1:C:131:VAL:HG12	1:C:131:VAL:O	2.18	0.42
1:D:107:ILE:CG2	1:D:110:SER:HB3	2.49	0.42
1:A:56:GLU:HG2	1:A:58:LEU:HG	2.01	0.42
1:A:42:ASN:HD22	1:A:63:ALA:HA	1.84	0.42
1:B:235:SER:OG	2:F:187:HIS:CE1	2.72	0.42
1:D:289:ARG:HG3	1:D:294:ILE:HD11	2.00	0.42
1:B:66:ASP:O	1:B:67:ASN:HB2	2.20	0.42
1:B:30:LEU:HD22	1:B:160:MET:HE1	2.01	0.42
1:D:101:THR:HG22	1:D:102:LEU:N	2.35	0.42
2:E:148:VAL:HG21	2:E:182:LEU:HA	2.01	0.42
1:D:94:GLU:HG3	1:D:94:GLU:O	2.20	0.42
1:A:275:GLN:HB2	1:A:286:THR:HB	2.02	0.42
1:A:124:PRO:O	1:A:149:ARG:NH1	2.52	0.42
1:A:302:PRO:HD2	1:D:176:ASP:HB3	2.02	0.42
1:D:263:VAL:HG23	1:D:263:VAL:O	2.18	0.42
1:A:266:ASN:ND2	2:E:172:ARG:NH1	2.67	0.42
1:A:238:ARG:HB2	1:A:238:ARG:HH11	1.84	0.42
1:D:191:ASN:C	1:D:193:ASP:N	2.73	0.42
1:C:296:ILE:HD12	1:C:305:ALA:O	2.19	0.42
1:C:145:ARG:HG2	1:C:147:VAL:CG2	2.50	0.41
1:B:182:GLN:OE1	1:B:184:ARG:HD2	2.20	0.41
1:C:276:MET:O	1:C:277:LEU:HD23	2.20	0.41
1:C:229:GLN:CA	1:C:229:GLN:HE21	2.32	0.41
1:C:223:THR:HA	1:C:224:PRO:HD3	1.90	0.41
1:D:221:SER:N	4:D:395:HOH:O	2.53	0.41
1:C:220:PHE:CE2	1:C:250:GLU:HG2	2.55	0.41
1:B:70:LEU:C	1:B:198:MET:HE1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ASN:OD1	1:D:53:GLN:HB2	2.21	0.41
1:C:122:LEU:HA	1:C:125:TYR:CE2	2.55	0.41
2:F:172:ARG:HE	2:F:172:ARG:HB2	1.71	0.41
1:C:267:ARG:HA	4:C:320:HOH:O	2.20	0.41
1:C:271:SER:O	1:C:272:SER:C	2.58	0.41
1:A:48:ILE:HA	1:A:56:GLU:O	2.20	0.41
1:A:148:ALA:HB3	4:A:417:HOH:O	2.20	0.41
1:D:53:GLN:HG2	2:H:141:MET:HE3	2.01	0.41
1:D:284:VAL:HA	1:D:296:ILE:O	2.21	0.41
1:C:98:GLU:HA	1:C:99:PRO:HD3	1.76	0.41
1:D:268:ALA:N	1:D:291:ASN:O	2.54	0.41
1:A:247:MET:N	1:A:248:PRO:CD	2.84	0.41
1:A:265:VAL:HG11	1:A:314:PHE:HE2	1.86	0.41
1:C:82:GLU:HG3	1:C:93:PHE:HB2	2.02	0.41
1:C:288:VAL:HG22	1:C:293:GLU:HG3	2.03	0.41
1:D:209:LEU:O	1:D:210:LEU:CB	2.65	0.41
1:A:94:GLU:HB2	2:E:147:PRO:CG	2.51	0.41
1:C:73:LEU:HD22	1:C:110:SER:CA	2.50	0.41
1:A:36:LEU:HD12	1:A:40:SER:OG	2.20	0.41
1:C:154:TYR:OH	1:C:278:ARG:NH2	2.48	0.41
1:B:103:ASN:ND2	1:B:209:LEU:HD11	2.36	0.41
1:B:53:GLN:HG3	2:F:140:PRO:HB2	2.03	0.40
1:D:291:ASN:CG	1:D:292:ALA:N	2.75	0.40
1:D:133:ARG:CZ	4:D:330:HOH:O	2.69	0.40
1:C:159:TRP:HB2	1:C:169:ARG:HB3	2.03	0.40
2:F:173:ILE:HA	2:F:173:ILE:HD13	1.88	0.40
1:B:53:GLN:HE21	1:B:53:GLN:HB3	1.52	0.40
1:C:102:LEU:HD12	1:C:102:LEU:N	2.37	0.40
1:C:107:ILE:CG2	1:C:110:SER:HB3	2.52	0.40
1:D:169:ARG:HG3	1:D:184:ARG:HG2	2.03	0.40
1:C:48:ILE:HD12	1:C:50:ILE:HD11	2.04	0.40
1:A:156:TYR:CD2	1:A:258:LEU:HD21	2.56	0.40
1:B:61:ARG:O	1:B:71:ALA:HA	2.22	0.40
1:D:279:THR:HG23	1:D:282:ARG:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	280/295 (95%)	260 (93%)	19 (7%)	1 (0%)	39 48
1	B	280/295 (95%)	271 (97%)	9 (3%)	0	100 100
1	C	270/295 (92%)	257 (95%)	11 (4%)	2 (1%)	26 31
1	D	263/295 (89%)	242 (92%)	19 (7%)	2 (1%)	24 27
2	E	38/96 (40%)	36 (95%)	1 (3%)	1 (3%)	7 4
2	F	38/96 (40%)	31 (82%)	5 (13%)	2 (5%)	2 1
2	G	32/96 (33%)	29 (91%)	2 (6%)	1 (3%)	5 3
2	H	27/96 (28%)	23 (85%)	4 (15%)	0	100 100
All	All	1228/1564 (78%)	1149 (94%)	70 (6%)	9 (1%)	26 31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	270	PRO
2	G	188	SER
1	C	270	PRO
2	F	149	SER
1	D	269	THR
1	C	272	SER
2	F	134	PRO
1	A	151	GLY
2	E	134	PRO

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	254/263 (97%)	241 (95%)	13 (5%)	29 39
1	B	254/263 (97%)	242 (95%)	12 (5%)	32 43
1	C	247/263 (94%)	233 (94%)	14 (6%)	25 34
1	D	242/263 (92%)	220 (91%)	22 (9%)	12 13
2	E	38/83 (46%)	33 (87%)	5 (13%)	5 5
2	F	38/83 (46%)	31 (82%)	7 (18%)	2 1
2	G	33/83 (40%)	30 (91%)	3 (9%)	12 13
2	H	28/83 (34%)	25 (89%)	3 (11%)	8 9
All	All	1134/1384 (82%)	1055 (93%)	79 (7%)	19 23

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	121	ARG
1	A	122	LEU
1	A	129	ILE
1	A	194	ILE
1	A	205	ASN
1	A	206	LEU
1	A	219	LYS
1	A	247	MET
1	A	252	ARG
1	A	273	THR
1	A	281	ARG
1	A	289	ARG
1	B	52	LYS
1	B	53	GLN
1	B	86	ARG
1	B	88	ASN
1	B	153	ARG
1	B	238	ARG
1	B	239	ARG
1	B	267	ARG
1	B	274	ASP
1	B	277	LEU
1	B	281	ARG
1	B	291	ASN

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Mol	Chain	Res	Type
1	C	30	LEU
1	C	94	GLU
1	C	105	ASP
1	C	153	ARG
1	C	193	ASP
1	C	219	LYS
1	C	220	PHE
1	C	229	GLN
1	C	236	SER
1	C	238	ARG
1	C	267	ARG
1	C	273	THR
1	C	274	ASP
1	C	313	LYS
1	D	24	THR
1	D	39	GLN
1	D	53	GLN
1	D	57	SER
1	D	65	LEU
1	D	94	GLU
1	D	97	LEU
1	D	98	GLU
1	D	109	ASP
1	D	127	ASP
1	D	198	MET
1	D	199	GLN
1	D	265	VAL
1	D	269	THR
1	D	273	THR
1	D	274	ASP
1	D	279	THR
1	D	290	ASP
1	D	291	ASN
1	D	306	LYS
1	D	311	ASN
1	D	314	PHE
2	E	135	VAL
2	E	142	MET
2	E	182	LEU
2	E	183	GLN
2	E	190	GLN
2	F	133	THR

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Mol	Chain	Res	Type
2	F	141	MET
2	F	142	MET
2	F	174	ASN
2	F	178	GLN
2	F	183	GLN
2	F	190	GLN
2	G	141	MET
2	G	171	ARG
2	G	190	GLN
2	H	141	MET
2	H	174	ASN
2	H	183	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	42	ASN
1	A	266	ASN
1	A	291	ASN
1	B	39	GLN
1	B	88	ASN
1	B	103	ASN
1	B	189	ASN
1	B	191	ASN
1	B	199	GLN
1	B	266	ASN
1	B	275	GLN
1	B	291	ASN
1	C	192	GLN
1	C	199	GLN
1	C	229	GLN
1	C	303	GLN
1	D	103	ASN
1	D	182	GLN
1	D	191	ASN
1	D	199	GLN
1	D	291	ASN
2	E	174	ASN
2	E	183	GLN
2	F	178	GLN
2	F	187	HIS

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Mol	Chain	Res	Type
2	F	190	GLN
2	H	174	ASN
2	H	183	GLN

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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	284/295 (96%)	0.57	31 (10%) 7 11	22, 44, 71, 102	0
1	B	284/295 (96%)	0.51	23 (8%) 15 21	23, 43, 72, 98	0
1	C	276/295 (93%)	0.63	38 (13%) 4 6	22, 44, 91, 111	0
1	D	269/295 (91%)	0.90	41 (15%) 3 5	24, 51, 91, 115	0
2	E	42/96 (43%)	1.19	7 (16%) 2 4	36, 60, 89, 97	0
2	F	42/96 (43%)	1.04	9 (21%) 1 2	39, 60, 83, 97	0
2	G	36/96 (37%)	1.74	13 (36%) 0 0	48, 75, 109, 113	0
2	H	31/96 (32%)	2.10	16 (51%) 0 0	51, 75, 96, 108	0
All	All	1264/1564 (80%)	0.75	178 (14%) 4 6	22, 48, 88, 115	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	271	SER	8.7
1	B	270	PRO	7.6
1	A	270	PRO	6.5
1	D	292	ALA	6.4
1	C	315	GLY	6.4
2	G	141	MET	6.2
1	C	271	SER	5.9
1	C	219	LYS	5.8
2	E	171	ARG	5.7
1	C	220	PHE	5.7
1	A	271	SER	5.7
2	G	171	ARG	5.6
1	C	314	PHE	5.5
1	D	222	TRP	5.5
1	D	96	GLY	5.4
1	B	193	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
2	E	132	GLU	5.3
2	H	140	PRO	4.8
1	C	96	GLY	4.7
2	H	141	MET	4.7
1	D	221	SER	4.6
1	D	267	ARG	4.6
1	B	194	ILE	4.5
1	B	267	ARG	4.5
1	D	202	ALA	4.4
2	H	137	ASN	4.3
2	E	134	PRO	4.2
2	F	132	GLU	4.2
2	F	171	ARG	4.2
1	B	271	SER	4.2
1	D	272	SER	4.1
2	G	170	ARG	4.0
1	D	234	VAL	4.0
1	D	95	PRO	4.0
1	B	192	GLN	3.9
1	D	270	PRO	3.8
1	D	205	ASN	3.8
2	E	141	MET	3.8
1	D	111	LEU	3.7
1	C	239	ARG	3.7
2	H	188	SER	3.7
1	D	210	LEU	3.7
1	D	314	PHE	3.7
1	D	254	TYR	3.7
1	D	287	SER	3.6
1	A	268	ALA	3.6
1	A	315	GLY	3.6
1	D	291	ASN	3.6
1	C	250	GLU	3.6
1	C	291	ASN	3.6
1	C	238	ARG	3.6
2	G	172	ARG	3.6
1	A	247	MET	3.5
2	H	139	LEU	3.5
2	F	170	ARG	3.5
1	D	269	THR	3.4
2	G	142	MET	3.4
1	B	25	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	272	SER	3.3
2	G	140	PRO	3.3
1	C	97	LEU	3.3
2	H	175	ALA	3.3
1	C	267	ARG	3.3
1	D	193	ASP	3.3
2	H	146	SER	3.2
2	G	137	ASN	3.2
2	F	141	MET	3.2
1	D	268	ALA	3.2
2	F	133	THR	3.2
2	H	136	PHE	3.2
2	G	139	LEU	3.1
1	A	194	ILE	3.1
1	D	204	ALA	3.1
1	C	221	SER	3.0
2	H	147	PRO	3.0
1	A	291	ASN	3.0
1	C	66	ASP	3.0
2	H	187	HIS	3.0
1	B	292	ALA	3.0
1	D	197	SER	3.0
1	C	112	PRO	3.0
1	D	226	TRP	3.0
1	D	125	TYR	2.9
2	H	148	VAL	2.9
1	A	97	LEU	2.9
2	H	144	LYS	2.8
2	E	170	ARG	2.8
1	C	288	VAL	2.8
2	F	172	ARG	2.8
1	A	267	ARG	2.8
1	A	273	THR	2.8
1	D	208	PRO	2.8
1	A	269	THR	2.8
1	C	111	LEU	2.7
1	A	192	GLN	2.7
2	G	188	SER	2.7
1	D	288	VAL	2.7
1	C	270	PRO	2.7
1	D	112	PRO	2.7
1	B	96	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	151	GLY	2.7
2	H	142	MET	2.7
1	C	193	ASP	2.7
1	B	48	ILE	2.6
1	A	125	TYR	2.6
1	D	265	VAL	2.6
1	B	83	VAL	2.6
1	B	269	THR	2.6
1	D	185	VAL	2.5
1	A	96	GLY	2.5
1	B	266	ASN	2.5
1	B	111	LEU	2.5
1	C	269	THR	2.5
1	D	58	LEU	2.5
1	D	196	SER	2.4
2	G	187	HIS	2.4
1	A	48	ILE	2.4
2	G	190	GLN	2.4
1	D	110	SER	2.4
2	H	138	THR	2.4
2	F	150	LEU	2.4
1	A	108	VAL	2.4
1	A	287	SER	2.4
1	B	313	LYS	2.4
1	D	156	TYR	2.4
1	C	236	SER	2.3
1	C	108	VAL	2.3
1	C	149	ARG	2.3
1	D	289	ARG	2.3
1	B	67	ASN	2.3
1	A	45	LEU	2.3
1	C	67	ASN	2.3
1	B	45	LEU	2.3
1	B	107	ILE	2.3
2	G	173	ILE	2.3
1	D	24	THR	2.3
1	D	45	LEU	2.3
1	C	290	ASP	2.3
1	A	248	PRO	2.3
1	B	219	LYS	2.3
1	A	239	ARG	2.3
1	D	123	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	134	PRO	2.2
1	D	48	ILE	2.2
2	H	186	LEU	2.2
1	A	221	SER	2.2
2	H	174	ASN	2.2
1	C	156	TYR	2.2
1	B	247	MET	2.2
1	B	291	ASN	2.2
1	C	292	ALA	2.2
1	A	249	ILE	2.2
2	F	175	ALA	2.2
1	A	111	LEU	2.2
1	B	84	VAL	2.1
1	A	25	PRO	2.1
1	A	60	TYR	2.1
1	C	46	SER	2.1
1	C	289	ARG	2.1
1	A	67	ASN	2.1
1	D	93	PHE	2.1
1	C	210	LEU	2.1
1	A	193	ASP	2.1
2	E	133	THR	2.1
1	C	218	ALA	2.1
2	G	189	GLU	2.1
1	C	194	ILE	2.1
1	B	221	SER	2.1
1	C	225	THR	2.1
1	C	235	SER	2.1
1	C	47	PHE	2.1
1	D	100	PHE	2.1
1	A	272	SER	2.1
1	C	261	PHE	2.0
1	A	277	LEU	2.0
1	A	185	VAL	2.0
1	A	220	PHE	2.0
1	C	273	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	1	1/1	0.99	0.08	-1.43	60,60,60,60	0
3	ZN	B	2	1/1	0.98	0.09	-1.46	55,55,55,55	0
3	ZN	E	4	1/1	0.97	0.10	-2.08	76,76,76,76	0
3	ZN	F	3	1/1	0.94	0.09	-5.48	71,71,71,71	0
3	ZN	A	5	1/1	0.97	0.15	-	108,108,108,108	0
3	ZN	B	6	1/1	0.85	0.17	-	123,123,123,123	0

6.5 Other polymers (i)

There are no such residues in this entry.