Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 11:11 pm BST

PDB ID	:	4BIA
Title	:	Crystal structure of SCP2 thiolase from Trypanosoma brucei: The C337A mutant.
Authors	:	Harijan, R.K.; Kiema, T.-R.; Weiss, M.S.; Michels, P.A.M.; Wierenga, R.K.
Deposited on	:	2013-04-10
Resolution	:	2.90 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.

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.268
Clashscore		24
Ramachandran outliers		4.4%
Sidechain outliers		6.9%
RSRZ outliers		4.0%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
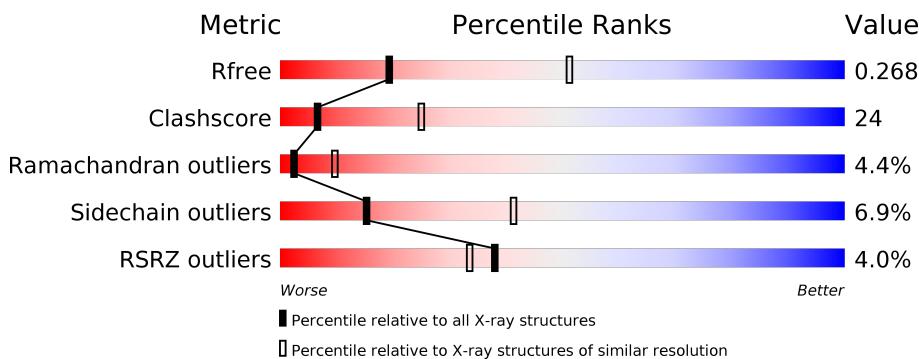
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	454	4% / 48% / 39% / 6% / 8%
1	B	454	4% / 48% / 37% / 6% · / 8%
1	C	454	2% / 48% / 39% / 6% / 8%
1	D	454	5% / 47% / 38% / 6% / 8%
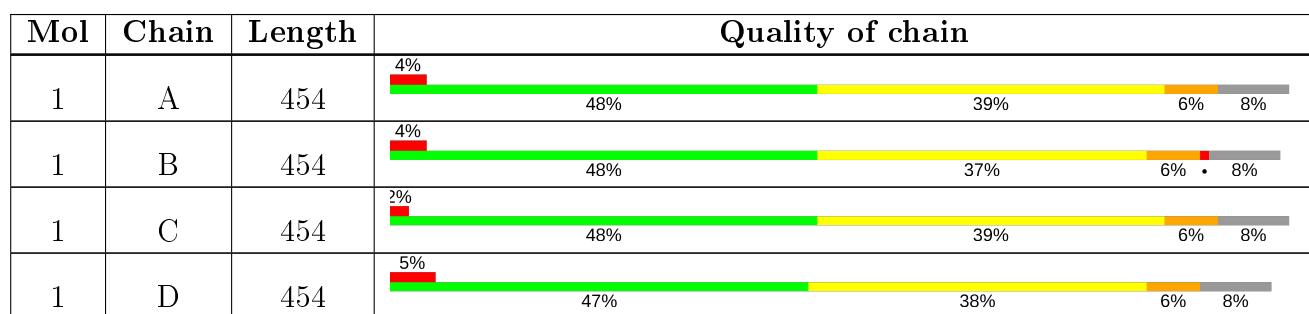
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12319 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 3-KETOACYL-COA THIOLASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3072	1924	540	592	16			
1	B	416	Total	C	N	O	S	0	0	0
			3068	1921	542	589	16			
1	C	419	Total	C	N	O	S	0	0	0
			3086	1931	545	594	16			
1	D	416	Total	C	N	O	S	0	0	0
			3065	1920	541	588	16			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q57XD5
A	-14	HIS	-	expression tag	UNP Q57XD5
A	-13	HIS	-	expression tag	UNP Q57XD5
A	-12	HIS	-	expression tag	UNP Q57XD5
A	-11	HIS	-	expression tag	UNP Q57XD5
A	-10	HIS	-	expression tag	UNP Q57XD5
A	-9	SER	-	expression tag	UNP Q57XD5
A	-8	SER	-	expression tag	UNP Q57XD5
A	-7	GLY	-	expression tag	UNP Q57XD5
A	-6	LEU	-	expression tag	UNP Q57XD5
A	-5	VAL	-	expression tag	UNP Q57XD5
A	-4	PRO	-	expression tag	UNP Q57XD5
A	-3	ARG	-	expression tag	UNP Q57XD5
A	-2	GLY	-	expression tag	UNP Q57XD5
A	-1	SER	-	expression tag	UNP Q57XD5
A	0	HIS	-	expression tag	UNP Q57XD5
A	337	ALA	CYS	engineered mutation	UNP Q57XD5
B	-15	HIS	-	expression tag	UNP Q57XD5
B	-14	HIS	-	expression tag	UNP Q57XD5
B	-13	HIS	-	expression tag	UNP Q57XD5
B	-12	HIS	-	expression tag	UNP Q57XD5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP Q57XD5
B	-10	HIS	-	expression tag	UNP Q57XD5
B	-9	SER	-	expression tag	UNP Q57XD5
B	-8	SER	-	expression tag	UNP Q57XD5
B	-7	GLY	-	expression tag	UNP Q57XD5
B	-6	LEU	-	expression tag	UNP Q57XD5
B	-5	VAL	-	expression tag	UNP Q57XD5
B	-4	PRO	-	expression tag	UNP Q57XD5
B	-3	ARG	-	expression tag	UNP Q57XD5
B	-2	GLY	-	expression tag	UNP Q57XD5
B	-1	SER	-	expression tag	UNP Q57XD5
B	0	HIS	-	expression tag	UNP Q57XD5
B	337	ALA	CYS	engineered mutation	UNP Q57XD5
C	-15	HIS	-	expression tag	UNP Q57XD5
C	-14	HIS	-	expression tag	UNP Q57XD5
C	-13	HIS	-	expression tag	UNP Q57XD5
C	-12	HIS	-	expression tag	UNP Q57XD5
C	-11	HIS	-	expression tag	UNP Q57XD5
C	-10	HIS	-	expression tag	UNP Q57XD5
C	-9	SER	-	expression tag	UNP Q57XD5
C	-8	SER	-	expression tag	UNP Q57XD5
C	-7	GLY	-	expression tag	UNP Q57XD5
C	-6	LEU	-	expression tag	UNP Q57XD5
C	-5	VAL	-	expression tag	UNP Q57XD5
C	-4	PRO	-	expression tag	UNP Q57XD5
C	-3	ARG	-	expression tag	UNP Q57XD5
C	-2	GLY	-	expression tag	UNP Q57XD5
C	-1	SER	-	expression tag	UNP Q57XD5
C	0	HIS	-	expression tag	UNP Q57XD5
C	337	ALA	CYS	engineered mutation	UNP Q57XD5
D	-15	HIS	-	expression tag	UNP Q57XD5
D	-14	HIS	-	expression tag	UNP Q57XD5
D	-13	HIS	-	expression tag	UNP Q57XD5
D	-12	HIS	-	expression tag	UNP Q57XD5
D	-11	HIS	-	expression tag	UNP Q57XD5
D	-10	HIS	-	expression tag	UNP Q57XD5
D	-9	SER	-	expression tag	UNP Q57XD5
D	-8	SER	-	expression tag	UNP Q57XD5
D	-7	GLY	-	expression tag	UNP Q57XD5
D	-6	LEU	-	expression tag	UNP Q57XD5
D	-5	VAL	-	expression tag	UNP Q57XD5
D	-4	PRO	-	expression tag	UNP Q57XD5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP Q57XD5
D	-2	GLY	-	expression tag	UNP Q57XD5
D	-1	SER	-	expression tag	UNP Q57XD5
D	0	HIS	-	expression tag	UNP Q57XD5
D	337	ALA	CYS	engineered mutation	UNP Q57XD5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total 5	O 5	0	0
2	B	1	Total 1	O 1	0	0
2	C	8	Total 8	O 8	0	0
2	D	14	Total 14	O 14	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: 3-KETOACYL-COA THIOLASE, PUTATIVE
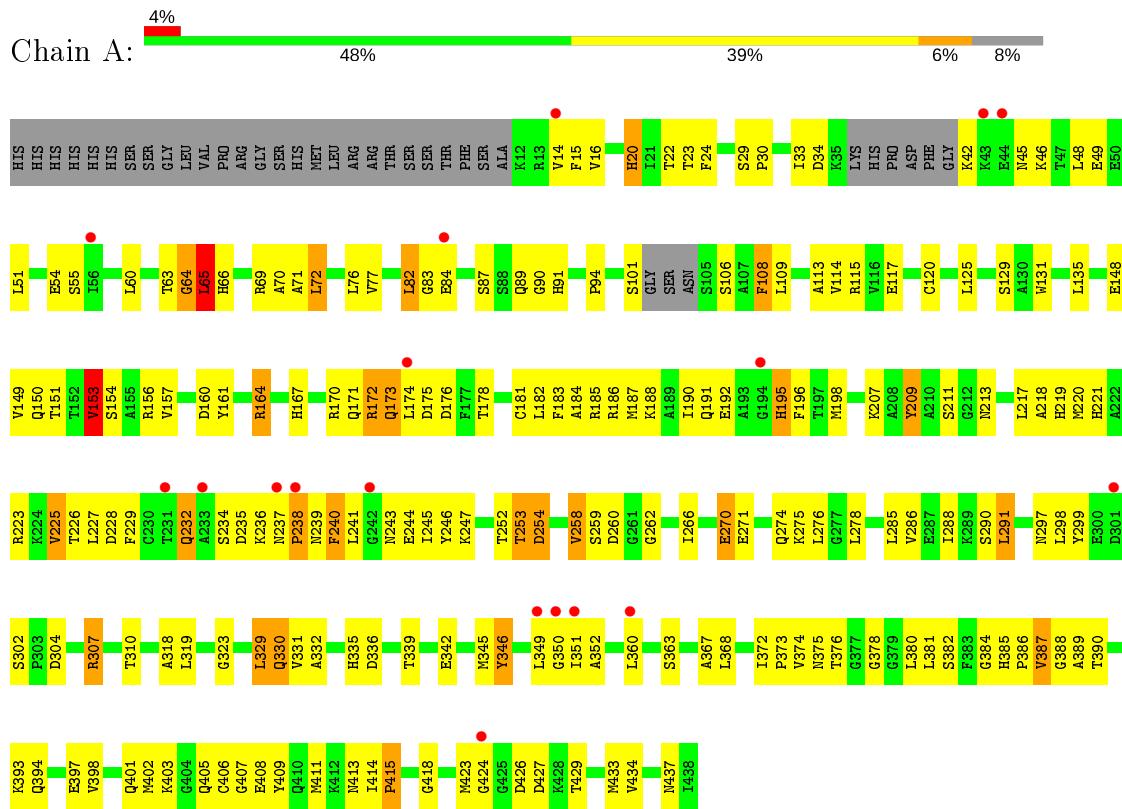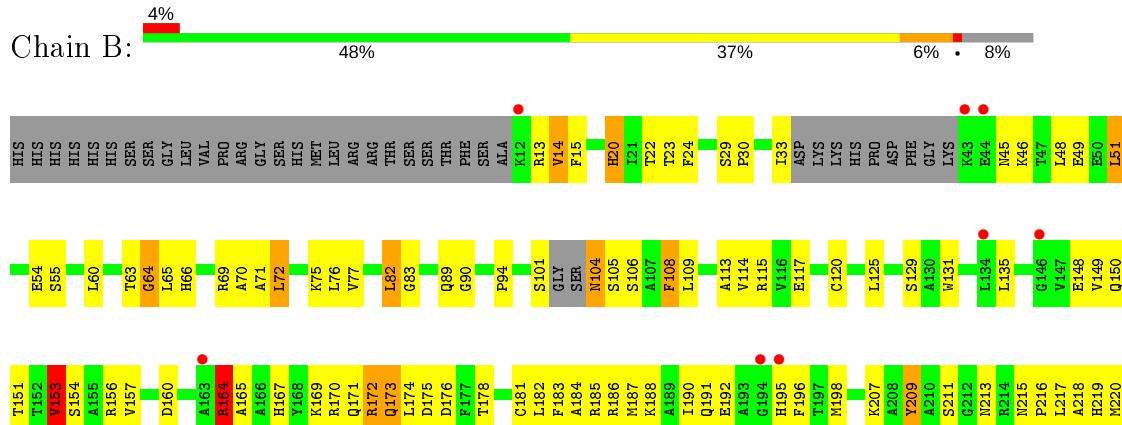

- Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

Chain C:

• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

Chain D:
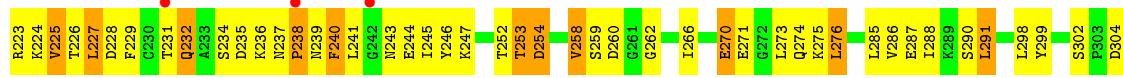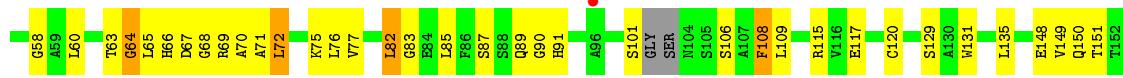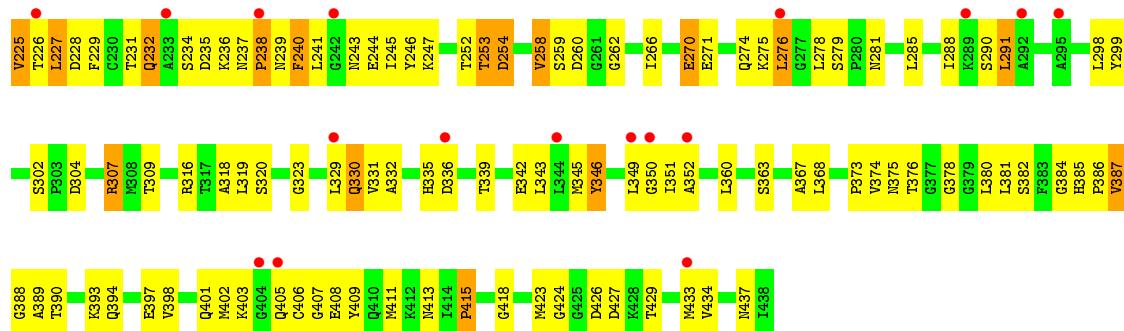
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	60.13Å 60.13Å 375.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.36 – 2.90 41.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.36-2.90) 92.1 (41.72-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.267 , 0.296 0.254 , 0.268	Depositor DCC
R_{free} test set	1704 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 37.0	EDS
L-test for twinning[2]	$< |L| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.438 for -h,-k,l 0.440 for h,-h-k,-l 0.448 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 33651 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12319	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.30	0/3118	0.60	7/4217 (0.2%)
1	B	0.33	0/3114	0.93	9/4210 (0.2%)
1	C	0.30	0/3133	0.61	8/4238 (0.2%)
1	D	0.31	0/3111	0.78	7/4206 (0.2%)
All	All	0.31	0/12476	0.74	31/16871 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	164	ARG	NE-CZ-NH1	25.62	133.11	120.30
1	D	185	ARG	NE-CZ-NH1	24.16	132.38	120.30
1	D	185	ARG	NE-CZ-NH2	-23.90	108.35	120.30
1	B	164	ARG	NE-CZ-NH2	-23.42	108.59	120.30
1	B	307	ARG	NE-CZ-NH1	23.31	131.95	120.30
1	B	307	ARG	NE-CZ-NH2	-20.24	110.18	120.30
1	D	185	ARG	CD-NE-CZ	9.04	136.26	123.60
1	B	164	ARG	CD-NE-CZ	8.45	135.43	123.60
1	B	307	ARG	CD-NE-CZ	7.67	134.33	123.60
1	C	164	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	135	LEU	CA-CB-CG	7.53	132.62	115.30
1	D	164	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	164	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	164	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	164	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	164	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	185	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	65	LEU	CA-CB-CG	6.68	130.67	115.30
1	D	307	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	307	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	185	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	185	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	D	307	ARG	NE-CZ-NH1	6.18	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	185	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	307	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	319	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	307	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	185	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	185	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	276	LEU	CB-CG-CD1	5.15	119.75	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3072	0	3058	148	1
1	B	3068	0	3067	149	0
1	C	3086	0	3076	151	0
1	D	3065	0	3063	148	1
2	A	5	0	0	0	0
2	B	1	0	0	0	0
2	C	8	0	0	0	0
2	D	14	0	0	0	0
All	All	12319	0	12264	580	1

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 24.

All (580) 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:C:20:HIS:HD2	1:C:58:GLY:HA3	1.40	0.85
1:B:51:LEU:HD21	1:B:260:ASP:HB3	1.58	0.84
1:D:20:HIS:HD2	1:D:58:GLY:HA3	1.43	0.82
1:C:403:LYS:HE3	1:C:437:ASN:HD21	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:LYS:HE3	1:D:437:ASN:HD21	1.45	0.80
1:A:403:LYS:HE3	1:A:437:ASN:HD21	1.45	0.80
1:B:403:LYS:HE3	1:B:437:ASN:HD21	1.46	0.79
1:C:13:ARG:NH1	1:C:287:GLU:OE2	2.20	0.75
1:A:209:TYR:O	1:A:213:ASN:ND2	2.20	0.73
1:B:209:TYR:O	1:B:213:ASN:ND2	2.20	0.73
1:C:20:HIS:CD2	1:C:58:GLY:HA3	2.24	0.73
1:D:209:TYR:O	1:D:213:ASN:ND2	2.20	0.72
1:D:20:HIS:CD2	1:D:58:GLY:HA3	2.25	0.71
1:C:209:TYR:O	1:C:213:ASN:ND2	2.20	0.71
1:A:51:LEU:HD11	1:A:260:ASP:HB3	1.72	0.71
1:D:304:ASP:HB3	1:D:307:ARG:HB2	1.73	0.70
1:D:160:ASP:O	1:D:164:ARG:NH1	2.24	0.70
1:A:304:ASP:HB3	1:A:307:ARG:HB2	1.74	0.69
1:D:51:LEU:HD11	1:D:260:ASP:HB3	1.73	0.69
1:C:160:ASP:O	1:C:164:ARG:NH1	2.25	0.69
1:C:304:ASP:HB3	1:C:307:ARG:HB2	1.73	0.69
1:B:304:ASP:HB3	1:B:307:ARG:HB2	1.76	0.68
1:B:167:HIS:O	1:B:171:GLN:N	2.27	0.68
1:A:160:ASP:O	1:A:164:ARG:NH1	2.26	0.68
1:C:51:LEU:HD11	1:C:260:ASP:HB3	1.73	0.68
1:B:401:GLN:NE2	1:B:411:MET:SD	2.68	0.67
1:C:167:HIS:O	1:C:171:GLN:N	2.27	0.67
1:A:167:HIS:O	1:A:171:GLN:N	2.26	0.67
1:A:401:GLN:NE2	1:A:411:MET:SD	2.68	0.67
1:D:101:SER:HB2	1:D:106:SER:HB2	1.78	0.66
1:C:401:GLN:NE2	1:C:411:MET:SD	2.68	0.66
1:D:401:GLN:NE2	1:D:411:MET:SD	2.68	0.66
1:B:101:SER:HB2	1:B:106:SER:HB2	1.77	0.66
1:D:167:HIS:O	1:D:171:GLN:N	2.27	0.66
1:A:101:SER:HB2	1:A:106:SER:HB2	1.78	0.65
1:B:390:THR:HG23	1:B:393:LYS:HE3	1.78	0.65
1:B:46:LYS:NZ	1:B:54:GLU:OE2	2.29	0.65
1:B:30:PRO:O	1:C:224:LYS:NZ	2.22	0.65
1:C:239:ASN:HD22	1:C:247:LYS:HG2	1.61	0.65
1:A:46:LYS:NZ	1:A:54:GLU:OE2	2.30	0.65
1:D:46:LYS:NZ	1:D:54:GLU:OE2	2.29	0.65
1:C:101:SER:HB2	1:C:106:SER:HB2	1.78	0.65
1:C:46:LYS:NZ	1:C:54:GLU:OE2	2.30	0.65
1:A:198:MET:SD	1:A:232:GLN:NE2	2.70	0.64
1:A:239:ASN:HD22	1:A:247:LYS:HG2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:PHE:HA	1:C:186:ARG:HB2	1.79	0.64
1:C:51:LEU:HD12	1:C:149:VAL:HG22	1.81	0.63
1:D:239:ASN:HD22	1:D:247:LYS:HG2	1.62	0.63
1:A:156:ARG:NH2	1:A:176:ASP:OD2	2.28	0.63
1:A:183:PHE:HA	1:A:186:ARG:HB2	1.79	0.63
1:A:390:THR:HG23	1:A:393:LYS:HE3	1.78	0.63
1:C:390:THR:HG23	1:C:393:LYS:HE3	1.80	0.63
1:D:183:PHE:HA	1:D:186:ARG:HB2	1.80	0.63
1:D:20:HIS:ND1	1:D:20:HIS:C	2.51	0.63
1:B:183:PHE:HA	1:B:186:ARG:HB2	1.79	0.63
1:B:239:ASN:HD22	1:B:247:LYS:HG2	1.63	0.63
1:B:198:MET:SD	1:B:232:GLN:NE2	2.71	0.63
1:C:20:HIS:ND1	1:C:20:HIS:C	2.51	0.63
1:D:198:MET:SD	1:D:232:GLN:NE2	2.72	0.63
1:C:175:ASP:O	1:C:178:THR:OG1	2.17	0.62
1:D:175:ASP:O	1:D:178:THR:OG1	2.17	0.62
1:D:390:THR:HG23	1:D:393:LYS:HE3	1.80	0.62
1:D:51:LEU:HD12	1:D:149:VAL:HG22	1.80	0.62
1:B:213:ASN:HA	1:B:221:HIS:HD2	1.65	0.62
1:C:198:MET:SD	1:C:232:GLN:NE2	2.72	0.62
1:B:175:ASP:O	1:B:178:THR:OG1	2.18	0.61
1:B:183:PHE:O	1:B:187:MET:N	2.34	0.61
1:C:170:ARG:O	1:C:173:GLN:NE2	2.25	0.61
1:B:64:GLY:O	1:B:69:ARG:NH2	2.29	0.61
1:A:175:ASP:O	1:A:178:THR:OG1	2.18	0.61
1:A:51:LEU:HD12	1:A:149:VAL:HG22	1.81	0.61
1:D:182:LEU:HD13	1:D:426:ASP:HB2	1.83	0.61
1:D:213:ASN:HA	1:D:221:HIS:HD2	1.65	0.61
1:A:183:PHE:O	1:A:187:MET:N	2.34	0.60
1:A:64:GLY:O	1:A:69:ARG:NH2	2.29	0.60
1:D:156:ARG:NH2	1:D:176:ASP:OD2	2.29	0.60
1:A:213:ASN:HA	1:A:221:HIS:HD2	1.65	0.60
1:C:402:MET:HG2	1:C:437:ASN:HD22	1.67	0.60
1:A:182:LEU:HD13	1:A:426:ASP:HB2	1.83	0.60
1:C:213:ASN:HA	1:C:221:HIS:HD2	1.65	0.60
1:C:243:ASN:O	1:C:247:LYS:N	2.32	0.60
1:B:29:SER:HB2	1:B:219:HIS:HD2	1.67	0.60
1:A:402:MET:HG2	1:A:437:ASN:HD22	1.67	0.60
1:B:402:MET:HG2	1:B:437:ASN:HD22	1.67	0.60
1:A:114:VAL:HG13	1:B:125:LEU:HD13	1.83	0.59
1:C:60:LEU:HD23	1:C:266:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LEU:HD13	1:C:426:ASP:HB2	1.83	0.59
1:C:64:GLY:O	1:C:69:ARG:NH2	2.29	0.59
1:B:14:VAL:HG22	1:B:288:ILE:HB	1.85	0.59
1:B:156:ARG:NH2	1:B:176:ASP:OD2	2.29	0.59
1:D:29:SER:HB2	1:D:219:HIS:HD2	1.67	0.59
1:A:29:SER:HB2	1:A:219:HIS:HD2	1.67	0.59
1:D:60:LEU:HD23	1:D:266:ILE:HD11	1.85	0.59
1:D:424:GLY:HA3	1:D:429:THR:HB	1.84	0.59
1:C:29:SER:HB2	1:C:219:HIS:HD2	1.68	0.59
1:B:104:ASN:O	1:B:106:SER:N	2.35	0.59
1:A:424:GLY:HA3	1:A:429:THR:HB	1.84	0.58
1:D:402:MET:HG2	1:D:437:ASN:HD22	1.68	0.58
1:C:424:GLY:HA3	1:C:429:THR:HB	1.84	0.58
1:A:94:PRO:HG2	1:B:298:LEU:HD23	1.84	0.58
1:B:60:LEU:HD23	1:B:266:ILE:HD11	1.86	0.58
1:A:60:LEU:HD23	1:A:266:ILE:HD11	1.86	0.58
1:B:14:VAL:HG11	1:B:131:TRP:HD1	1.68	0.58
1:B:182:LEU:HD13	1:B:426:ASP:HB2	1.84	0.58
1:C:183:PHE:O	1:C:187:MET:N	2.36	0.58
1:D:243:ASN:O	1:D:247:LYS:N	2.32	0.58
1:B:424:GLY:HA3	1:B:429:THR:HB	1.85	0.58
1:C:156:ARG:NH2	1:C:176:ASP:OD2	2.29	0.58
1:B:45:ASN:OD1	1:B:46:LYS:N	2.37	0.57
1:C:14:VAL:HG21	1:C:131:TRP:HD1	1.69	0.57
1:D:14:VAL:HG21	1:D:131:TRP:HD1	1.69	0.57
1:C:243:ASN:O	1:C:245:ILE:N	2.37	0.57
1:D:183:PHE:O	1:D:187:MET:N	2.36	0.57
1:A:14:VAL:HG21	1:A:131:TRP:HD1	1.70	0.57
1:B:243:ASN:O	1:B:247:LYS:N	2.33	0.57
1:B:237:ASN:HD21	1:B:253:THR:H	1.52	0.57
1:A:45:ASN:OD1	1:A:46:LYS:N	2.37	0.57
1:B:243:ASN:O	1:B:245:ILE:N	2.37	0.57
1:C:273:LEU:HA	1:C:276:LEU:HD12	1.87	0.57
1:B:151:THR:OG1	1:B:260:ASP:OD2	2.22	0.56
1:A:125:LEU:HD13	1:B:114:VAL:HG13	1.87	0.56
1:C:237:ASN:HD21	1:C:253:THR:H	1.53	0.56
1:D:237:ASN:HD21	1:D:253:THR:H	1.53	0.56
1:D:243:ASN:O	1:D:245:ILE:N	2.38	0.56
1:A:243:ASN:O	1:A:247:LYS:N	2.33	0.55
1:A:243:ASN:O	1:A:245:ILE:N	2.38	0.55
1:C:45:ASN:OD1	1:C:46:LYS:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:HD21	1:A:253:THR:H	1.53	0.55
1:B:319:LEU:O	1:B:323:GLY:N	2.40	0.55
1:D:89:GLN:NE2	1:D:90:GLY:O	2.40	0.55
1:A:319:LEU:O	1:A:323:GLY:N	2.40	0.55
1:D:48:LEU:HD13	1:D:149:VAL:HG23	1.89	0.55
1:C:319:LEU:O	1:C:323:GLY:N	2.40	0.55
1:C:89:GLN:NE2	1:C:90:GLY:O	2.40	0.55
1:A:20:HIS:ND1	1:A:20:HIS:C	2.60	0.55
1:C:330:GLN:HB2	1:C:415:PRO:HB3	1.89	0.55
1:C:239:ASN:ND2	1:C:247:LYS:HG2	2.22	0.55
1:B:89:GLN:NE2	1:B:90:GLY:O	2.40	0.55
1:D:51:LEU:O	1:D:55:SER:OG	2.22	0.55
1:A:298:LEU:HD23	1:B:94:PRO:HG2	1.89	0.54
1:C:285:LEU:O	1:C:403:LYS:NZ	2.40	0.54
1:D:330:GLN:HB2	1:D:415:PRO:HB3	1.89	0.54
1:D:45:ASN:OD1	1:D:46:LYS:N	2.39	0.54
1:B:170:ARG:O	1:B:173:GLN:NE2	2.26	0.54
1:A:51:LEU:O	1:A:55:SER:OG	2.21	0.54
1:C:48:LEU:HD13	1:C:149:VAL:HG23	1.89	0.54
1:D:319:LEU:O	1:D:323:GLY:N	2.40	0.54
1:A:170:ARG:O	1:A:173:GLN:NE2	2.28	0.54
1:A:49:GLU:OE1	1:A:49:GLU:N	2.40	0.54
1:B:20:HIS:C	1:B:20:HIS:ND1	2.62	0.54
1:D:239:ASN:ND2	1:D:247:LYS:HG2	2.22	0.54
1:B:14:VAL:O	1:B:288:ILE:N	2.34	0.54
1:A:15:PHE:HE1	1:A:270:GLU:HG3	1.73	0.53
1:A:285:LEU:O	1:A:403:LYS:NZ	2.40	0.53
1:C:386:PRO:HB2	1:C:389:ALA:HB3	1.90	0.53
1:B:48:LEU:HD13	1:B:149:VAL:HG23	1.90	0.53
1:A:14:VAL:O	1:A:288:ILE:N	2.34	0.53
1:B:239:ASN:ND2	1:B:247:LYS:HG2	2.23	0.53
1:D:15:PHE:HE1	1:D:270:GLU:HG3	1.73	0.53
1:C:407:GLY:O	1:C:409:TYR:N	2.42	0.53
1:D:285:LEU:O	1:D:403:LYS:NZ	2.41	0.53
1:A:48:LEU:HD13	1:A:149:VAL:HG23	1.91	0.53
1:A:174:LEU:HB2	1:A:178:THR:HG23	1.91	0.53
1:C:174:LEU:HB2	1:C:178:THR:HG23	1.91	0.53
1:C:386:PRO:O	1:C:389:ALA:N	2.33	0.53
1:C:209:TYR:HE1	1:C:223:ARG:HB3	1.74	0.53
1:D:174:LEU:HB2	1:D:178:THR:HG23	1.91	0.53
1:D:209:TYR:HE1	1:D:223:ARG:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASN:ND2	1:A:247:LYS:HG2	2.23	0.53
1:B:76:LEU:HD21	1:B:108:PHE:CZ	2.44	0.53
1:D:209:TYR:CE1	1:D:223:ARG:HB3	2.44	0.53
1:A:151:THR:OG1	1:A:260:ASP:OD2	2.23	0.53
1:A:89:GLN:NE2	1:A:90:GLY:O	2.42	0.53
1:A:386:PRO:HB2	1:A:389:ALA:HB3	1.91	0.53
1:D:407:GLY:O	1:D:409:TYR:N	2.42	0.52
1:A:34:ASP:O	1:A:42:LYS:N	2.42	0.52
1:B:209:TYR:CE1	1:B:223:ARG:HB3	2.44	0.52
1:B:386:PRO:O	1:B:389:ALA:N	2.34	0.52
1:B:386:PRO:HB2	1:B:389:ALA:HB3	1.89	0.52
1:A:209:TYR:CE1	1:A:223:ARG:HB3	2.44	0.52
1:B:285:LEU:O	1:B:403:LYS:NZ	2.41	0.52
1:A:76:LEU:HD21	1:A:108:PHE:CZ	2.44	0.52
1:B:15:PHE:HE1	1:B:270:GLU:HG3	1.75	0.52
1:B:49:GLU:OE1	1:B:49:GLU:N	2.41	0.52
1:C:49:GLU:OE1	1:C:49:GLU:N	2.41	0.52
1:D:151:THR:OG1	1:D:260:ASP:OD2	2.26	0.52
1:C:15:PHE:HE1	1:C:270:GLU:HG3	1.74	0.52
1:A:336:ASP:OD1	1:A:375:ASN:ND2	2.43	0.52
1:D:154:SER:HB3	1:D:157:VAL:HB	1.92	0.52
1:A:209:TYR:HE1	1:A:223:ARG:HB3	1.74	0.52
1:C:336:ASP:OD1	1:C:375:ASN:ND2	2.43	0.52
1:B:170:ARG:NH2	1:B:298:LEU:O	2.43	0.52
1:B:336:ASP:OD1	1:B:375:ASN:ND2	2.43	0.52
1:C:403:LYS:HE3	1:C:437:ASN:ND2	2.21	0.52
1:D:336:ASP:OD1	1:D:375:ASN:ND2	2.43	0.52
1:A:170:ARG:NH2	1:A:298:LEU:O	2.43	0.52
1:A:220:MET:O	1:A:382:SER:OG	2.28	0.52
1:C:209:TYR:CE1	1:C:223:ARG:HB3	2.44	0.52
1:A:407:GLY:O	1:A:409:TYR:N	2.43	0.51
1:B:174:LEU:HB2	1:B:178:THR:HG23	1.92	0.51
1:C:154:SER:HB3	1:C:157:VAL:HB	1.91	0.51
1:C:220:MET:O	1:C:382:SER:OG	2.27	0.51
1:D:219:HIS:ND1	1:D:259:SER:HB3	2.26	0.51
1:B:51:LEU:HD22	1:B:149:VAL:HG22	1.92	0.51
1:B:70:ALA:O	1:B:72:LEU:N	2.43	0.51
1:C:241:LEU:HB2	1:C:247:LYS:HA	1.93	0.51
1:D:64:GLY:O	1:D:69:ARG:NH2	2.29	0.51
1:A:219:HIS:ND1	1:A:259:SER:HB3	2.26	0.51
1:A:330:GLN:HB2	1:A:415:PRO:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:HIS:ND1	1:C:259:SER:HB3	2.25	0.51
1:A:70:ALA:O	1:A:72:LEU:N	2.43	0.51
1:D:220:MET:O	1:D:382:SER:OG	2.27	0.51
1:D:241:LEU:HB2	1:D:247:LYS:HA	1.93	0.51
1:B:330:GLN:HB2	1:B:415:PRO:HB3	1.91	0.51
1:C:51:LEU:O	1:C:55:SER:OG	2.22	0.51
1:D:386:PRO:HB2	1:D:389:ALA:HB3	1.91	0.51
1:D:403:LYS:HE3	1:D:437:ASN:ND2	2.21	0.51
1:D:76:LEU:HD21	1:D:108:PHE:CZ	2.45	0.51
1:A:23:THR:HA	1:A:217:LEU:HB2	1.92	0.51
1:A:87:SER:O	1:B:169:LYS:NZ	2.32	0.51
1:B:407:GLY:O	1:B:409:TYR:N	2.44	0.51
1:D:14:VAL:O	1:D:288:ILE:N	2.35	0.51
1:D:170:ARG:O	1:D:173:GLN:NE2	2.26	0.51
1:D:49:GLU:OE1	1:D:49:GLU:N	2.41	0.51
1:B:209:TYR:HE1	1:B:223:ARG:HB3	1.74	0.51
1:D:23:THR:HA	1:D:217:LEU:HB2	1.93	0.51
1:B:109:LEU:HD12	1:B:109:LEU:H	1.76	0.51
1:B:241:LEU:HB2	1:B:247:LYS:HA	1.93	0.51
1:C:170:ARG:NH2	1:C:298:LEU:O	2.44	0.51
1:C:76:LEU:HD21	1:C:108:PHE:CZ	2.45	0.50
1:A:154:SER:HB3	1:A:157:VAL:HB	1.93	0.50
1:D:70:ALA:O	1:D:72:LEU:N	2.44	0.50
1:A:241:LEU:HB2	1:A:247:LYS:HA	1.93	0.50
1:B:219:HIS:ND1	1:B:259:SER:HB3	2.26	0.50
1:B:290:SER:HB2	1:B:434:VAL:HB	1.94	0.50
1:C:151:THR:OG1	1:C:260:ASP:OD2	2.25	0.50
1:C:131:TRP:CG	1:C:291:LEU:HD23	2.47	0.50
1:B:23:THR:HA	1:B:217:LEU:HB2	1.92	0.49
1:B:259:SER:OG	1:B:385:HIS:N	2.41	0.49
1:C:70:ALA:O	1:C:72:LEU:N	2.44	0.49
1:D:170:ARG:NH2	1:D:298:LEU:O	2.44	0.49
1:B:211:SER:HB2	1:B:378:GLY:HA2	1.93	0.49
1:C:290:SER:HB2	1:C:434:VAL:HB	1.94	0.49
1:D:290:SER:HB2	1:D:434:VAL:HB	1.94	0.49
1:B:342:GLU:HA	1:B:345:MET:HG2	1.94	0.49
1:A:211:SER:HB2	1:A:378:GLY:HA2	1.93	0.49
1:B:154:SER:HB3	1:B:157:VAL:HB	1.93	0.49
1:C:23:THR:HA	1:C:217:LEU:HB2	1.93	0.49
1:D:181:CYS:HA	1:D:184:ALA:HB3	1.95	0.49
1:A:167:HIS:HB3	1:A:170:ARG:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:OD1	1:A:254:ASP:N	2.45	0.49
1:A:24:PHE:HD2	1:A:384:GLY:HA3	1.77	0.49
1:C:181:CYS:HA	1:C:184:ALA:HB3	1.95	0.49
1:C:24:PHE:HD2	1:C:384:GLY:HA3	1.78	0.49
1:C:386:PRO:O	1:C:388:GLY:N	2.46	0.49
1:A:109:LEU:H	1:A:109:LEU:HD12	1.76	0.49
1:A:238:PRO:O	1:A:252:THR:N	2.46	0.49
1:A:386:PRO:O	1:A:388:GLY:N	2.45	0.49
1:A:84:GLU:O	1:B:164:ARG:NH1	2.24	0.49
1:D:131:TRP:CG	1:D:291:LEU:HD23	2.48	0.49
1:A:161:TYR:O	1:A:164:ARG:HG2	2.12	0.49
1:B:51:LEU:O	1:B:55:SER:OG	2.23	0.49
1:D:24:PHE:HD2	1:D:384:GLY:HA3	1.78	0.49
1:D:254:ASP:OD1	1:D:254:ASP:N	2.46	0.49
1:B:181:CYS:HA	1:B:184:ALA:HB3	1.95	0.48
1:B:220:MET:O	1:B:382:SER:OG	2.29	0.48
1:B:386:PRO:O	1:B:388:GLY:N	2.45	0.48
1:C:109:LEU:HD12	1:C:109:LEU:H	1.77	0.48
1:C:238:PRO:O	1:C:252:THR:N	2.46	0.48
1:D:167:HIS:HB3	1:D:170:ARG:HB3	1.95	0.48
1:D:51:LEU:CD1	1:D:260:ASP:HB3	2.42	0.48
1:A:342:GLU:HA	1:A:345:MET:HG2	1.95	0.48
1:B:167:HIS:HB3	1:B:170:ARG:HB3	1.95	0.48
1:B:238:PRO:O	1:B:252:THR:N	2.46	0.48
1:D:386:PRO:O	1:D:388:GLY:N	2.46	0.48
1:B:368:LEU:HA	1:B:373:PRO:HB3	1.95	0.48
1:C:254:ASP:N	1:C:254:ASP:OD1	2.46	0.48
1:B:401:GLN:HG3	1:B:406:CYS:SG	2.54	0.48
1:C:211:SER:HB2	1:C:378:GLY:HA2	1.95	0.48
1:D:109:LEU:HD12	1:D:109:LEU:H	1.77	0.48
1:D:190:ILE:HG12	1:D:196:PHE:CZ	2.49	0.48
1:B:243:ASN:O	1:B:246:TYR:N	2.45	0.48
1:C:167:HIS:HB3	1:C:170:ARG:HB3	1.95	0.48
1:D:339:THR:HG22	1:D:381:LEU:HD21	1.96	0.48
1:A:131:TRP:CG	1:A:291:LEU:HD23	2.49	0.48
1:C:259:SER:OG	1:C:385:HIS:N	2.42	0.48
1:B:254:ASP:OD1	1:B:254:ASP:N	2.46	0.48
1:B:339:THR:HG22	1:B:381:LEU:HD21	1.95	0.48
1:C:339:THR:HG22	1:C:381:LEU:HD21	1.96	0.48
1:C:190:ILE:HG12	1:C:196:PHE:CZ	2.49	0.48
1:D:238:PRO:O	1:D:252:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HG12	1:A:196:PHE:CZ	2.49	0.48
1:A:368:LEU:HA	1:A:373:PRO:HB3	1.96	0.48
1:A:290:SER:HB2	1:A:434:VAL:HB	1.94	0.48
1:C:13:ARG:HD2	1:C:270:GLU:HG2	1.95	0.48
1:C:169:LYS:NZ	1:D:87:SER:O	2.38	0.48
1:A:181:CYS:HA	1:A:184:ALA:HB3	1.96	0.48
1:A:51:LEU:CD1	1:A:260:ASP:HB3	2.41	0.48
1:A:403:LYS:HE3	1:A:437:ASN:ND2	2.22	0.47
1:B:190:ILE:HG12	1:B:196:PHE:CZ	2.49	0.47
1:C:172:ARG:C	1:C:174:LEU:H	2.18	0.47
1:C:243:ASN:O	1:C:246:TYR:N	2.46	0.47
1:B:24:PHE:HD2	1:B:384:GLY:HA3	1.77	0.47
1:C:82:LEU:N	1:C:148:GLU:OE2	2.45	0.47
1:C:164:ARG:HA	1:D:89:GLN:HA	1.95	0.47
1:D:167:HIS:CD2	1:D:298:LEU:HD12	2.49	0.47
1:D:211:SER:HB2	1:D:378:GLY:HA2	1.95	0.47
1:B:160:ASP:O	1:B:164:ARG:NH2	2.40	0.47
1:C:342:GLU:HA	1:C:345:MET:HG2	1.96	0.47
1:D:368:LEU:HA	1:D:373:PRO:HB3	1.96	0.47
1:D:332:ALA:HB3	1:D:374:VAL:HG22	1.96	0.47
1:A:401:GLN:HG3	1:A:406:CYS:SG	2.54	0.47
1:C:14:VAL:HG21	1:C:131:TRP:CD1	2.49	0.47
1:C:191:GLN:HE22	1:C:198:MET:N	2.12	0.47
1:C:401:GLN:HG3	1:C:406:CYS:SG	2.55	0.47
1:D:342:GLU:HA	1:D:345:MET:HG2	1.96	0.47
1:B:131:TRP:CG	1:B:291:LEU:HD23	2.49	0.47
1:C:161:TYR:O	1:C:164:ARG:HG2	2.15	0.47
1:C:368:LEU:HA	1:C:373:PRO:HB3	1.96	0.47
1:C:335:HIS:HB2	1:C:394:GLN:HE22	1.80	0.47
1:D:172:ARG:C	1:D:174:LEU:H	2.18	0.47
1:B:29:SER:HB2	1:B:219:HIS:CD2	2.49	0.47
1:C:20:HIS:ND1	1:C:21:ILE:N	2.63	0.47
1:C:51:LEU:CD1	1:C:260:ASP:HB3	2.42	0.47
1:A:339:THR:HG22	1:A:381:LEU:HD21	1.96	0.47
1:A:386:PRO:O	1:A:389:ALA:N	2.34	0.47
1:B:335:HIS:HB2	1:B:394:GLN:HE22	1.80	0.47
1:D:234:SER:OG	1:D:235:ASP:N	2.48	0.47
1:A:191:GLN:HE22	1:A:198:MET:N	2.13	0.47
1:B:191:GLN:HE22	1:B:198:MET:N	2.13	0.47
1:B:297:ASN:OD1	1:B:299:TYR:N	2.40	0.47
1:D:243:ASN:O	1:D:246:TYR:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:GLN:HE22	1:D:198:MET:N	2.12	0.47
1:D:335:HIS:HB2	1:D:394:GLN:HE22	1.80	0.46
1:A:186:ARG:HH22	1:A:302:SER:HB2	1.81	0.46
1:C:29:SER:HB2	1:C:219:HIS:CD2	2.50	0.46
1:C:380:LEU:H	1:C:380:LEU:HD12	1.80	0.46
1:A:172:ARG:C	1:A:174:LEU:H	2.19	0.46
1:D:150:GLN:HB3	1:D:258:VAL:HG13	1.97	0.46
1:D:380:LEU:H	1:D:380:LEU:HD12	1.80	0.46
1:C:170:ARG:NH1	1:C:299:TYR:O	2.48	0.46
1:A:335:HIS:HB2	1:A:394:GLN:HE22	1.80	0.46
1:D:401:GLN:HG3	1:D:406:CYS:SG	2.55	0.46
1:B:13:ARG:HG2	1:B:287:GLU:OE2	2.15	0.46
1:C:167:HIS:CD2	1:C:298:LEU:HD12	2.51	0.46
1:A:63:THR:O	1:A:65:LEU:N	2.43	0.46
1:B:14:VAL:HG11	1:B:131:TRP:CD1	2.49	0.46
1:D:213:ASN:ND2	1:D:223:ARG:O	2.27	0.46
1:A:33:ILE:HD13	1:A:33:ILE:HA	1.89	0.46
1:B:218:ALA:HB3	1:B:221:HIS:HB2	1.98	0.46
1:D:20:HIS:ND1	1:D:21:ILE:N	2.63	0.46
1:B:82:LEU:N	1:B:148:GLU:OE2	2.45	0.46
1:D:161:TYR:O	1:D:164:ARG:HG2	2.15	0.46
1:D:29:SER:HB2	1:D:219:HIS:CD2	2.49	0.46
1:A:360:LEU:O	1:A:363:SER:OG	2.28	0.46
1:B:380:LEU:HD12	1:B:380:LEU:H	1.81	0.46
1:A:120:CYS:HB2	1:A:423:MET:O	2.16	0.45
1:B:63:THR:HG21	1:B:266:ILE:HD12	1.98	0.45
1:C:120:CYS:HA	1:C:387:VAL:HG12	1.98	0.45
1:D:14:VAL:HG21	1:D:131:TRP:CD1	2.49	0.45
1:A:237:ASN:ND2	1:A:237:ASN:O	2.49	0.45
1:B:172:ARG:C	1:B:174:LEU:H	2.19	0.45
1:D:291:LEU:HD13	1:D:433:MET:HG2	1.98	0.45
1:A:82:LEU:N	1:A:148:GLU:OE2	2.45	0.45
1:B:167:HIS:CD2	1:B:299:TYR:HA	2.51	0.45
1:D:170:ARG:NH1	1:D:299:TYR:O	2.49	0.45
1:A:259:SER:OG	1:A:385:HIS:N	2.41	0.45
1:B:373:PRO:HB2	1:B:376:THR:CG2	2.46	0.45
1:C:332:ALA:HB3	1:C:374:VAL:HG22	1.97	0.45
1:D:237:ASN:ND2	1:D:253:THR:OG1	2.49	0.45
1:A:20:HIS:HE1	1:A:22:THR:HG22	1.81	0.45
1:C:271:GLU:O	1:C:274:GLN:HG2	2.16	0.45
1:C:89:GLN:HA	1:D:164:ARG:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ALA:HB3	1:A:374:VAL:HG22	1.98	0.45
1:C:226:THR:HG22	1:C:228:ASP:H	1.82	0.45
1:C:150:GLN:HB3	1:C:258:VAL:HG13	1.97	0.45
1:C:291:LEU:HD13	1:C:433:MET:HG2	1.97	0.45
1:D:55:SER:OG	1:D:262:GLY:HA3	2.17	0.45
1:A:167:HIS:CD2	1:A:298:LEU:HD12	2.52	0.45
1:A:167:HIS:CD2	1:A:299:TYR:HA	2.51	0.45
1:A:373:PRO:HB2	1:A:376:THR:CG2	2.47	0.45
1:B:120:CYS:HB3	1:B:335:HIS:CE1	2.52	0.45
1:B:167:HIS:CD2	1:B:298:LEU:HD12	2.51	0.45
1:C:87:SER:O	1:D:169:LYS:NZ	2.35	0.45
1:A:115:ARG:NH1	1:A:117:GLU:HB2	2.32	0.45
1:A:243:ASN:O	1:A:246:TYR:N	2.46	0.45
1:B:76:LEU:HD21	1:B:108:PHE:CE2	2.52	0.45
1:B:120:CYS:HA	1:B:387:VAL:HG12	1.99	0.45
1:B:332:ALA:HB3	1:B:374:VAL:HG22	1.98	0.45
1:C:234:SER:OG	1:C:235:ASP:N	2.48	0.45
1:A:380:LEU:HD12	1:A:380:LEU:H	1.81	0.45
1:A:63:THR:HG21	1:A:266:ILE:HD12	1.98	0.45
1:B:291:LEU:HD13	1:B:433:MET:HG2	1.99	0.45
1:C:14:VAL:O	1:C:288:ILE:N	2.36	0.45
1:C:120:CYS:HB3	1:C:335:HIS:CE1	2.52	0.45
1:D:167:HIS:CD2	1:D:299:TYR:HA	2.52	0.45
1:A:120:CYS:HB3	1:A:335:HIS:CE1	2.51	0.45
1:B:115:ARG:NH1	1:B:117:GLU:HB2	2.31	0.45
1:B:20:HIS:HE1	1:B:22:THR:HG22	1.82	0.45
1:C:167:HIS:CD2	1:C:299:TYR:HA	2.51	0.45
1:C:55:SER:OG	1:C:262:GLY:HA3	2.17	0.45
1:C:77:VAL:HG11	1:C:129:SER:HB3	1.99	0.45
1:D:115:ARG:NH1	1:D:117:GLU:HB2	2.32	0.45
1:D:67:ASP:HB3	1:D:68:GLY:H	1.63	0.45
1:A:329:LEU:HB3	1:A:372:ILE:HD13	1.99	0.44
1:A:76:LEU:HD21	1:A:108:PHE:CE2	2.52	0.44
1:B:329:LEU:HB3	1:B:372:ILE:HD13	1.98	0.44
1:D:271:GLU:O	1:D:274:GLN:HG2	2.17	0.44
1:D:386:PRO:O	1:D:389:ALA:N	2.34	0.44
1:A:234:SER:OG	1:A:235:ASP:N	2.50	0.44
1:B:65:LEU:HD22	1:B:72:LEU:HD11	1.99	0.44
1:D:82:LEU:N	1:D:148:GLU:OE2	2.46	0.44
1:D:227:LEU:O	1:D:231:THR:HG23	2.17	0.44
1:A:218:ALA:HB3	1:A:221:HIS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:CYS:HB2	1:B:423:MET:O	2.17	0.44
1:B:215:ASN:HA	1:B:216:PRO:HD2	1.81	0.44
1:B:234:SER:OG	1:B:235:ASP:N	2.50	0.44
1:B:403:LYS:HE3	1:B:437:ASN:ND2	2.22	0.44
1:C:227:LEU:O	1:C:231:THR:HG23	2.18	0.44
1:D:237:ASN:ND2	1:D:237:ASN:O	2.50	0.44
1:A:310:THR:OG1	1:A:427:ASP:O	2.28	0.44
1:B:186:ARG:HH22	1:B:302:SER:HB2	1.81	0.44
1:C:229:PHE:HZ	1:C:236:LYS:HB2	1.82	0.44
1:D:226:THR:HG22	1:D:228:ASP:H	1.82	0.44
1:A:153:VAL:HB	1:A:154:SER:H	1.63	0.44
1:C:72:LEU:HD22	1:C:275:LYS:HE3	2.00	0.44
1:A:55:SER:OG	1:A:262:GLY:HA3	2.18	0.44
1:B:77:VAL:HG11	1:B:129:SER:HB3	2.00	0.44
1:C:76:LEU:HD21	1:C:108:PHE:CE2	2.52	0.44
1:D:120:CYS:HB3	1:D:335:HIS:CE1	2.53	0.44
1:D:76:LEU:HD21	1:D:108:PHE:CE2	2.52	0.44
1:D:218:ALA:HB3	1:D:221:HIS:HB2	2.00	0.44
1:D:229:PHE:HZ	1:D:236:LYS:HB2	1.83	0.44
1:D:259:SER:OG	1:D:385:HIS:N	2.42	0.44
1:C:218:ALA:HB3	1:C:221:HIS:HB2	2.00	0.44
1:C:65:LEU:HD22	1:C:72:LEU:HD11	2.00	0.44
1:A:120:CYS:HA	1:A:387:VAL:HG12	1.99	0.43
1:D:373:PRO:HB2	1:D:376:THR:CG2	2.48	0.43
1:C:115:ARG:NH1	1:C:117:GLU:HB2	2.32	0.43
1:D:276:LEU:HB3	1:D:278:LEU:HG	1.99	0.43
1:C:373:PRO:HB2	1:C:376:THR:CG2	2.48	0.43
1:A:291:LEU:HD13	1:A:433:MET:HG2	1.99	0.43
1:A:29:SER:HB2	1:A:219:HIS:CD2	2.49	0.43
1:A:72:LEU:HD22	1:A:275:LYS:HE3	2.01	0.43
1:B:188:LYS:NZ	1:B:192:GLU:OE2	2.51	0.43
1:C:237:ASN:ND2	1:C:237:ASN:O	2.51	0.43
1:D:72:LEU:HD22	1:D:275:LYS:HE3	1.99	0.43
1:D:330:GLN:O	1:D:373:PRO:HD2	2.19	0.43
1:A:188:LYS:NZ	1:A:192:GLU:OE2	2.51	0.43
1:A:226:THR:HG22	1:A:228:ASP:H	1.82	0.43
1:B:213:ASN:ND2	1:B:223:ARG:O	2.28	0.43
1:B:237:ASN:ND2	1:B:253:THR:OG1	2.50	0.43
1:C:153:VAL:HB	1:C:154:SER:H	1.63	0.43
1:D:316:ARG:O	1:D:320:SER:OG	2.24	0.43
1:A:120:CYS:HB3	1:A:335:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG21	1:A:131:TRP:CD1	2.50	0.43
1:A:77:VAL:HG11	1:A:129:SER:HB3	2.00	0.43
1:B:276:LEU:HB3	1:B:278:LEU:HG	2.00	0.43
1:B:55:SER:OG	1:B:262:GLY:HA3	2.17	0.43
1:C:120:CYS:HB3	1:C:335:HIS:NE2	2.34	0.43
1:C:398:VAL:HG11	1:C:418:GLY:HA3	2.00	0.43
1:D:120:CYS:HA	1:D:387:VAL:HG12	1.98	0.43
1:D:31:LEU:HA	1:D:31:LEU:HD12	1.87	0.43
1:D:120:CYS:HB3	1:D:335:HIS:NE2	2.34	0.43
1:D:398:VAL:HG11	1:D:418:GLY:HA3	2.00	0.43
1:A:297:ASN:OD1	1:A:299:TYR:N	2.41	0.43
1:B:150:GLN:HB3	1:B:258:VAL:HG13	2.00	0.43
1:B:72:LEU:HD22	1:B:275:LYS:HE3	2.00	0.43
1:B:414:ILE:HA	1:B:415:PRO:HD3	1.92	0.43
1:D:65:LEU:HD22	1:D:72:LEU:HD11	2.00	0.43
1:A:150:GLN:HB3	1:A:258:VAL:HG13	2.00	0.43
1:C:120:CYS:HB2	1:C:423:MET:O	2.19	0.43
1:D:77:VAL:HG11	1:D:129:SER:HB3	2.00	0.43
1:D:215:ASN:HA	1:D:216:PRO:HD2	1.83	0.43
1:A:237:ASN:ND2	1:A:253:THR:OG1	2.50	0.43
1:B:373:PRO:HB2	1:B:376:THR:HG22	2.01	0.43
1:C:330:GLN:O	1:C:373:PRO:HD2	2.18	0.43
1:D:120:CYS:HB2	1:D:423:MET:O	2.19	0.43
1:A:170:ARG:NH1	1:A:299:TYR:O	2.52	0.43
1:A:398:VAL:HG11	1:A:418:GLY:HA3	2.01	0.43
1:B:237:ASN:ND2	1:B:237:ASN:O	2.50	0.43
1:C:237:ASN:ND2	1:C:253:THR:OG1	2.49	0.43
1:C:186:ARG:HH22	1:C:302:SER:HB2	1.83	0.43
1:C:349:LEU:HG	1:C:351:ILE:HG12	2.01	0.43
1:B:153:VAL:HB	1:B:154:SER:H	1.63	0.42
1:B:63:THR:O	1:B:65:LEU:N	2.47	0.42
1:C:63:THR:HG21	1:C:266:ILE:HD12	2.01	0.42
1:A:207:LYS:HE2	1:A:367:ALA:HA	2.01	0.42
1:D:15:PHE:CE1	1:D:270:GLU:HG3	2.52	0.42
1:A:15:PHE:CE1	1:A:270:GLU:HG3	2.52	0.42
1:A:225:VAL:HG12	1:A:226:THR:H	1.84	0.42
1:B:226:THR:HG22	1:B:228:ASP:H	1.83	0.42
1:C:15:PHE:CE1	1:C:270:GLU:HG3	2.53	0.42
1:D:207:LYS:HE2	1:D:367:ALA:HA	2.00	0.42
1:A:229:PHE:HZ	1:A:236:LYS:HB2	1.84	0.42
1:B:15:PHE:CE1	1:B:270:GLU:HG3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:CYS:HB3	1:B:335:HIS:NE2	2.33	0.42
1:C:207:LYS:HE2	1:C:367:ALA:HA	2.01	0.42
1:D:229:PHE:CZ	1:D:236:LYS:HB2	2.54	0.42
1:D:63:THR:HG21	1:D:266:ILE:HD12	2.01	0.42
1:A:349:LEU:HG	1:A:351:ILE:HG12	2.00	0.42
1:B:225:VAL:HG12	1:B:226:THR:H	1.84	0.42
1:D:188:LYS:NZ	1:D:192:GLU:OE2	2.52	0.42
1:D:239:ASN:OD1	1:D:239:ASN:N	2.53	0.42
1:A:243:ASN:C	1:A:245:ILE:H	2.23	0.42
1:B:76:LEU:O	1:B:113:ALA:HA	2.20	0.42
1:B:170:ARG:NH1	1:B:299:TYR:O	2.52	0.42
1:C:243:ASN:C	1:C:245:ILE:H	2.23	0.42
1:C:402:MET:SD	1:C:437:ASN:HB2	2.59	0.42
1:D:186:ARG:HH22	1:D:302:SER:HB2	1.83	0.42
1:C:67:ASP:HB3	1:C:68:GLY:H	1.63	0.42
1:A:373:PRO:HB2	1:A:376:THR:HG22	2.01	0.42
1:B:190:ILE:HG12	1:B:196:PHE:CE2	2.55	0.42
1:C:360:LEU:HD12	1:C:360:LEU:H	1.85	0.42
1:D:153:VAL:HB	1:D:154:SER:H	1.63	0.42
1:A:190:ILE:HG12	1:A:196:PHE:CE2	2.55	0.42
1:A:213:ASN:ND2	1:A:223:ARG:O	2.28	0.42
1:A:91:HIS:HB2	1:B:165:ALA:HA	2.01	0.42
1:B:243:ASN:C	1:B:245:ILE:H	2.22	0.42
1:B:398:VAL:HG11	1:B:418:GLY:HA3	2.01	0.42
1:C:188:LYS:NZ	1:C:192:GLU:OE2	2.52	0.42
1:D:349:LEU:HG	1:D:351:ILE:HG12	2.02	0.42
1:C:190:ILE:HG12	1:C:196:PHE:CE2	2.55	0.42
1:C:229:PHE:CZ	1:C:236:LYS:HB2	2.54	0.42
1:D:243:ASN:C	1:D:245:ILE:H	2.23	0.42
1:D:373:PRO:HB2	1:D:376:THR:HG22	2.02	0.42
1:A:76:LEU:O	1:A:113:ALA:HA	2.20	0.41
1:C:373:PRO:HB2	1:C:376:THR:HG22	2.02	0.41
1:C:393:LYS:O	1:C:397:GLU:N	2.54	0.41
1:C:309:THR:N	1:C:427:ASP:OD2	2.53	0.41
1:D:402:MET:SD	1:D:437:ASN:HB2	2.60	0.41
1:C:16:VAL:N	1:C:286:VAL:O	2.41	0.41
1:D:190:ILE:HG12	1:D:196:PHE:CE2	2.55	0.41
1:B:229:PHE:HZ	1:B:236:LYS:HB2	1.84	0.41
1:B:271:GLU:O	1:B:274:GLN:HG2	2.20	0.41
1:A:131:TRP:O	1:A:135:LEU:HD12	2.19	0.41
1:A:16:VAL:N	1:A:286:VAL:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TYR:HB2	1:A:352:ALA:HB3	2.03	0.41
1:A:331:VAL:HG21	1:A:401:GLN:NE2	2.36	0.41
1:B:131:TRP:O	1:B:135:LEU:HD12	2.20	0.41
1:B:222:ALA:HB2	1:C:222:ALA:CB	2.51	0.41
1:C:75:LYS:HE2	1:C:76:LEU:O	2.21	0.41
1:A:330:GLN:O	1:A:373:PRO:HD2	2.21	0.41
1:A:393:LYS:O	1:A:397:GLU:N	2.54	0.41
1:D:63:THR:O	1:D:65:LEU:N	2.47	0.41
1:B:222:ALA:HB2	1:C:222:ALA:HB1	2.03	0.41
1:C:414:ILE:HA	1:C:415:PRO:HD3	1.91	0.41
1:A:229:PHE:CZ	1:A:236:LYS:HB2	2.55	0.41
1:A:271:GLU:O	1:A:274:GLN:HG2	2.21	0.41
1:A:164:ARG:HA	1:B:89:GLN:HA	2.03	0.41
1:D:279:SER:O	1:D:281:ASN:N	2.50	0.41
1:D:360:LEU:O	1:D:363:SER:OG	2.25	0.41
1:C:91:HIS:CE1	1:D:429:THR:HG1	2.32	0.41
1:A:414:ILE:HD12	1:A:414:ILE:HA	1.98	0.41
1:B:393:LYS:O	1:B:397:GLU:N	2.54	0.41
1:C:331:VAL:HG21	1:C:401:GLN:NE2	2.36	0.41
1:C:335:HIS:HA	1:C:380:LEU:HD11	2.03	0.41
1:D:225:VAL:HG12	1:D:226:THR:H	1.85	0.41
1:D:360:LEU:H	1:D:360:LEU:HD12	1.85	0.41
1:C:346:TYR:HB2	1:C:352:ALA:HB3	2.03	0.41
1:D:309:THR:N	1:D:427:ASP:OD2	2.54	0.41
1:A:403:LYS:HD3	1:A:403:LYS:HA	1.95	0.40
1:B:207:LYS:HE2	1:B:367:ALA:HA	2.01	0.40
1:C:215:ASN:HA	1:C:216:PRO:HD2	1.83	0.40
1:D:393:LYS:O	1:D:397:GLU:N	2.54	0.40
1:B:33:ILE:HD13	1:B:33:ILE:HA	1.95	0.40
1:B:310:THR:N	1:B:427:ASP:OD2	2.41	0.40
1:A:190:ILE:HD11	1:A:195:HIS:HB3	2.04	0.40
1:B:227:LEU:O	1:B:231:THR:HG23	2.21	0.40
1:B:349:LEU:HG	1:B:351:ILE:HG12	2.02	0.40
1:B:75:LYS:HE2	1:B:76:LEU:O	2.21	0.40
1:C:225:VAL:HG12	1:C:226:THR:H	1.85	0.40
1:A:335:HIS:HA	1:A:380:LEU:HD11	2.04	0.40
1:B:51:LEU:CD2	1:B:149:VAL:HG22	2.52	0.40
1:B:330:GLN:O	1:B:373:PRO:HD2	2.21	0.40
1:D:346:TYR:HB2	1:D:352:ALA:HB3	2.03	0.40
1:C:167:HIS:HD2	1:C:298:LEU:O	2.04	0.40
1:C:63:THR:O	1:C:65:LEU:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:HIS:HD2	1:D:298:LEU:O	2.05	0.40
1:D:331:VAL:HG21	1:D:401:GLN:NE2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:O	1:D:224:LYS:NZ[2_425]	2.17	0.03

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	412/454 (91%)	341 (83%)	53 (13%)	18 (4%)	2	10
1	B	410/454 (90%)	338 (82%)	54 (13%)	18 (4%)	2	10
1	C	415/454 (91%)	341 (82%)	56 (14%)	18 (4%)	2	10
1	D	410/454 (90%)	338 (82%)	54 (13%)	18 (4%)	2	10
All	All	1647/1816 (91%)	1358 (82%)	217 (13%)	72 (4%)	2	10

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ALA
1	A	108	PHE
1	A	387	VAL
1	B	71	ALA
1	B	105	SER
1	B	108	PHE
1	B	387	VAL
1	C	108	PHE

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Mol	Chain	Res	Type
1	C	387	VAL
1	D	108	PHE
1	D	387	VAL
1	A	72	LEU
1	A	244	GLU
1	A	408	GLU
1	B	72	LEU
1	B	244	GLU
1	B	408	GLU
1	C	71	ALA
1	C	72	LEU
1	C	244	GLU
1	C	408	GLU
1	D	71	ALA
1	D	72	LEU
1	D	244	GLU
1	D	408	GLU
1	A	83	GLY
1	A	238	PRO
1	B	83	GLY
1	B	238	PRO
1	C	83	GLY
1	C	238	PRO
1	D	83	GLY
1	D	238	PRO
1	A	173	GLN
1	A	232	GLN
1	A	350	GLY
1	A	413	ASN
1	B	173	GLN
1	B	232	GLN
1	B	350	GLY
1	B	413	ASN
1	C	173	GLN
1	C	232	GLN
1	C	413	ASN
1	D	173	GLN
1	D	232	GLN
1	D	413	ASN
1	A	240	PHE
1	A	318	ALA
1	B	240	PHE

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Mol	Chain	Res	Type
1	C	318	ALA
1	D	240	PHE
1	D	318	ALA
1	C	240	PHE
1	C	350	GLY
1	A	64	GLY
1	D	350	GLY
1	A	153	VAL
1	A	258	VAL
1	B	64	GLY
1	B	153	VAL
1	C	153	VAL
1	C	258	VAL
1	D	153	VAL
1	D	258	VAL
1	B	258	VAL
1	C	64	GLY
1	D	64	GLY
1	C	415	PRO
1	D	415	PRO
1	A	415	PRO
1	B	415	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	314/349 (90%)	293 (93%)	21 (7%)	16	43
1	B	315/349 (90%)	290 (92%)	25 (8%)	12	34
1	C	316/349 (90%)	297 (94%)	19 (6%)	19	49
1	D	314/349 (90%)	292 (93%)	22 (7%)	15	41
All	All	1259/1396 (90%)	1172 (93%)	87 (7%)	15	41

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	65	LEU
1	A	66	HIS
1	A	82	LEU
1	A	153	VAL
1	A	172	ARG
1	A	195	HIS
1	A	209	TYR
1	A	225	VAL
1	A	227	LEU
1	A	240	PHE
1	A	253	THR
1	A	254	ASP
1	A	270	GLU
1	A	276	LEU
1	A	278	LEU
1	A	291	LEU
1	A	329	LEU
1	A	330	GLN
1	A	346	TYR
1	A	405	GLN
1	B	14	VAL
1	B	20	HIS
1	B	51	LEU
1	B	66	HIS
1	B	82	LEU
1	B	104	ASN
1	B	153	VAL
1	B	164	ARG
1	B	172	ARG
1	B	195	HIS
1	B	209	TYR
1	B	225	VAL
1	B	227	LEU
1	B	240	PHE
1	B	253	THR
1	B	254	ASP
1	B	270	GLU
1	B	276	LEU
1	B	291	LEU
1	B	307	ARG
1	B	319	LEU
1	B	329	LEU

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Mol	Chain	Res	Type
1	B	330	GLN
1	B	346	TYR
1	B	405	GLN
1	C	20	HIS
1	C	66	HIS
1	C	82	LEU
1	C	85	LEU
1	C	153	VAL
1	C	157	VAL
1	C	172	ARG
1	C	195	HIS
1	C	209	TYR
1	C	225	VAL
1	C	227	LEU
1	C	240	PHE
1	C	253	THR
1	C	254	ASP
1	C	270	GLU
1	C	291	LEU
1	C	329	LEU
1	C	346	TYR
1	C	405	GLN
1	D	20	HIS
1	D	66	HIS
1	D	82	LEU
1	D	135	LEU
1	D	153	VAL
1	D	157	VAL
1	D	172	ARG
1	D	195	HIS
1	D	209	TYR
1	D	225	VAL
1	D	227	LEU
1	D	240	PHE
1	D	253	THR
1	D	254	ASP
1	D	270	GLU
1	D	276	LEU
1	D	291	LEU
1	D	329	LEU
1	D	330	GLN
1	D	343	LEU

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Mol	Chain	Res	Type
1	D	346	TYR
1	D	405	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	221	HIS
1	A	232	GLN
1	A	437	ASN
1	B	191	GLN
1	B	221	HIS
1	B	232	GLN
1	B	437	ASN
1	C	191	GLN
1	C	221	HIS
1	C	232	GLN
1	C	437	ASN
1	D	191	GLN
1	D	221	HIS
1	D	232	GLN
1	D	437	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 carbohydrates 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	418/454 (92%)	0.15	18 (4%)	35	31	28, 68, 94, 122	0
1	B	416/454 (91%)	0.23	16 (3%)	40	36	28, 67, 95, 123	0
1	C	419/454 (92%)	0.15	10 (2%)	59	56	29, 67, 95, 121	0
1	D	416/454 (91%)	0.23	22 (5%)	26	22	30, 66, 95, 121	0
All	All	1669/1816 (91%)	0.19	66 (3%)	38	33	28, 67, 95, 123	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	GLY	6.1
1	A	194	GLY	5.0
1	A	174	LEU	4.8
1	C	201	ALA	4.5
1	D	194	GLY	4.4
1	B	194	GLY	4.1
1	B	263	ALA	4.0
1	D	173	GLN	3.9
1	C	346	TYR	3.8
1	A	237	ASN	3.8
1	D	404	GLY	3.8
1	A	242	GLY	3.5
1	D	329	LEU	3.5
1	B	241	LEU	3.5
1	A	14	VAL	3.4
1	B	44	GLU	3.4
1	B	240	PHE	3.3
1	B	12	LYS	3.3
1	D	242	GLY	3.3
1	D	350	GLY	3.2
1	D	233	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	146	GLY	3.1
1	B	43	LYS	3.1
1	B	195	HIS	3.0
1	B	242	GLY	3.0
1	C	350	GLY	2.9
1	D	147	VAL	2.8
1	A	238	PRO	2.8
1	A	301	ASP	2.8
1	D	352	ALA	2.8
1	A	44	GLU	2.8
1	C	173	GLN	2.8
1	C	96	ALA	2.7
1	D	336	ASP	2.7
1	A	233	ALA	2.7
1	D	292	ALA	2.7
1	D	295	ALA	2.6
1	A	360	LEU	2.6
1	B	134	LEU	2.6
1	D	238	PRO	2.5
1	D	433	MET	2.5
1	A	424	GLY	2.4
1	B	163	ALA	2.4
1	C	231	THR	2.3
1	A	56	ILE	2.3
1	B	333	GLU	2.3
1	B	334	VAL	2.3
1	D	276	LEU	2.3
1	D	211	SER	2.3
1	C	238	PRO	2.3
1	D	349	LEU	2.2
1	D	67	ASP	2.2
1	D	289	LYS	2.2
1	C	242	GLY	2.2
1	C	342	GLU	2.2
1	B	239	ASN	2.1
1	B	268	ALA	2.1
1	D	344	LEU	2.1
1	A	84	GLU	2.1
1	D	405	GLN	2.1
1	A	231	THR	2.1
1	D	226	THR	2.1
1	A	351	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	167	HIS	2.0
1	A	43	LYS	2.0
1	A	349	LEU	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.