Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2016 – 03:16 PM EST

PDB ID	:	5B58
Title	:	Inward-facing conformation of ABC heme importer BhuUV in complex with periplasmic heme binding protein BhuT from Burkholderia cenocepacia
Authors	:	Naoe, Y.; Nakamura, N.; Doi, A.; Shiro, Y.; Sugimoto, H.
Deposited on	:	2016-04-25
Resolution	:	3.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

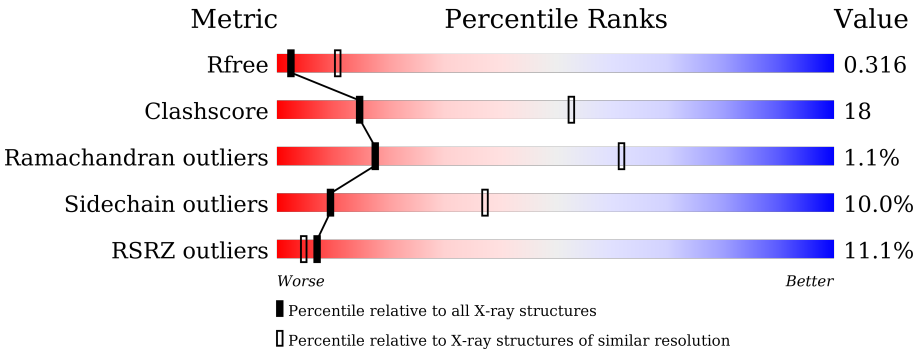
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 3.21 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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	385	6% 48% 34% 14%
1	B	385	4% 53% 29% 14%
2	C	273	3% 51% 40% 5%
2	D	273	3% 55% 33% 5% 7%
3	T	271	39% 77% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10446 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 Putative hemin ABC transport system, membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2326	1512	413	393	8			
1	B	331	Total	C	N	O	S	0	0	0
			2326	1512	413	393	8			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP B4EKB4
A	-21	GLY	-	expression tag	UNP B4EKB4
A	-20	HIS	-	expression tag	UNP B4EKB4
A	-19	HIS	-	expression tag	UNP B4EKB4
A	-18	HIS	-	expression tag	UNP B4EKB4
A	-17	HIS	-	expression tag	UNP B4EKB4
A	-16	HIS	-	expression tag	UNP B4EKB4
A	-15	HIS	-	expression tag	UNP B4EKB4
A	-14	HIS	-	expression tag	UNP B4EKB4
A	-13	HIS	-	expression tag	UNP B4EKB4
A	-12	HIS	-	expression tag	UNP B4EKB4
A	-11	HIS	-	expression tag	UNP B4EKB4
A	-10	SER	-	expression tag	UNP B4EKB4
A	-9	SER	-	expression tag	UNP B4EKB4
A	-8	GLY	-	expression tag	UNP B4EKB4
A	-7	HIS	-	expression tag	UNP B4EKB4
A	-6	ILE	-	expression tag	UNP B4EKB4
A	-5	ASP	-	expression tag	UNP B4EKB4
A	-4	ASP	-	expression tag	UNP B4EKB4
A	-3	ASP	-	expression tag	UNP B4EKB4
A	-2	ASP	-	expression tag	UNP B4EKB4
A	-1	LYS	-	expression tag	UNP B4EKB4
A	0	HIS	-	expression tag	UNP B4EKB4
B	-22	MET	-	expression tag	UNP B4EKB4
B	-21	GLY	-	expression tag	UNP B4EKB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP B4EKB4
B	-19	HIS	-	expression tag	UNP B4EKB4
B	-18	HIS	-	expression tag	UNP B4EKB4
B	-17	HIS	-	expression tag	UNP B4EKB4
B	-16	HIS	-	expression tag	UNP B4EKB4
B	-15	HIS	-	expression tag	UNP B4EKB4
B	-14	HIS	-	expression tag	UNP B4EKB4
B	-13	HIS	-	expression tag	UNP B4EKB4
B	-12	HIS	-	expression tag	UNP B4EKB4
B	-11	HIS	-	expression tag	UNP B4EKB4
B	-10	SER	-	expression tag	UNP B4EKB4
B	-9	SER	-	expression tag	UNP B4EKB4
B	-8	GLY	-	expression tag	UNP B4EKB4
B	-7	HIS	-	expression tag	UNP B4EKB4
B	-6	ILE	-	expression tag	UNP B4EKB4
B	-5	ASP	-	expression tag	UNP B4EKB4
B	-4	ASP	-	expression tag	UNP B4EKB4
B	-3	ASP	-	expression tag	UNP B4EKB4
B	-2	ASP	-	expression tag	UNP B4EKB4
B	-1	LYS	-	expression tag	UNP B4EKB4
B	0	HIS	-	expression tag	UNP B4EKB4

- Molecule 2 is a protein called Hemin import ATP-binding protein HmuV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	258	Total	C	N	O	S	0	0	0
			1951	1228	370	346	7			
2	D	253	Total	C	N	O	S	0	0	0
			1907	1203	357	340	7			

- Molecule 3 is a protein called Putative hemin transport system, substrate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	265	Total	C	N	O	S	0	0	0
			1936	1216	361	356	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	35	GLY	-	expression tag	UNP B4EKB3
T	36	PRO	-	expression tag	UNP B4EKB3
T	37	LEU	-	expression tag	UNP B4EKB3

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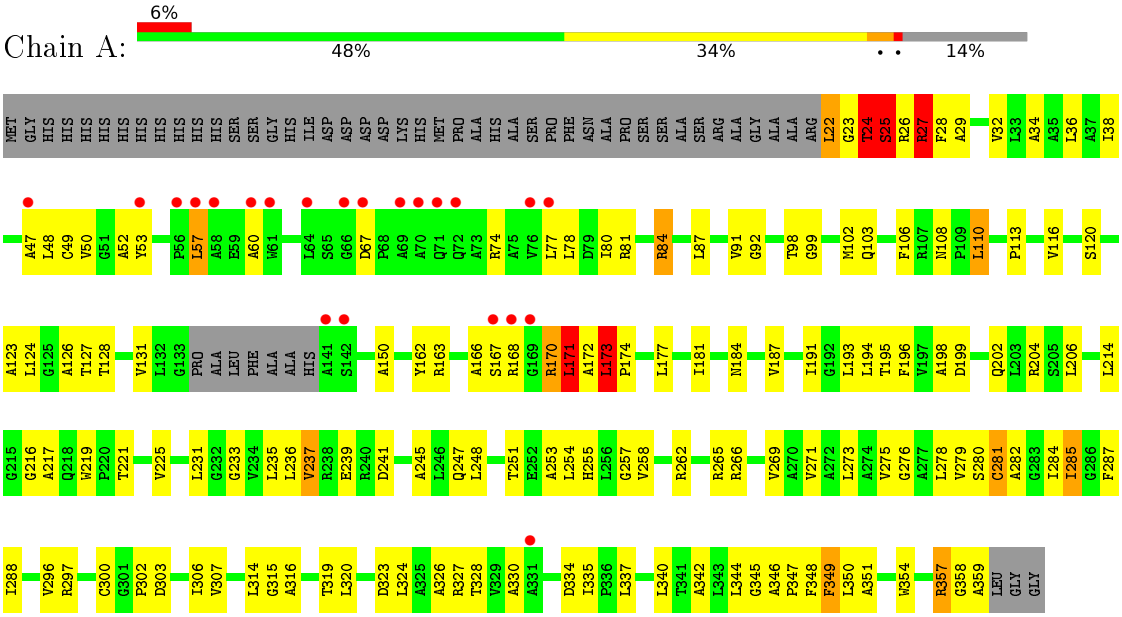
Chain	Residue	Modelled	Actual	Comment	Reference
T	38	GLY	-	expression tag	UNP B4EKB3
T	39	SER	-	expression tag	UNP B4EKB3

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.

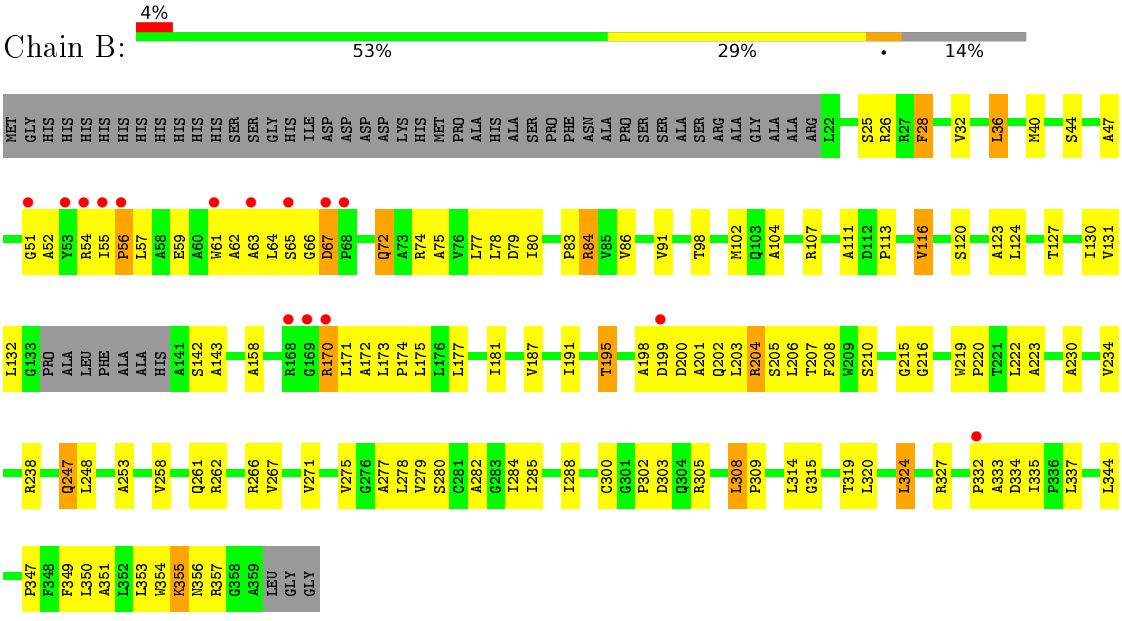
• Molecule 1: Putative hemin ABC transport system, membrane protein

Chain A:



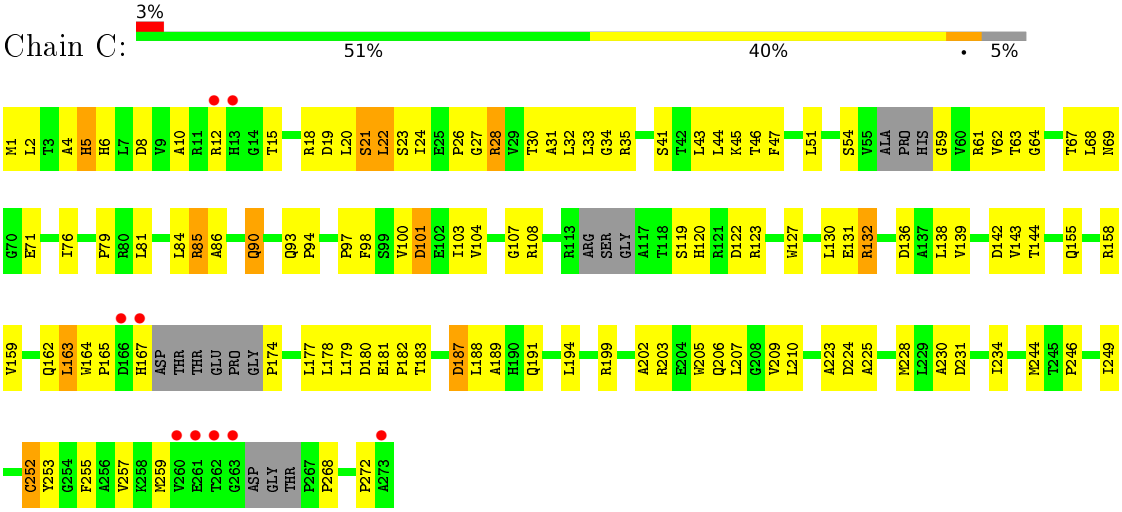
• Molecule 1: Putative hemin ABC transport system, membrane protein

Chain B:



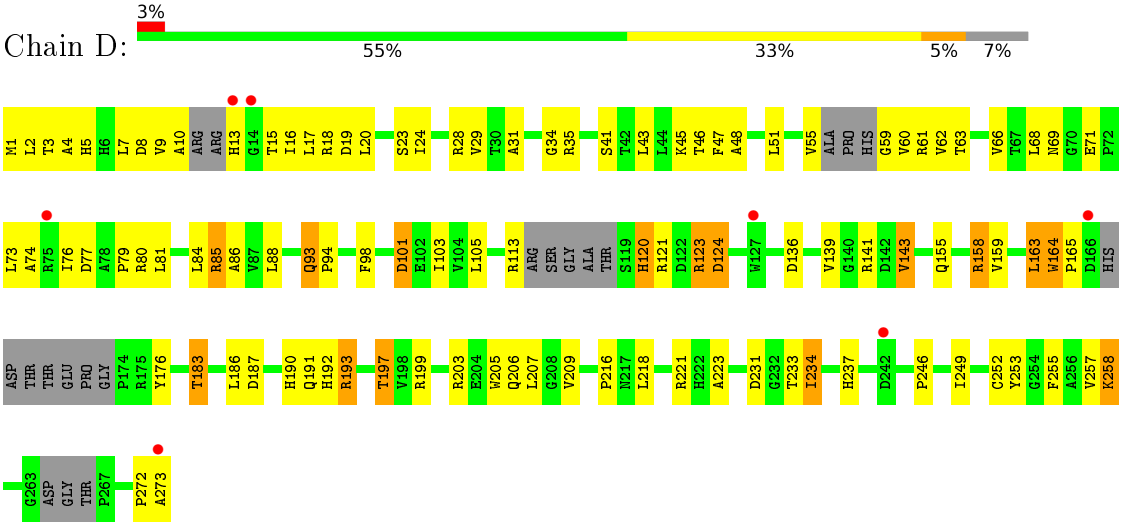
• Molecule 2: Hemin import ATP-binding protein HmuV

Chain C:



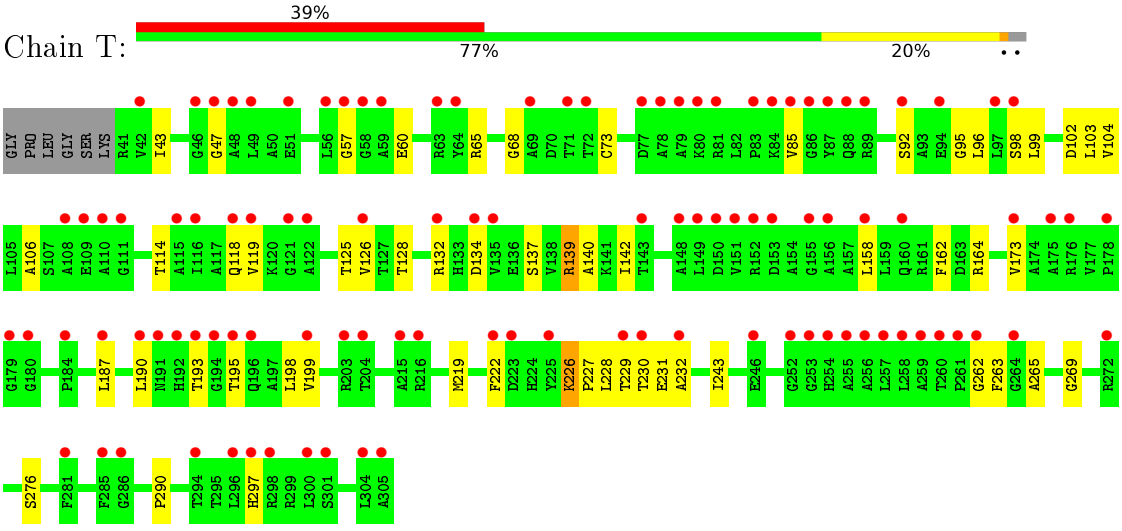
• Molecule 2: Hemin import ATP-binding protein HmuV

Chain D:



• Molecule 3: Putative hemin transport system, substrate-binding protein

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.02Å 99.75Å 253.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.61 – 3.21 32.61 – 3.21	Depositor EDS
% Data completeness (in resolution range)	76.1 (32.61-3.21) 76.1 (32.61-3.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.269 , 0.309 0.271 , 0.316	Depositor DCC
R_{free} test set	1065 reflections (4.75%)	DCC
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 30.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	10446	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/2363	0.64	2/3232 (0.1%)
1	B	0.42	0/2363	0.69	2/3232 (0.1%)
2	C	0.44	0/1988	0.65	0/2704
2	D	0.43	1/1942 (0.1%)	0.69	0/2641
3	T	0.26	0/1970	0.46	0/2684
All	All	0.40	1/10626 (0.0%)	0.63	4/14493 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	143	VAL	CB-CG1	-5.36	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	204	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	248	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	173	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	344	LEU	CA-CB-CG	5.42	127.75	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	PHE	Peptide
1	A	52	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2326	0	2502	106	0
1	B	2326	0	2502	111	0
2	C	1951	0	1987	86	0
2	D	1907	0	1941	71	0
3	T	1936	0	1974	49	0
All	All	10446	0	10906	378	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 18.

All (378) 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:27:ARG:O	1:A:29:ALA:N	1.90	1.03
1:A:334:ASP:HB2	3:T:92:SER:HB2	1.42	1.00
1:B:63:ALA:HB1	1:B:74:ARG:HB2	1.51	0.91
1:B:59:GLU:HG2	1:B:72:GLN:HB3	1.52	0.89
1:B:84:ARG:HH22	1:B:215:GLY:HA2	1.38	0.89
1:A:23:GLY:HA2	1:A:24:THR:HB	1.59	0.84
1:B:61:TRP:HB3	1:B:67:ASP:HB3	1.61	0.81
2:C:183:THR:HG22	2:C:194:LEU:HD23	1.64	0.80
2:C:1:MET:N	2:C:69:ASN:OD1	2.17	0.78
1:B:247:GLN:HB2	2:D:98:PHE:HE2	1.47	0.78
2:D:48:ALA:O	2:D:85:ARG:NH1	2.17	0.78
2:D:155:GLN:OE1	2:D:158:ARG:NH1	2.18	0.77
1:B:78:LEU:O	1:B:219:TRP:NE1	2.17	0.77
1:B:201:ALA:O	1:B:205:SER:OG	2.03	0.76
2:D:187:ASP:OD1	2:D:190:HIS:ND1	2.18	0.76
2:C:2:LEU:HD23	2:C:24:ILE:HD12	1.68	0.75
2:C:8:ASP:OD1	2:C:19:ASP:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:199:ARG:HH21	2:C:203:ARG:HH22	1.32	0.75
1:A:204:ARG:HD2	1:B:203:LEU:HD22	1.69	0.74
2:C:119:SER:HB2	2:C:120:HIS:HA	1.67	0.74
1:B:333:ALA:HB2	3:T:226:LYS:HD3	1.69	0.74
3:T:68:GLY:HA3	3:T:99:LEU:HD13	1.68	0.74
1:B:28:PHE:H	1:B:28:PHE:HD1	1.35	0.72
2:C:32:LEU:HD21	2:C:43:LEU:HD13	1.73	0.71
1:B:120:SER:HB3	1:B:187:VAL:HG11	1.72	0.71
1:B:63:ALA:HB1	1:B:74:ARG:CB	2.21	0.71
1:A:29:ALA:HA	1:A:32:VAL:HG12	1.73	0.70
3:T:43:ILE:HD11	3:T:99:LEU:HB2	1.73	0.68
1:A:288:ILE:HG12	1:A:319:THR:HG22	1.76	0.68
1:B:26:ARG:HH11	1:B:300:CYS:HA	1.57	0.68
1:A:323:ASP:O	1:A:326:ALA:N	2.25	0.68
1:A:204:ARG:NH2	1:B:198:ALA:O	2.26	0.68
1:A:170:ARG:HH22	2:C:59:GLY:N	1.92	0.67
2:D:120:HIS:HA	2:D:123:ARG:HB2	1.75	0.67
2:D:101:ASP:O	2:D:105:LEU:HB2	1.94	0.66
1:A:98:THR:HB	1:A:271:VAL:HG23	1.77	0.66
1:B:52:ALA:HB3	3:T:231:GLU:HB3	1.77	0.66
1:A:253:ALA:O	1:A:258:VAL:HG13	1.96	0.66
2:D:15:THR:HG21	2:D:18:ARG:HH12	1.59	0.66
2:D:193:ARG:O	2:D:197:THR:OG1	2.13	0.65
1:A:27:ARG:HB2	1:A:27:ARG:HH11	1.61	0.65
1:A:78:LEU:O	1:A:219:TRP:NE1	2.28	0.65
1:B:170:ARG:HH22	2:D:59:GLY:N	1.94	0.65
2:D:203:ARG:HA	2:D:203:ARG:HH21	1.62	0.65
3:T:96:LEU:HD13	3:T:119:VAL:HG21	1.78	0.64
1:B:62:ALA:N	1:B:67:ASP:OD1	2.31	0.64
1:B:332:PRO:HB2	3:T:232:ALA:HB2	1.80	0.64
2:D:2:LEU:HD23	2:D:24:ILE:HD13	1.80	0.64
1:A:124:LEU:HB2	1:A:187:VAL:HG13	1.80	0.64
2:C:187:ASP:N	2:C:187:ASP:OD1	2.29	0.64
1:A:357:ARG:HA	1:B:175:LEU:HD11	1.80	0.63
3:T:164:ARG:O	3:T:164:ARG:NH1	2.32	0.63
1:A:25:SER:HA	1:A:27:ARG:NH1	2.14	0.63
2:D:164:TRP:HB3	2:D:165:PRO:HA	1.80	0.63
2:D:77:ASP:HB3	2:D:79:PRO:HD2	1.80	0.63
1:B:40:MET:O	1:B:44:SER:OG	2.16	0.62
2:C:24:ILE:HD13	2:C:210:LEU:HB2	1.82	0.62
2:C:46:THR:HG22	2:C:51:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:132:ARG:HB2	3:T:137:SER:HB2	1.82	0.62
1:A:255:HIS:O	2:C:85:ARG:NH2	2.33	0.61
1:B:253:ALA:O	1:B:258:VAL:HG13	2.00	0.61
1:A:199:ASP:C	1:B:204:ARG:HH22	2.04	0.61
2:C:98:PHE:O	2:C:143:VAL:HG22	2.00	0.61
1:B:335:ILE:H	1:B:335:ILE:HD12	1.64	0.61
1:A:196:PHE:CE1	3:T:227:PRO:HD2	2.36	0.60
1:B:63:ALA:O	1:B:74:ARG:NE	2.34	0.60
1:B:84:ARG:HE	1:B:327:ARG:HD2	1.66	0.60
1:B:98:THR:HB	1:B:271:VAL:HG23	1.83	0.60
2:C:199:ARG:HH21	2:C:203:ARG:NH2	1.98	0.60
1:A:181:ILE:HA	1:A:184:ASN:HB2	1.83	0.60
1:A:202:GLN:O	1:A:206:LEU:HG	2.02	0.60
1:B:36:LEU:HD21	1:B:314:LEU:HB2	1.84	0.60
1:B:142:SER:OG	1:B:143:ALA:N	2.34	0.59
1:B:61:TRP:HB3	1:B:67:ASP:CB	2.29	0.59
1:B:91:VAL:HG11	1:B:285:ILE:HD12	1.84	0.59
1:B:282:ALA:HB1	1:B:285:ILE:HD11	1.85	0.59
2:D:120:HIS:ND1	2:D:120:HIS:O	2.35	0.59
1:B:102:MET:HG3	1:B:113:PRO:HA	1.85	0.59
1:B:204:ARG:HD2	3:T:198:LEU:HD22	1.85	0.58
1:B:75:ALA:HB1	3:T:265:ALA:HB1	1.85	0.58
1:B:124:LEU:HD22	1:B:187:VAL:HG23	1.86	0.58
2:D:86:ALA:HB3	2:D:163:LEU:HD21	1.85	0.58
1:B:80:ILE:HD11	3:T:262:GLY:HA2	1.85	0.58
2:C:189:ALA:HB2	2:D:255:PHE:HB2	1.84	0.58
2:C:108:ARG:NE	2:C:122:ASP:OD1	2.33	0.58
2:C:132:ARG:HG2	2:C:164:TRP:HH2	1.69	0.58
2:D:7:LEU:HD21	2:D:46:THR:HG21	1.86	0.58
1:A:275:VAL:O	1:A:279:VAL:HG12	2.04	0.58
1:B:59:GLU:CG	1:B:72:GLN:HB3	2.31	0.58
1:A:265:ARG:O	1:A:269:VAL:HG23	2.03	0.57
2:D:93:GLN:CD	2:D:94:PRO:HD2	2.24	0.57
1:A:23:GLY:HA2	1:A:24:THR:CB	2.33	0.57
1:A:204:ARG:HH12	1:B:199:ASP:C	2.07	0.57
2:C:249:ILE:HG21	2:C:257:VAL:HG21	1.85	0.57
1:A:326:ALA:HB2	1:A:340:LEU:HD13	1.85	0.57
1:A:91:VAL:HA	1:A:278:LEU:HD22	1.86	0.57
1:A:131:VAL:HG21	1:A:194:LEU:HD22	1.85	0.56
1:B:216:GLY:HA3	3:T:195:THR:OG1	2.04	0.56
1:B:347:PRO:O	1:B:351:ALA:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HG	1:B:77:LEU:HD21	1.87	0.56
2:C:178:LEU:HD23	2:C:210:LEU:HB3	1.86	0.56
2:D:81:LEU:O	2:D:84:LEU:N	2.37	0.56
2:C:103:ILE:HD12	2:C:143:VAL:HG11	1.87	0.56
1:B:247:GLN:HB2	2:D:98:PHE:CE2	2.35	0.56
1:B:285:ILE:HD13	1:B:337:LEU:HD11	1.87	0.56
1:B:47:ALA:HA	1:B:324:LEU:CD1	2.36	0.56
2:C:28:ARG:HG2	2:C:224:ASP:HB2	1.88	0.56
1:B:198:ALA:HB1	1:B:202:GLN:CB	2.35	0.56
1:A:49:CYS:SG	1:A:57:LEU:HD12	2.46	0.56
1:A:303:ASP:O	1:A:307:VAL:HG23	2.06	0.55
2:D:9:VAL:HG22	2:D:17:LEU:HB3	1.89	0.55
3:T:222:PHE:CE2	3:T:226:LYS:HD2	2.41	0.55
2:D:255:PHE:CZ	2:D:272:PRO:HB3	2.42	0.55
2:D:2:LEU:HD21	2:D:47:PHE:HB3	1.88	0.55
1:A:102:MET:HG3	1:A:113:PRO:HA	1.89	0.54
1:A:162:TYR:CE1	1:A:166:ALA:HB2	2.43	0.54
1:B:191:ILE:O	1:B:195:THR:HG23	2.07	0.54
1:B:219:TRP:CE3	1:B:222:LEU:HD11	2.42	0.54
2:D:15:THR:HG21	2:D:18:ARG:NH1	2.22	0.54
1:A:199:ASP:C	1:B:204:ARG:NH2	2.61	0.54
3:T:187:LEU:HD11	3:T:199:VAL:HG11	1.90	0.54
1:A:191:ILE:O	1:A:195:THR:HG23	2.08	0.54
1:B:84:ARG:NH2	1:B:215:GLY:HA2	2.17	0.54
2:C:68:LEU:HD11	2:C:84:LEU:HD13	1.89	0.54
1:B:28:PHE:N	1:B:28:PHE:CD1	2.76	0.53
1:B:303:ASP:OD1	1:B:305:ARG:HB2	2.07	0.53
2:C:93:GLN:HE21	2:C:144:THR:HB	1.73	0.53
2:D:51:LEU:HA	2:D:55:VAL:HG22	1.90	0.53
1:A:126:ALA:HB2	1:A:150:ALA:HB2	1.90	0.53
2:C:183:THR:HB	2:C:191:GLN:HG2	1.89	0.53
2:C:8:ASP:HB2	2:C:63:THR:OG1	2.09	0.53
2:D:1:MET:HA	2:D:176:TYR:OH	2.08	0.53
2:D:234:ILE:HD11	2:D:237:HIS:HB2	1.90	0.53
1:A:214:LEU:HG	1:A:337:LEU:HD21	1.91	0.53
1:A:84:ARG:NH2	1:A:327:ARG:HG2	2.24	0.53
1:B:308:LEU:HB3	1:B:309:PRO:HD3	1.89	0.53
2:C:188:LEU:HD11	2:D:216:PRO:HG2	1.91	0.53
3:T:263:PHE:O	3:T:269:GLY:HA3	2.09	0.53
2:C:107:GLY:O	2:C:162:GLN:HG3	2.09	0.52
1:A:167:SER:HB2	1:A:170:ARG:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLY:O	1:A:237:VAL:HG12	2.10	0.52
3:T:162:PHE:CE2	3:T:290:PRO:HD3	2.44	0.52
1:A:262:ARG:O	1:A:266:ARG:HG3	2.10	0.52
2:D:4:ALA:HA	2:D:66:VAL:HA	1.92	0.52
1:A:103:GLN:OE1	1:A:297:ARG:NH2	2.43	0.52
1:A:173:LEU:HG	1:A:174:PRO:HD3	1.92	0.52
2:D:249:ILE:HG21	2:D:257:VAL:HG21	1.92	0.52
1:A:27:ARG:HH11	1:A:27:ARG:CB	2.23	0.51
1:B:267:VAL:O	1:B:271:VAL:HG12	2.10	0.51
2:C:4:ALA:HB2	2:C:47:PHE:HE1	1.76	0.51
1:A:170:ARG:O	1:A:171:LEU:HB2	2.10	0.51
1:A:87:LEU:HD23	1:A:214:LEU:HB3	1.92	0.51
2:C:120:HIS:O	2:C:123:ARG:N	2.43	0.51
2:D:9:VAL:HG12	2:D:62:VAL:HG22	1.91	0.51
1:A:24:THR:HG23	1:A:25:SER:N	2.26	0.51
2:D:98:PHE:O	2:D:143:VAL:HG23	2.10	0.51
1:B:32:VAL:HG11	1:B:300:CYS:SG	2.50	0.51
1:B:344:LEU:O	1:B:347:PRO:HD2	2.10	0.51
1:A:24:THR:HG22	2:C:101:ASP:OD2	2.11	0.51
1:A:302:PRO:HG2	2:C:98:PHE:CD1	2.46	0.50
2:C:94:PRO:HG3	2:C:143:VAL:HG21	1.92	0.50
2:C:22:LEU:HG	2:C:234:ILE:CD1	2.41	0.50
1:B:107:ARG:NH1	1:B:107:ARG:HB2	2.27	0.50
2:C:31:ALA:HB2	2:C:223:ALA:HB2	1.93	0.50
1:A:50:VAL:HG11	1:A:328:THR:HG21	1.93	0.50
2:C:230:ALA:HB2	2:C:252:CYS:HA	1.93	0.50
1:A:315:GLY:O	1:A:319:THR:HG23	2.12	0.50
2:C:155:GLN:OE1	2:C:158:ARG:NH1	2.45	0.50
1:B:170:ARG:HA	1:B:261:GLN:OE1	2.12	0.50
3:T:229:THR:HB	3:T:231:GLU:OE1	2.11	0.49
2:C:2:LEU:HA	2:C:68:LEU:HA	1.93	0.49
2:D:136:ASP:O	2:D:139:VAL:HG13	2.12	0.49
2:D:203:ARG:NH2	2:D:203:ARG:HA	2.25	0.49
2:D:2:LEU:HD13	2:D:68:LEU:HD13	1.94	0.49
3:T:95:GLY:O	3:T:98:SER:OG	2.26	0.49
1:A:236:LEU:O	1:A:239:GLU:N	2.40	0.49
1:B:332:PRO:HB2	3:T:232:ALA:CB	2.43	0.49
2:D:34:GLY:HA2	2:D:252:CYS:SG	2.52	0.49
1:A:163:ARG:NH1	1:A:168:ARG:HH12	2.11	0.49
1:B:275:VAL:O	1:B:279:VAL:HG12	2.12	0.49
1:B:84:ARG:HH11	1:B:84:ARG:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:LEU:HD23	2:C:228:MET:HE3	1.94	0.49
1:A:282:ALA:HB3	1:A:285:ILE:HD11	1.94	0.49
1:B:173:LEU:HB3	1:B:174:PRO:HD3	1.95	0.49
2:C:94:PRO:HG3	2:C:143:VAL:CG2	2.43	0.49
1:A:351:ALA:O	1:A:354:TRP:HB3	2.12	0.49
2:C:97:PRO:HB3	2:C:142:ASP:OD2	2.13	0.49
1:A:99:GLY:O	1:A:103:GLN:HG3	2.13	0.48
2:D:101:ASP:N	2:D:101:ASP:OD1	2.45	0.48
2:D:164:TRP:HB3	2:D:165:PRO:CA	2.42	0.48
1:B:177:LEU:O	1:B:181:ILE:HG12	2.13	0.48
1:B:44:SER:HA	1:B:320:LEU:HD21	1.94	0.48
2:C:130:LEU:HD13	2:C:139:VAL:HG12	1.95	0.48
1:B:208:PHE:CD2	3:T:227:PRO:HG3	2.48	0.48
1:B:277:ALA:O	1:B:280:SER:OG	2.21	0.48
2:D:205:TRP:HE3	2:D:207:LEU:HD13	1.78	0.48
2:C:5:HIS:HA	2:C:21:SER:HB3	1.95	0.48
2:D:35:ARG:NH1	2:D:253:TYR:O	2.46	0.48
1:A:330:ALA:HB3	1:A:335:ILE:HD11	1.95	0.48
1:A:113:PRO:HB3	1:A:275:VAL:HG21	1.96	0.48
1:B:104:ALA:CB	1:B:247:GLN:HE22	2.27	0.48
1:B:26:ARG:NH1	1:B:300:CYS:O	2.47	0.48
1:A:346:ALA:HB3	1:A:347:PRO:HD3	1.96	0.48
1:B:355:LYS:O	1:B:355:LYS:HG2	2.14	0.48
2:C:206:GLN:OE1	2:C:206:GLN:HA	2.14	0.47
1:B:80:ILE:HD13	3:T:230:THR:HB	1.96	0.47
3:T:60:GLU:HB3	3:T:65:ARG:HG2	1.96	0.47
1:A:196:PHE:HZ	1:B:333:ALA:HB1	1.79	0.47
1:B:130:ILE:HG22	1:B:202:GLN:OE1	2.14	0.47
2:D:191:GLN:OE1	2:D:218:LEU:HD11	2.14	0.47
3:T:243:ILE:O	3:T:276:SER:HA	2.15	0.47
1:B:91:VAL:HA	1:B:278:LEU:HD22	1.95	0.47
2:D:8:ASP:HB2	2:D:63:THR:OG1	2.14	0.47
1:A:231:LEU:HD23	1:A:273:LEU:HD21	1.96	0.47
1:B:123:ALA:O	1:B:127:THR:HG22	2.13	0.47
2:D:29:VAL:HG22	2:D:209:VAL:HB	1.95	0.47
2:D:85:ARG:HG2	2:D:86:ALA:N	2.29	0.47
3:T:104:VAL:HB	3:T:126:VAL:HG22	1.96	0.47
1:B:204:ARG:HD2	3:T:198:LEU:CD2	2.45	0.47
1:B:84:ARG:NE	1:B:327:ARG:HD2	2.28	0.46
1:B:210:SER:O	1:B:284:ILE:HB	2.15	0.46
2:C:41:SER:O	2:C:45:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:142:ILE:HG23	3:T:158:LEU:HD23	1.97	0.46
1:B:315:GLY:O	1:B:319:THR:HG23	2.15	0.46
1:A:216:GLY:CA	3:T:114:THR:HB	2.46	0.46
1:A:47:ALA:HA	1:A:324:LEU:CD1	2.46	0.46
1:B:104:ALA:HB1	1:B:247:GLN:HE22	1.79	0.46
2:C:10:ALA:HB2	2:C:15:THR:HG22	1.96	0.46
1:B:86:VAL:HG13	1:B:222:LEU:HD22	1.98	0.46
2:C:86:ALA:HB1	2:C:159:VAL:HG23	1.97	0.46
2:D:76:ILE:HG21	2:D:81:LEU:HD13	1.97	0.46
1:A:60:ALA:HB1	1:A:77:LEU:HD11	1.98	0.46
1:B:220:PRO:HA	1:B:223:ALA:HB3	1.96	0.46
2:C:71:GLU:HG3	2:C:76:ILE:HD11	1.98	0.46
3:T:173:VAL:HG13	3:T:297:HIS:CD2	2.50	0.46
2:C:131:GLU:HB3	2:C:132:ARG:HH11	1.81	0.46
3:T:190:LEU:HD23	3:T:198:LEU:HD23	1.97	0.46
1:A:245:ALA:O	1:A:253:ALA:HB2	2.15	0.46
1:A:92:GLY:HA3	1:A:316:ALA:HA	1.96	0.46
1:B:57:LEU:HG	1:B:77:LEU:CD2	2.46	0.46
2:D:31:ALA:HB2	2:D:223:ALA:HB2	1.98	0.45
1:A:22:LEU:HD12	2:C:127:TRP:CG	2.51	0.45
2:C:26:PRO:HB3	2:C:206:GLN:O	2.16	0.45
1:B:205:SER:HA	3:T:193:THR:OG1	2.16	0.45
1:B:195:THR:O	1:B:203:LEU:HD11	2.16	0.45
2:D:3:THR:O	2:D:66:VAL:HA	2.16	0.45
1:A:262:ARG:O	1:A:265:ARG:HB2	2.16	0.45
1:B:124:LEU:HA	1:B:127:THR:HG22	1.99	0.45
1:B:332:PRO:O	3:T:232:ALA:HB2	2.16	0.45
1:A:34:ALA:O	1:A:38:ILE:HG12	2.16	0.45
1:A:358:GLY:HA2	1:A:359:ALA:HA	1.63	0.45
2:C:249:ILE:HG23	2:C:253:TYR:HD2	1.81	0.45
1:A:29:ALA:HB1	1:A:306:ILE:HG21	1.99	0.45
2:D:192:HIS:HE1	2:D:221:ARG:NE	2.15	0.45
1:A:25:SER:HA	1:A:27:ARG:CZ	2.47	0.45
1:B:230:ALA:O	1:B:234:VAL:HG23	2.17	0.45
2:C:90:GLN:OE1	2:C:90:GLN:N	2.50	0.45
2:D:69:ASN:OD1	2:D:176:TYR:OH	2.11	0.45
1:A:225:VAL:HG21	1:A:281:CYS:SG	2.57	0.45
2:C:34:GLY:HA2	2:C:252:CYS:SG	2.56	0.45
1:B:302:PRO:HG2	2:D:98:PHE:CD1	2.52	0.44
2:C:30:THR:HA	2:C:225:ALA:O	2.17	0.44
2:D:20:LEU:HD13	2:D:43:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:O	1:A:127:THR:HG22	2.17	0.44
1:B:247:GLN:HG2	1:B:247:GLN:H	1.42	0.44
2:C:90:GLN:HG3	2:C:180:ASP:O	2.17	0.44
2:D:183:THR:O	2:D:186:LEU:HB2	2.17	0.44
2:D:246:PRO:HB3	2:D:257:VAL:O	2.17	0.44
2:C:2:LEU:CD1	2:C:68:LEU:HB3	2.48	0.44
2:D:1:MET:H2	2:D:69:ASN:HA	1.82	0.44
2:C:100:VAL:O	2:C:104:VAL:HG23	2.17	0.44
2:C:47:PHE:HD2	2:C:210:LEU:HD22	1.82	0.44
2:C:35:ARG:HG3	2:C:252:CYS:O	2.18	0.44
2:C:2:LEU:HD12	2:C:68:LEU:HB3	1.99	0.44
2:C:93:GLN:HE21	2:C:144:THR:CB	2.30	0.44
3:T:60:GLU:CB	3:T:65:ARG:HG2	2.48	0.44
2:C:179:LEU:HD13	2:C:182:PRO:HG3	1.99	0.44
3:T:132:ARG:H	3:T:137:SER:CB	2.31	0.44
1:B:219:TRP:HE3	1:B:222:LEU:HD11	1.82	0.44
1:B:262:ARG:HD2	1:B:266:ARG:HG3	2.00	0.44
2:C:255:PHE:CZ	2:C:272:PRO:HB3	2.52	0.44
1:A:124:LEU:HA	1:A:127:THR:HG22	1.99	0.44
1:A:287:PHE:CD2	1:A:342:ALA:HA	2.53	0.44
1:A:345:GLY:O	1:A:349:PHE:N	2.51	0.44
1:B:302:PRO:HG2	2:D:98:PHE:CE1	2.53	0.44
3:T:173:VAL:HG22	3:T:297:HIS:CG	2.52	0.44
1:B:171:LEU:HD23	1:B:261:GLN:HE22	1.83	0.43
1:B:63:ALA:CB	1:B:74:ARG:HB2	2.35	0.43
3:T:103:LEU:HD12	3:T:125:THR:O	2.17	0.43
1:A:163:ARG:HH12	1:A:168:ARG:HH12	1.66	0.43
1:A:287:PHE:CD1	1:A:287:PHE:N	2.86	0.43
1:A:24:THR:O	1:A:26:ARG:N	2.51	0.43
1:A:198:ALA:HB1	1:A:202:GLN:HB2	2.00	0.43
1:B:203:LEU:O	1:B:207:THR:HG23	2.19	0.43
2:C:69:ASN:ND2	2:C:174:PRO:HD2	2.33	0.43
1:B:351:ALA:O	1:B:354:TRP:N	2.52	0.43
2:C:20:LEU:HD11	2:C:234:ILE:HG13	1.99	0.43
2:D:3:THR:HG23	2:D:23:SER:HB3	2.00	0.43
1:A:288:ILE:HG12	1:A:319:THR:CG2	2.45	0.43
2:D:121:ARG:HG3	2:D:121:ARG:HH11	1.84	0.43
2:C:20:LEU:HD12	2:C:20:LEU:HA	1.79	0.43
2:D:3:THR:OG1	2:D:23:SER:HB2	2.19	0.43
1:A:80:ILE:HG23	3:T:118:GLN:HE21	1.84	0.43
1:B:355:LYS:HE2	1:B:356:ASN:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:ARG:HG3	2:C:122:ASP:HB3	2.01	0.43
2:C:67:THR:HG23	2:C:71:GLU:C	2.39	0.43
2:D:73:LEU:O	2:D:76:ILE:N	2.51	0.43
1:A:251:THR:HG22	1:A:255:HIS:CE1	2.54	0.42
2:D:120:HIS:CG	2:D:120:HIS:O	2.71	0.42
2:D:41:SER:O	2:D:45:LYS:HG3	2.19	0.42
1:A:247:GLN:HG2	1:A:247:GLN:H	1.60	0.42
1:B:170:ARG:HG3	1:B:170:ARG:H	1.42	0.42
3:T:106:ALA:O	3:T:128:THR:HA	2.19	0.42
1:A:108:ASN:OD1	1:A:110:LEU:HB2	2.19	0.42
1:A:198:ALA:O	1:B:204:ARG:NH1	2.47	0.42
3:T:222:PHE:CD2	3:T:226:LYS:HD2	2.55	0.42
3:T:199:VAL:HG13	3:T:228:LEU:HB2	2.00	0.42
1:A:47:ALA:CB	1:A:320:LEU:HD11	2.48	0.42
1:B:116:VAL:O	1:B:158:ALA:HA	2.18	0.42
2:C:246:PRO:HB3	2:C:257:VAL:O	2.19	0.42
2:C:68:LEU:HD21	2:C:81:LEU:HD11	1.99	0.42
1:A:214:LEU:HG	1:A:337:LEU:CD2	2.49	0.42
3:T:47:GLY:HA2	3:T:73:CYS:SG	2.59	0.42
2:C:132:ARG:N	2:C:132:ARG:HD3	2.34	0.42
1:B:62:ALA:HB2	1:B:67:ASP:O	2.19	0.42
2:D:206:GLN:OE1	2:D:206:GLN:HA	2.19	0.42
3:T:164:ARG:HA	3:T:164:ARG:HD2	1.94	0.42
1:A:25:SER:HA	1:A:27:ARG:HH12	1.83	0.42
2:D:258:LYS:HB3	2:D:273:ALA:HB2	2.00	0.42
1:A:80:ILE:HG23	3:T:118:GLN:NE2	2.34	0.42
1:B:131:VAL:HG22	1:B:202:GLN:OE1	2.20	0.42
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.87	0.42
1:B:79:ASP:O	1:B:83:PRO:HG2	2.19	0.42
2:C:120:HIS:ND1	2:C:120:HIS:C	2.73	0.42
2:C:6:HIS:O	2:C:64:GLY:HA3	2.20	0.42
2:C:163:LEU:HA	2:C:163:LEU:HD12	1.89	0.41
2:C:2:LEU:O	2:C:23:SER:HA	2.20	0.41
2:D:88:LEU:HD23	2:D:159:VAL:HG11	2.01	0.41
1:A:106:PHE:CE2	1:A:177:LEU:HD21	2.55	0.41
1:B:107:ARG:HB2	1:B:107:ARG:HH11	1.85	0.41
2:C:27:GLY:HA2	2:C:202:ALA:O	2.20	0.41
2:D:81:LEU:HA	2:D:81:LEU:HD12	1.86	0.41
1:A:127:THR:HG21	1:A:191:ILE:HG12	2.01	0.41
1:B:288:ILE:HG12	1:B:319:THR:HG22	2.02	0.41
1:A:276:GLY:O	1:A:280:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TRP:O	1:B:66:GLY:N	2.53	0.41
1:A:247:GLN:HB2	2:C:98:PHE:HE2	1.86	0.41
1:A:87:LEU:HD22	1:A:217:ALA:HB2	2.02	0.41
1:B:55:ILE:HA	1:B:56:PRO:HD3	1.93	0.41
3:T:139:ARG:HG3	3:T:140:ALA:N	2.36	0.41
1:A:235:LEU:O	1:A:239:GLU:HG2	2.21	0.41
1:A:247:GLN:HB2	2:C:98:PHE:CE2	2.56	0.41
1:A:284:ILE:H	1:A:284:ILE:HG12	1.70	0.41
2:D:55:VAL:HG11	2:D:60:VAL:HG22	2.03	0.41
1:B:333:ALA:HB2	3:T:226:LYS:CD	2.45	0.41
1:A:196:PHE:HA	1:B:208:PHE:CE1	2.56	0.41
1:A:257:GLY:HA3	2:C:79:PRO:HA	2.03	0.41
1:A:335:ILE:H	1:A:335:ILE:HG12	1.61	0.41
2:D:10:ALA:HB2	2:D:15:THR:HG22	2.03	0.41
2:D:120:HIS:HE1	2:D:124:ASP:OD2	2.04	0.41
3:T:219:MET:HE3	3:T:222:PHE:HE1	1.85	0.41
1:A:23:GLY:N	2:C:123:ARG:NH2	2.69	0.41
1:A:84:ARG:HH21	1:A:327:ARG:HG2	1.83	0.41
2:C:205:TRP:CD1	2:C:205:TRP:N	2.87	0.41
1:A:163:ARG:HH11	1:A:168:ARG:HH22	1.69	0.41
2:D:71:GLU:HG3	2:D:76:ILE:HD11	2.03	0.41
1:A:48:LEU:O	1:A:81:ARG:HD2	2.21	0.40
2:C:136:ASP:C	2:C:138:LEU:H	2.25	0.40
1:A:23:GLY:O	2:C:123:ARG:NH2	2.54	0.40
1:B:198:ALA:HB1	1:B:202:GLN:HB2	2.03	0.40
3:T:134:ASP:N	3:T:134:ASP:OD1	2.53	0.40
3:T:85:VAL:HG13	3:T:99:LEU:HD11	2.03	0.40
2:C:244:MET:HG3	2:C:259:MET:HE3	2.03	0.40
2:D:1:MET:N	2:D:69:ASN:HA	2.35	0.40
2:C:8:ASP:O	2:C:62:VAL:HA	2.21	0.40
2:D:71:GLU:OE1	2:D:80:ARG:NH2	2.55	0.40
1:B:204:ARG:HG2	1:B:208:PHE:CE2	2.56	0.40
2:C:177:LEU:O	2:C:209:VAL:HA	2.21	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	327/385 (85%)	284 (87%)	37 (11%)	6 (2%)	11	51
1	B	327/385 (85%)	294 (90%)	28 (9%)	5 (2%)	13	55
2	C	248/273 (91%)	232 (94%)	14 (6%)	2 (1%)	24	69
2	D	241/273 (88%)	227 (94%)	12 (5%)	2 (1%)	24	69
3	T	263/271 (97%)	255 (97%)	7 (3%)	1 (0%)	39	80
All	All	1406/1587 (89%)	1292 (92%)	98 (7%)	16 (1%)	17	62

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	28	PHE
1	A	171	LEU
1	B	357	ARG
2	D	164	TRP
1	A	27	ARG
2	D	74	ALA
1	A	24	THR
1	A	172	ALA
1	B	111	ALA
1	B	172	ALA
3	T	57	GLY
2	C	165	PRO
1	B	56	PRO
2	C	268	PRO
1	B	51	GLY

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	220/259 (85%)	189 (86%)	31 (14%)	4 20
1	B	220/259 (85%)	197 (90%)	23 (10%)	8 35
2	C	198/209 (95%)	178 (90%)	20 (10%)	9 37
2	D	194/209 (93%)	169 (87%)	25 (13%)	5 24
3	T	186/190 (98%)	183 (98%)	3 (2%)	70 90
All	All	1018/1126 (90%)	916 (90%)	102 (10%)	9 37

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	24	THR
1	A	25	SER
1	A	27	ARG
1	A	36	LEU
1	A	53	TYR
1	A	57	LEU
1	A	67	ASP
1	A	74	ARG
1	A	84	ARG
1	A	110	LEU
1	A	116	VAL
1	A	120	SER
1	A	128	THR
1	A	170	ARG
1	A	171	LEU
1	A	173	LEU
1	A	193	LEU
1	A	221	THR
1	A	237	VAL
1	A	241	ASP
1	A	248	LEU
1	A	254	LEU
1	A	281	CYS
1	A	285	ILE
1	A	296	VAL
1	A	300	CYS

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Mol	Chain	Res	Type
1	A	314	LEU
1	A	349	PHE
1	A	350	LEU
1	A	357	ARG
1	B	25	SER
1	B	28	PHE
1	B	36	LEU
1	B	54	ARG
1	B	64	LEU
1	B	65	SER
1	B	67	ASP
1	B	72	GLN
1	B	84	ARG
1	B	116	VAL
1	B	132	LEU
1	B	170	ARG
1	B	195	THR
1	B	200	ASP
1	B	238	ARG
1	B	247	GLN
1	B	308	LEU
1	B	324	LEU
1	B	334	ASP
1	B	349	PHE
1	B	350	LEU
1	B	353	LEU
1	B	355	LYS
2	C	5	HIS
2	C	12	ARG
2	C	18	ARG
2	C	21	SER
2	C	22	LEU
2	C	28	ARG
2	C	44	LEU
2	C	54	SER
2	C	61	ARG
2	C	85	ARG
2	C	90	GLN
2	C	101	ASP
2	C	132	ARG
2	C	163	LEU
2	C	167	HIS

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Mol	Chain	Res	Type
2	C	181	GLU
2	C	187	ASP
2	C	207	LEU
2	C	231	ASP
2	C	252	CYS
2	D	5	HIS
2	D	13	HIS
2	D	16	ILE
2	D	19	ASP
2	D	28	ARG
2	D	61	ARG
2	D	85	ARG
2	D	93	GLN
2	D	101	ASP
2	D	103	ILE
2	D	113	ARG
2	D	120	HIS
2	D	123	ARG
2	D	124	ASP
2	D	141	ARG
2	D	158	ARG
2	D	163	LEU
2	D	183	THR
2	D	193	ARG
2	D	197	THR
2	D	199	ARG
2	D	231	ASP
2	D	233	THR
2	D	234	ILE
2	D	258	LYS
3	T	102	ASP
3	T	139	ARG
3	T	226	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	93	GLN
2	D	192	HIS
3	T	118	GLN
3	T	192	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	331/385 (85%)	-0.11	22 (6%) 22 13	34, 64, 170, 254	0
1	B	331/385 (85%)	-0.32	15 (4%) 37 25	13, 52, 166, 199	0
2	C	258/273 (94%)	-0.20	9 (3%) 48 34	27, 59, 124, 170	0
2	D	253/273 (92%)	-0.32	7 (2%) 56 44	13, 52, 107, 143	0
3	T	265/271 (97%)	2.06	107 (40%) 0 0	76, 108, 128, 141	265 (100%)
All	All	1438/1587 (90%)	0.19	160 (11%) 7 5	13, 67, 137, 254	265 (18%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	254	HIS	10.5
3	T	193	THR	10.2
3	T	215	ALA	10.2
3	T	191	ASN	9.8
2	C	166	ASP	8.9
3	T	58	GLY	8.8
1	A	57	LEU	8.7
3	T	77	ASP	8.4
3	T	122	ALA	8.4
3	T	64	TYR	7.3
3	T	149	LEU	7.1
2	C	167	HIS	6.9
3	T	151	VAL	6.9
3	T	192	HIS	6.6
3	T	59	ALA	6.5
3	T	80	LYS	6.1
3	T	179	GLY	6.1
1	A	64	LEU	6.0
1	A	66	GLY	5.9
3	T	196	GLN	5.8

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Mol	Chain	Res	Type	RSRZ
3	T	48	ALA	5.7
3	T	81	ARG	5.7
3	T	156	ALA	5.5
3	T	47	GLY	5.5
2	C	13	HIS	5.4
3	T	46	GLY	5.3
3	T	78	ALA	5.3
3	T	57	GLY	5.2
3	T	255	ALA	5.2
3	T	150	ASP	5.2
1	A	56	PRO	5.0
3	T	216	ARG	5.0
1	A	69	ALA	4.9
3	T	256	ALA	4.7
3	T	153	ASP	4.7
1	A	61	TRP	4.6
3	T	87	TYR	4.6
3	T	49	LEU	4.6
3	T	178	PRO	4.5
1	A	60	ALA	4.4
3	T	195	THR	4.2
3	T	134	ASP	4.2
3	T	252	GLY	4.2
3	T	175	ALA	4.2
3	T	155	GLY	4.1
1	B	56	PRO	4.0
3	T	85	VAL	4.0
3	T	79	ALA	3.9
3	T	286	GLY	3.9
1	A	72	GLN	3.9
1	A	67	ASP	3.8
3	T	184	PRO	3.8
2	D	75	ARG	3.8
3	T	223	ASP	3.8
1	A	70	ALA	3.7
1	B	54	ARG	3.7
2	C	262	THR	3.7
3	T	63	ARG	3.6
3	T	98	SER	3.6
3	T	194	GLY	3.6
1	A	168	ARG	3.5
1	A	71	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	169	GLY	3.5
3	T	173	VAL	3.4
1	B	68	PRO	3.4
3	T	148	ALA	3.3
1	B	51	GLY	3.2
1	B	170	ARG	3.2
3	T	304	LEU	3.2
3	T	298	ARG	3.2
1	B	169	GLY	3.2
3	T	305	ALA	3.2
2	C	12	ARG	3.2
3	T	258	LEU	3.2
1	B	53	TYR	3.2
3	T	180	GLY	3.1
2	D	13	HIS	3.1
3	T	301	SER	3.0
3	T	51	GLU	3.0
3	T	158	LEU	3.0
3	T	272	ARG	3.0
3	T	92	SER	2.9
3	T	115	ALA	2.9
3	T	116	ILE	2.9
1	A	58	ALA	2.9
3	T	297	HIS	2.9
3	T	294	THR	2.8
3	T	222	PHE	2.8
3	T	264	GLY	2.8
3	T	262	GLY	2.8
2	C	263	GLY	2.8
2	C	260	VAL	2.8
3	T	135	VAL	2.7
3	T	126	VAL	2.7
3	T	204	THR	2.7
2	D	242	ASP	2.7
3	T	143	THR	2.7
1	A	47	ALA	2.7
1	A	53	TYR	2.7
3	T	72	THR	2.7
3	T	118	GLN	2.6
1	B	168	ARG	2.6
3	T	152	ARG	2.6
3	T	229	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	T	296	LEU	2.6
3	T	42	VAL	2.6
3	T	281	PHE	2.6
3	T	300	LEU	2.6
3	T	132	ARG	2.5
3	T	203	ARG	2.5
3	T	257	LEU	2.5
2	D	127	TRP	2.5
3	T	56	LEU	2.5
3	T	190	LEU	2.5
1	A	141	ALA	2.5
1	B	55	ILE	2.5
3	T	260	THR	2.5
2	C	261	GLU	2.5
2	C	273	ALA	2.4
3	T	246	GLU	2.4
3	T	253	GLY	2.4
3	T	160	GLN	2.4
3	T	176	ARG	2.4
1	A	142	SER	2.4
3	T	121	GLY	2.4
3	T	199	VAL	2.4
3	T	109	GLU	2.4
1	A	167	SER	2.3
3	T	285	PHE	2.3
3	T	261	PRO	2.3
3	T	230	THR	2.3
3	T	88	GLN	2.2
3	T	86	GLY	2.2
3	T	97	LEU	2.2
1	B	332	PRO	2.2
3	T	71	THR	2.2
3	T	84	LYS	2.2
3	T	69	ALA	2.1
3	T	232	ALA	2.1
1	B	199	ASP	2.1
3	T	111	GLY	2.1
3	T	119	VAL	2.1
1	A	77	LEU	2.1
1	B	67	ASP	2.1
3	T	110	ALA	2.1
2	D	166	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	14	GLY	2.1
3	T	94	GLU	2.1
3	T	89	ARG	2.1
1	B	63	ALA	2.1
2	D	273	ALA	2.1
1	B	61	TRP	2.1
3	T	187	LEU	2.1
1	B	65	SER	2.1
3	T	259	ALA	2.0
1	A	76	VAL	2.0
3	T	225	TYR	2.0
3	T	83	PRO	2.0
1	A	331	ALA	2.0
3	T	108	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.