Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2021 – 05:36 PM EST

PDB ID	:	3I3V
Title	:	Crystal Structure of probable secreted solute-binding lipoprotein from Streptomyces coelicolor
Authors	:	Damodharan, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-07-01
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

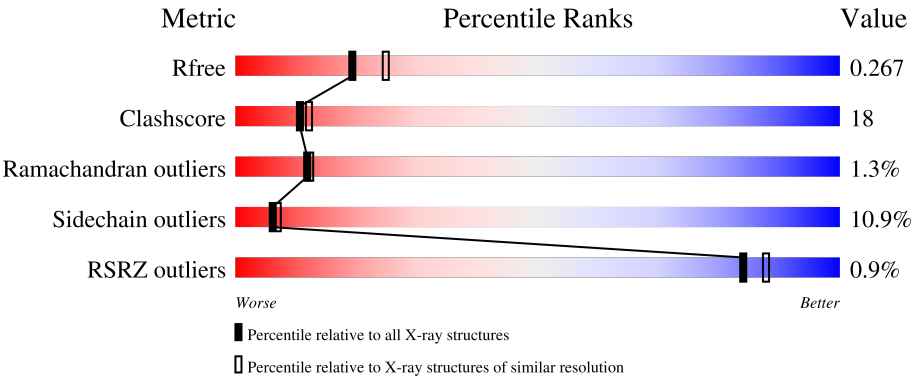
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	405	70% 23%
1	B	405	% 64% 27% 5%
1	C	405	% 67% 24% 5%
1	D	405	% 63% 28% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12244 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 Probable secreted solute-binding lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	Se	0	0	0
			2980	1883	528	564	5			
1	B	390	Total	C	N	O	Se	0	0	0
			2964	1875	527	557	5			
1	C	394	Total	C	N	O	Se	0	0	0
			2993	1890	528	570	5			
1	D	391	Total	C	N	O	Se	0	0	0
			2978	1882	528	563	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MSE	-	insertion	UNP Q9RL34
A	34	SER	-	insertion	UNP Q9RL34
A	35	LEU	-	insertion	UNP Q9RL34
A	430	GLU	-	insertion	UNP Q9RL34
A	431	GLY	-	insertion	UNP Q9RL34
A	432	HIS	-	insertion	UNP Q9RL34
A	433	HIS	-	insertion	UNP Q9RL34
A	434	HIS	-	insertion	UNP Q9RL34
A	435	HIS	-	insertion	UNP Q9RL34
A	436	HIS	-	insertion	UNP Q9RL34
A	437	HIS	-	insertion	UNP Q9RL34
B	33	MSE	-	insertion	UNP Q9RL34
B	34	SER	-	insertion	UNP Q9RL34
B	35	LEU	-	insertion	UNP Q9RL34
B	430	GLU	-	insertion	UNP Q9RL34
B	431	GLY	-	insertion	UNP Q9RL34
B	432	HIS	-	insertion	UNP Q9RL34
B	433	HIS	-	insertion	UNP Q9RL34
B	434	HIS	-	insertion	UNP Q9RL34
B	435	HIS	-	insertion	UNP Q9RL34
B	436	HIS	-	insertion	UNP Q9RL34

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Chain	Residue	Modelled	Actual	Comment	Reference
B	437	HIS	-	insertion	UNP Q9RL34
C	33	MSE	-	insertion	UNP Q9RL34
C	34	SER	-	insertion	UNP Q9RL34
C	35	LEU	-	insertion	UNP Q9RL34
C	430	GLU	-	insertion	UNP Q9RL34
C	431	GLY	-	insertion	UNP Q9RL34
C	432	HIS	-	insertion	UNP Q9RL34
C	433	HIS	-	insertion	UNP Q9RL34
C	434	HIS	-	insertion	UNP Q9RL34
C	435	HIS	-	insertion	UNP Q9RL34
C	436	HIS	-	insertion	UNP Q9RL34
C	437	HIS	-	insertion	UNP Q9RL34
D	33	MSE	-	insertion	UNP Q9RL34
D	34	SER	-	insertion	UNP Q9RL34
D	35	LEU	-	insertion	UNP Q9RL34
D	430	GLU	-	insertion	UNP Q9RL34
D	431	GLY	-	insertion	UNP Q9RL34
D	432	HIS	-	insertion	UNP Q9RL34
D	433	HIS	-	insertion	UNP Q9RL34
D	434	HIS	-	insertion	UNP Q9RL34
D	435	HIS	-	insertion	UNP Q9RL34
D	436	HIS	-	insertion	UNP Q9RL34
D	437	HIS	-	insertion	UNP Q9RL34

- Molecule 2 is water.

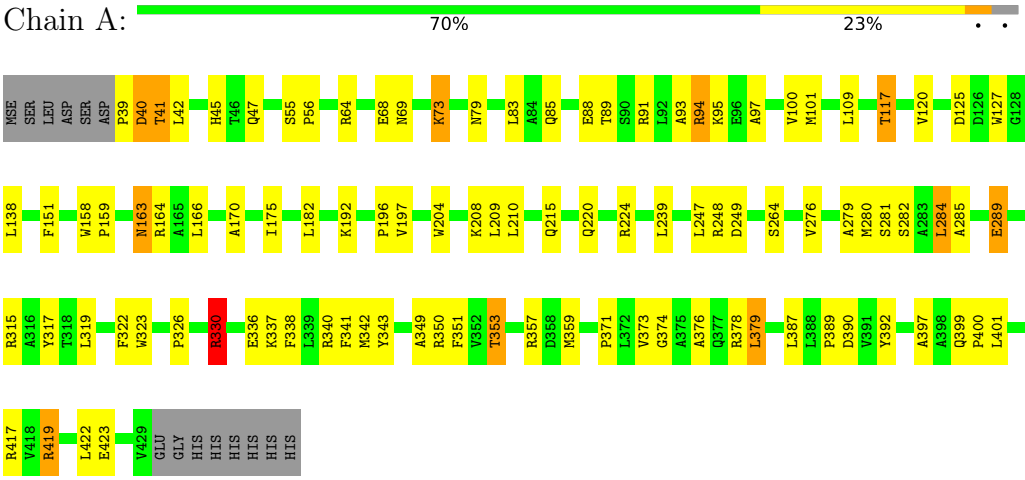
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	99	Total O 99 99	0	0
2	B	76	Total O 76 76	0	0
2	C	85	Total O 85 85	0	0
2	D	69	Total O 69 69	0	0

3 Residue-property plots (i)

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

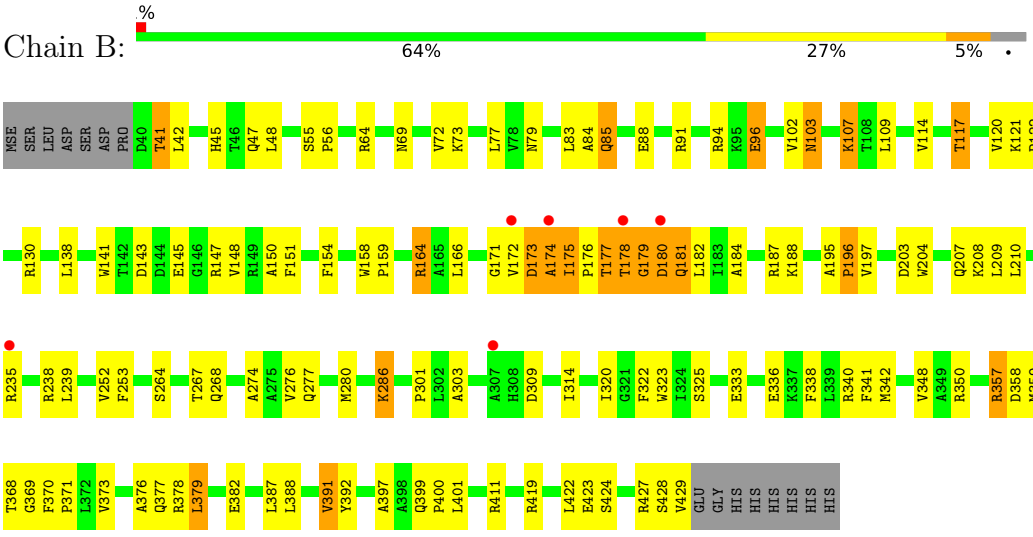
• Molecule 1: Probable secreted solute-binding lipoprotein

Chain A:



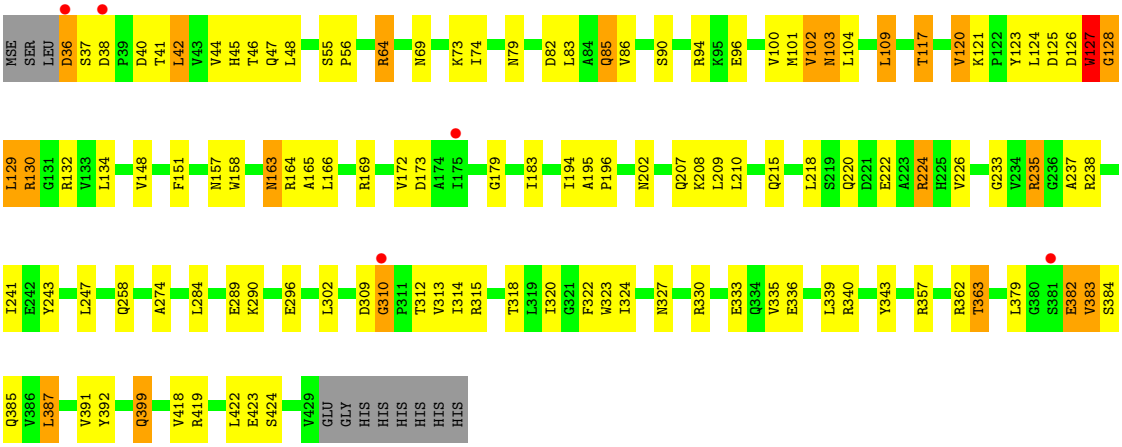
• Molecule 1: Probable secreted solute-binding lipoprotein

Chain B:



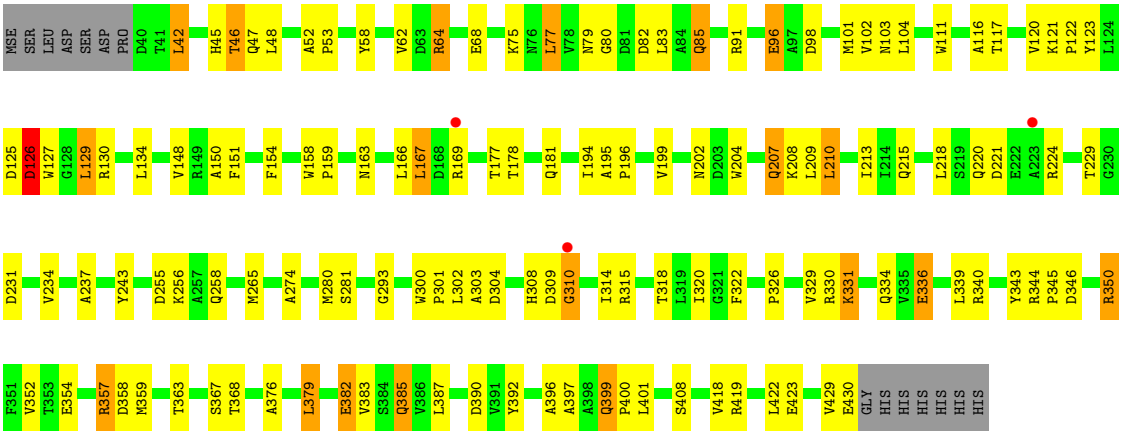
• Molecule 1: Probable secreted solute-binding lipoprotein

Chain C:



• Molecule 1: Probable secreted solute-binding lipoprotein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.31Å 91.31Å 370.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.70 – 2.30 45.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.0 (36.70-2.30) 98.1 (45.31-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.259 0.226 , 0.267	Depositor DCC
R_{free} test set	3997 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12244	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 40.83 % 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 2.5812e-04. 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, 0.333 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	0.37	0/3040	0.67	0/4138
1	B	0.34	0/3023	0.67	1/4116 (0.0%)
1	C	0.34	0/3053	0.65	1/4158 (0.0%)
1	D	0.36	0/3037	0.67	0/4134
All	All	0.35	0/12153	0.66	2/16546 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	388	LEU	N-CA-C	-5.69	95.64	111.00
1	C	37	SER	N-CA-C	5.54	125.95	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	ARG	Sidechain

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	2980	0	2949	82	0
1	B	2964	0	2938	118	0
1	C	2993	0	2948	121	0
1	D	2978	0	2951	119	0
2	A	99	0	0	5	0
2	B	76	0	0	3	0
2	C	85	0	0	7	0
2	D	69	0	0	4	0
All	All	12244	0	11786	436	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 (436) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ARG:HB3	1:D:359:MSE:HE3	1.20	1.14
1:D:125:ASP:O	1:D:126:ASP:HB3	1.51	1.09
1:D:399:GLN:HG2	1:D:400:PRO:HD3	1.34	1.02
1:B:357:ARG:HB3	1:B:359:MSE:HE3	1.42	1.01
1:A:357:ARG:HB2	1:A:359:MSE:CE	1.96	0.96
1:B:286:LYS:O	1:B:286:LYS:HD2	1.66	0.95
1:C:127:TRP:HB3	1:C:340:ARG:HH12	1.30	0.94
1:C:103:ASN:H	1:C:103:ASN:HD22	1.16	0.94
1:D:357:ARG:HB3	1:D:359:MSE:CE	1.99	0.93
1:B:85:GLN:H	1:B:85:GLN:HE21	0.97	0.93
1:D:358:ASP:O	1:D:359:MSE:HE2	1.70	0.91
1:D:45:HIS:HE1	1:D:79:ASN:HD22	1.16	0.91
1:B:91:ARG:HA	1:B:96:GLU:HG2	1.54	0.90
1:B:103:ASN:HD22	1:B:103:ASN:H	1.20	0.89
1:B:180:ASP:O	1:B:184:ALA:HB3	1.74	0.88
1:C:46:THR:HG22	1:C:48:LEU:H	1.36	0.87
1:B:178:THR:HG23	1:B:179:GLY:H	1.39	0.86
1:D:315:ARG:HB3	1:D:315:ARG:HH11	1.39	0.86
1:C:46:THR:HG23	1:C:101:MSE:HB2	1.56	0.85
1:B:358:ASP:O	1:B:359:MSE:HE2	1.76	0.85
1:C:85:GLN:HE21	1:C:85:GLN:H	1.22	0.85
1:B:85:GLN:N	1:B:85:GLN:HE21	1.75	0.84
1:C:117:THR:HG21	1:C:323:TRP:HE3	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLU:O	1:B:340:ARG:HG3	1.78	0.84
1:A:357:ARG:HB2	1:A:359:MSE:HE1	1.58	0.83
1:C:158:TRP:HB3	1:C:314:ILE:HB	1.61	0.82
1:C:127:TRP:HZ3	1:C:336:GLU:CB	1.92	0.82
1:D:46:THR:HG22	1:D:48:LEU:H	1.43	0.82
1:C:127:TRP:HB3	1:C:340:ARG:NH1	1.96	0.80
1:D:46:THR:HG23	1:D:101:MSE:HB2	1.61	0.80
1:B:215:GLN:HE22	1:B:387:LEU:H	1.31	0.79
1:C:85:GLN:NE2	1:C:85:GLN:H	1.79	0.79
1:A:357:ARG:HB2	1:A:359:MSE:HE2	1.62	0.79
1:A:248:ARG:HH12	1:A:412:GLY:H	1.29	0.79
1:C:302:LEU:HD11	1:C:310:GLY:HA3	1.66	0.77
1:D:326:PRO:O	1:D:329:VAL:HG22	1.85	0.77
1:D:47:GLN:HA	1:D:79:ASN:O	1.85	0.76
1:C:336:GLU:O	1:C:340:ARG:HG3	1.84	0.76
1:B:84:ALA:O	1:B:88:GLU:HG3	1.86	0.76
1:B:117:THR:HG21	1:B:323:TRP:HE3	1.50	0.76
1:A:117:THR:HG21	1:A:323:TRP:CE3	2.21	0.75
1:A:419:ARG:O	1:A:423:GLU:HG3	1.85	0.75
1:A:330:ARG:O	1:A:330:ARG:NH2	2.19	0.75
1:C:215:GLN:HE22	1:C:387:LEU:H	1.35	0.75
1:B:158:TRP:HB3	1:B:314:ILE:HB	1.67	0.75
1:A:350:ARG:HD3	2:A:446:HOH:O	1.87	0.75
1:A:117:THR:HG21	1:A:323:TRP:HE3	1.50	0.74
1:C:126:ASP:O	1:C:127:TRP:HD1	1.70	0.74
1:C:330:ARG:HD3	2:C:470:HOH:O	1.88	0.74
1:A:158:TRP:HB3	1:A:314:ILE:HB	1.70	0.73
1:B:172:VAL:HG12	1:B:173:ASP:H	1.51	0.73
1:B:197:VAL:HG22	1:B:252:VAL:O	1.89	0.73
1:B:176:PRO:HD2	1:B:181:GLN:OE1	1.87	0.73
1:C:126:ASP:C	1:C:127:TRP:CD1	2.62	0.73
1:C:126:ASP:C	1:C:127:TRP:HD1	1.90	0.73
1:C:166:LEU:HD12	1:C:194:ILE:HD13	1.71	0.73
1:D:111:TRP:HB3	1:D:117:THR:HG23	1.70	0.73
1:D:77:LEU:HD11	2:D:489:HOH:O	1.88	0.73
1:D:169:ARG:HG3	1:D:169:ARG:HH11	1.52	0.73
1:A:215:GLN:HE22	1:A:387:LEU:H	1.36	0.72
1:B:338:PHE:CE1	1:B:342:MSE:HE3	2.24	0.72
1:C:117:THR:HG21	1:C:323:TRP:CE3	2.23	0.72
1:C:163:ASN:C	1:C:163:ASN:HD22	1.92	0.71
1:D:209:LEU:O	1:D:213:ILE:HG12	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASN:HD22	1:A:163:ASN:C	1.95	0.71
1:B:348:VAL:HG11	1:B:363:THR:HG21	1.71	0.71
1:A:338:PHE:CE1	1:A:342:MSE:HE3	2.26	0.70
1:A:117:THR:CG2	2:A:499:HOH:O	2.39	0.69
1:A:351:PHE:HB3	1:A:359:MSE:HE1	1.73	0.69
1:A:351:PHE:HB3	1:A:359:MSE:CE	2.23	0.69
1:B:428:SER:O	1:B:429:VAL:HG23	1.93	0.69
1:C:123:TYR:O	1:C:127:TRP:NE1	2.26	0.69
1:B:103:ASN:HD22	1:B:103:ASN:N	1.90	0.69
1:A:248:ARG:HH11	1:A:411:ARG:HA	1.57	0.68
1:B:179:GLY:O	1:B:181:GLN:N	2.27	0.68
1:B:196:PRO:HB2	1:B:252:VAL:O	1.94	0.68
1:D:220:GLN:O	1:D:224:ARG:HG3	1.94	0.67
1:C:123:TYR:O	1:C:127:TRP:CD1	2.48	0.67
1:C:235:ARG:H	1:C:235:ARG:NE	1.93	0.67
1:C:290:LYS:NZ	1:C:290:LYS:HB3	2.09	0.67
1:A:387:LEU:HD11	1:A:392:TYR:CE1	2.31	0.66
1:C:233:GLY:HA2	1:C:419:ARG:HE	1.61	0.66
1:B:85:GLN:H	1:B:85:GLN:NE2	1.81	0.66
1:A:248:ARG:NH1	1:A:249:ASP:OD2	2.29	0.66
1:A:248:ARG:NH1	1:A:412:GLY:H	1.94	0.66
1:B:180:ASP:O	1:B:184:ALA:CB	2.43	0.66
1:C:100:VAL:HG12	1:C:102:VAL:HG22	1.78	0.66
1:B:197:VAL:HG12	1:B:276:VAL:HB	1.78	0.66
1:D:243:TYR:CE1	1:D:303:ALA:HB2	2.31	0.65
1:D:399:GLN:H	1:D:399:GLN:CD	1.98	0.65
1:C:357:ARG:HH11	1:C:357:ARG:HG2	1.61	0.64
1:C:123:TYR:HA	1:C:127:TRP:HE1	1.63	0.64
1:B:172:VAL:HG12	1:B:173:ASP:N	2.13	0.64
1:B:348:VAL:CG1	1:B:363:THR:HG21	2.27	0.64
1:D:204:TRP:CH2	1:D:280:MSE:HE2	2.32	0.64
1:B:235:ARG:HH11	1:B:238:ARG:HH22	1.46	0.64
1:A:88:GLU:OE1	1:B:107:LYS:HE2	1.97	0.63
1:D:45:HIS:HE1	1:D:79:ASN:ND2	1.93	0.63
1:D:98:ASP:CG	1:D:331:LYS:HE2	2.19	0.63
1:B:175:ILE:HD11	1:B:301:PRO:HG2	1.81	0.63
1:A:91:ARG:HH22	1:A:326:PRO:HG2	1.63	0.62
1:B:178:THR:HG23	1:B:179:GLY:N	2.13	0.62
1:C:83:LEU:C	1:C:83:LEU:HD23	2.20	0.61
1:C:127:TRP:HZ3	1:C:336:GLU:CG	2.13	0.61
1:D:204:TRP:HH2	1:D:280:MSE:HE2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:SER:O	1:B:427:ARG:HG3	2.01	0.61
1:A:376:ALA:HA	1:A:379:LEU:HD22	1.82	0.61
1:B:177:THR:HG22	1:B:181:GLN:HB2	1.83	0.61
1:D:397:ALA:O	1:D:401:LEU:HB2	2.01	0.61
1:A:170:ALA:HA	1:A:192:LYS:HG3	1.82	0.61
1:B:357:ARG:CB	1:B:359:MSE:HE3	2.24	0.60
1:C:237:ALA:O	1:C:241:ILE:HG13	2.01	0.60
1:C:302:LEU:HD11	1:C:310:GLY:CA	2.30	0.60
1:D:158:TRP:HB3	1:D:314:ILE:HB	1.82	0.60
1:D:45:HIS:CE1	1:D:79:ASN:HD22	2.08	0.60
1:D:220:GLN:HB3	1:D:224:ARG:HH21	1.67	0.60
1:A:397:ALA:O	1:A:401:LEU:HB2	2.02	0.60
1:C:127:TRP:HZ3	1:C:336:GLU:HB2	1.66	0.60
1:C:42:LEU:HB3	1:C:74:ILE:HD13	1.82	0.60
1:C:103:ASN:HD22	1:C:103:ASN:N	1.93	0.60
1:B:397:ALA:O	1:B:401:LEU:HB2	2.02	0.59
1:C:151:PHE:HB2	1:C:322:PHE:HB2	1.84	0.59
1:D:123:TYR:O	1:D:127:TRP:HB2	2.02	0.59
1:C:315:ARG:HD3	1:C:385:GLN:HG2	1.85	0.59
1:A:341:PHE:CD2	1:A:342:MSE:HE2	2.37	0.59
1:C:46:THR:HG23	1:C:101:MSE:CB	2.28	0.59
1:B:164:ARG:HH11	1:B:164:ARG:HG3	1.68	0.59
1:D:309:ASP:O	1:D:310:GLY:O	2.21	0.59
1:B:357:ARG:HB3	1:B:359:MSE:CE	2.26	0.59
1:D:210:LEU:HD22	1:D:210:LEU:O	2.03	0.59
1:C:47:GLN:HA	1:C:79:ASN:O	2.03	0.58
1:A:175:ILE:HD11	1:A:296:GLU:HG3	1.86	0.58
1:A:89:THR:HG23	1:B:114:VAL:HG11	1.84	0.58
1:B:341:PHE:CD2	1:B:342:MSE:HE2	2.38	0.58
1:B:177:THR:HB	1:B:181:GLN:CD	2.25	0.57
1:D:102:VAL:HG22	1:D:103:ASN:N	2.19	0.57
1:D:396:ALA:HB3	1:D:429:VAL:HG22	1.86	0.57
1:D:382:GLU:N	1:D:382:GLU:OE2	2.29	0.57
1:D:387:LEU:HD11	1:D:392:TYR:HE1	1.69	0.57
1:C:127:TRP:CZ3	1:C:336:GLU:CG	2.87	0.57
1:C:123:TYR:CA	1:C:127:TRP:HE1	2.17	0.57
1:B:197:VAL:HG23	1:B:253:PHE:HD1	1.70	0.57
1:D:429:VAL:HG12	1:D:430:GLU:H	1.70	0.57
1:D:127:TRP:CE2	1:D:336:GLU:OE2	2.58	0.56
1:B:428:SER:O	1:B:429:VAL:CB	2.53	0.56
1:C:127:TRP:CB	1:C:340:ARG:NH1	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:O	1:A:40:ASP:HB2	2.05	0.56
1:B:197:VAL:CG2	1:B:253:PHE:CD1	2.88	0.56
1:C:126:ASP:O	1:C:128:GLY:N	2.39	0.56
1:A:248:ARG:NH1	1:A:411:ARG:HA	2.20	0.56
1:B:363:THR:HG22	2:B:505:HOH:O	2.05	0.56
1:C:127:TRP:CZ3	1:C:336:GLU:HA	2.40	0.56
1:B:127:TRP:CZ2	1:B:336:GLU:HB2	2.41	0.56
1:C:357:ARG:NH1	1:C:357:ARG:HG2	2.20	0.56
1:A:399:GLN:HB2	1:A:400:PRO:HD3	1.89	0.55
1:C:419:ARG:O	1:C:423:GLU:HG3	2.06	0.55
1:C:82:ASP:O	1:C:86:VAL:HG23	2.07	0.55
1:A:336:GLU:OE1	1:A:340:ARG:NH1	2.39	0.55
1:C:103:ASN:H	1:C:103:ASN:ND2	1.95	0.55
1:B:103:ASN:H	1:B:103:ASN:ND2	1.98	0.55
1:B:117:THR:HG21	1:B:323:TRP:CE3	2.38	0.55
1:A:387:LEU:HD11	1:A:392:TYR:HE1	1.67	0.54
1:D:213:ILE:HD12	1:D:300:TRP:NE1	2.22	0.54
1:B:151:PHE:HB2	1:B:322:PHE:HB2	1.88	0.54
1:D:220:GLN:HE22	1:D:308:HIS:HE1	1.55	0.54
1:A:125:ASP:OD1	1:A:130:ARG:NH1	2.39	0.54
1:C:215:GLN:NE2	1:C:387:LEU:H	2.02	0.54
1:A:349:ALA:O	1:A:353:THR:HB	2.08	0.54
1:B:120:VAL:HG22	1:B:148:VAL:O	2.07	0.54
1:B:428:SER:O	1:B:429:VAL:CG2	2.55	0.54
1:B:45:HIS:NE2	1:B:79:ASN:ND2	2.53	0.54
1:B:223:ALA:HB3	1:B:387:LEU:CD1	2.39	0.53
1:B:277:GLN:O	1:B:277:GLN:HG3	2.08	0.53
1:C:117:THR:HG22	2:C:513:HOH:O	2.09	0.53
1:C:130:ARG:HG2	1:C:130:ARG:HH11	1.73	0.53
1:A:117:THR:HG23	2:A:499:HOH:O	2.04	0.53
1:A:341:PHE:HD2	1:A:342:MSE:HE2	1.73	0.53
1:C:117:THR:HG23	2:C:442:HOH:O	2.09	0.53
1:D:126:ASP:C	1:D:126:ASP:OD1	2.47	0.53
1:D:204:TRP:HA	1:D:207:GLN:HB3	1.89	0.52
1:D:163:ASN:CG	1:D:166:LEU:HD23	2.29	0.52
1:A:336:GLU:O	1:A:340:ARG:HG2	2.10	0.52
1:D:127:TRP:NE1	1:D:336:GLU:OE2	2.43	0.52
1:D:46:THR:HG23	1:D:101:MSE:CB	2.35	0.52
1:D:64:ARG:NE	1:D:68:GLU:OE2	2.42	0.52
1:C:165:ALA:O	1:C:169:ARG:HG3	2.10	0.52
1:C:419:ARG:HG2	1:C:419:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:VAL:O	1:D:367:SER:HB3	2.10	0.52
1:B:48:LEU:HD21	1:B:320:ILE:HD12	1.91	0.52
1:B:178:THR:CG2	1:B:179:GLY:H	2.19	0.52
1:D:127:TRP:O	1:D:340:ARG:NH2	2.43	0.52
1:C:129:LEU:O	1:C:132:ARG:HB2	2.10	0.51
1:A:282:SER:HG	1:A:357:ARG:HH22	1.57	0.51
1:C:222:GLU:O	1:C:226:VAL:HG23	2.11	0.51
1:C:224:ARG:HD3	1:C:387:LEU:CD1	2.39	0.51
1:C:44:VAL:HG12	1:C:46:THR:OG1	2.11	0.51
1:B:143:ASP:HB3	1:B:145:GLU:H	1.75	0.51
1:C:333:GLU:O	1:C:336:GLU:HB3	2.10	0.51
1:A:45:HIS:HB2	1:A:97:ALA:CB	2.41	0.51
1:B:121:LYS:CE	1:B:130:ARG:HH22	2.23	0.51
1:C:104:LEU:HD11	1:C:109:LEU:HD13	1.93	0.51
1:C:132:ARG:HD2	2:C:508:HOH:O	2.09	0.51
1:D:350:ARG:O	1:D:354:GLU:HB3	2.11	0.51
1:A:83:LEU:HD23	1:A:83:LEU:C	2.31	0.51
1:B:341:PHE:HD2	1:B:342:MSE:HE2	1.75	0.51
1:A:289:GLU:N	1:A:289:GLU:CD	2.64	0.51
1:B:204:TRP:HH2	1:B:280:MSE:HE2	1.75	0.51
1:C:121:LYS:HB2	1:C:148:VAL:HG23	1.92	0.51
1:C:224:ARG:HD2	1:C:392:TYR:CZ	2.46	0.51
1:D:125:ASP:O	1:D:126:ASP:CB	2.37	0.51
1:C:313:VAL:HG13	1:C:383:VAL:HG22	1.93	0.50
1:D:46:THR:CG2	1:D:48:LEU:H	2.19	0.50
1:C:104:LEU:HB3	1:C:318:THR:HB	1.92	0.50
1:B:264:SER:O	1:B:268:GLN:HG3	2.12	0.50
1:A:41:THR:HB	1:A:73:LYS:HB2	1.92	0.50
1:B:362:ARG:O	1:B:363:THR:HG22	2.11	0.50
1:B:223:ALA:HB3	1:B:387:LEU:HD12	1.94	0.50
1:C:127:TRP:HZ3	1:C:336:GLU:CA	2.25	0.50
1:B:235:ARG:HD3	1:B:238:ARG:HH12	1.77	0.50
1:D:399:GLN:CG	1:D:400:PRO:HD3	2.24	0.50
1:D:150:ALA:HB1	1:D:322:PHE:O	2.12	0.49
1:D:419:ARG:O	1:D:423:GLU:HG3	2.11	0.49
1:A:91:ARG:HH21	1:A:91:ARG:HG3	1.77	0.49
1:C:290:LYS:HB3	1:C:290:LYS:HZ2	1.77	0.49
1:D:315:ARG:CB	1:D:315:ARG:HH11	2.18	0.49
1:D:154:PHE:CD1	1:D:359:MSE:HE1	2.47	0.49
1:D:83:LEU:HD23	1:D:83:LEU:C	2.33	0.49
1:C:73:LYS:HB2	1:C:73:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ASP:OD1	1:D:130:ARG:HD2	2.13	0.49
1:D:129:LEU:HG	1:D:343:TYR:CD1	2.48	0.49
1:D:91:ARG:HA	1:D:96:GLU:HG2	1.94	0.49
1:C:309:ASP:O	1:C:310:GLY:O	2.31	0.49
1:B:69:ASN:HB3	1:B:72:VAL:HG23	1.95	0.49
1:C:127:TRP:CZ3	1:C:336:GLU:HB2	2.47	0.49
1:B:96:GLU:OE1	1:B:325:SER:HB2	2.13	0.48
1:D:302:LEU:HD11	1:D:310:GLY:HA3	1.94	0.48
1:C:47:GLN:HG3	1:C:83:LEU:HD13	1.95	0.48
1:B:121:LYS:HE2	1:B:130:ARG:HH22	1.78	0.48
1:C:333:GLU:CD	1:C:333:GLU:H	2.17	0.48
1:D:169:ARG:HD2	1:D:194:ILE:HD11	1.96	0.48
1:C:163:ASN:CG	1:C:166:LEU:HD23	2.34	0.48
1:D:315:ARG:NH1	1:D:315:ARG:HB3	2.19	0.48
1:D:429:VAL:HG12	1:D:430:GLU:N	2.29	0.48
1:A:39:PRO:O	1:A:40:ASP:CB	2.62	0.48
1:C:163:ASN:OD1	1:C:166:LEU:HD23	2.14	0.48
1:A:93:ALA:HB1	1:A:95:LYS:HE2	1.96	0.48
1:B:175:ILE:CD1	1:B:182:LEU:HA	2.44	0.48
1:B:175:ILE:O	1:B:301:PRO:HG3	2.14	0.48
1:D:46:THR:HG22	1:D:47:GLN:N	2.29	0.48
1:C:166:LEU:CD1	1:C:194:ILE:HD13	2.43	0.47
1:C:179:GLY:O	1:C:183:ILE:HG13	2.13	0.47
1:C:127:TRP:CZ3	1:C:336:GLU:HG3	2.48	0.47
1:D:82:ASP:HA	1:D:85:GLN:HE22	1.79	0.47
1:B:197:VAL:HG23	1:B:253:PHE:CD1	2.49	0.47
1:C:419:ARG:NH1	1:C:419:ARG:HG2	2.29	0.47
1:D:220:GLN:NE2	1:D:308:HIS:HE1	2.12	0.47
1:B:215:GLN:HE22	1:B:387:LEU:N	2.07	0.47
1:B:428:SER:O	1:B:429:VAL:HB	2.13	0.47
1:A:120:VAL:CG1	1:A:120:VAL:O	2.62	0.47
1:A:158:TRP:CE3	1:A:280:MSE:HG2	2.49	0.47
1:C:127:TRP:CD1	1:C:127:TRP:N	2.81	0.47
1:A:279:ALA:HB3	1:A:284:LEU:HD13	1.96	0.47
1:B:379:LEU:HA	1:B:379:LEU:HD12	1.74	0.47
1:D:408:SER:OG	1:D:418:VAL:HG13	2.15	0.47
1:D:98:ASP:OD2	1:D:331:LYS:HE2	2.14	0.47
1:A:68:GLU:HA	1:D:346:ASP:HB2	1.97	0.47
1:B:103:ASN:ND2	1:B:103:ASN:N	2.61	0.47
1:B:83:LEU:C	1:B:83:LEU:HD23	2.34	0.47
1:D:195:ALA:O	1:D:274:ALA:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:THR:HG23	1:D:101:MSE:SE	2.65	0.47
1:D:111:TRP:CE3	1:D:117:THR:HG21	2.50	0.47
1:D:220:GLN:HE22	1:D:308:HIS:CE1	2.32	0.47
1:B:179:GLY:O	1:B:180:ASP:C	2.53	0.47
1:D:120:VAL:HG22	1:D:148:VAL:O	2.14	0.47
1:B:399:GLN:HB3	1:B:400:PRO:HD3	1.97	0.47
1:C:382:GLU:H	1:C:382:GLU:CD	2.17	0.47
1:D:220:GLN:CD	1:D:220:GLN:H	2.18	0.47
1:D:151:PHE:HB2	1:D:322:PHE:HB2	1.97	0.46
1:D:213:ILE:HD12	1:D:300:TRP:CE2	2.49	0.46
1:B:370:PHE:O	1:B:373:VAL:HB	2.16	0.46
1:C:83:LEU:HD22	1:C:102:VAL:HG11	1.98	0.46
1:D:166:LEU:HD12	1:D:194:ILE:HD13	1.97	0.46
1:A:220:GLN:O	1:A:224:ARG:HG3	2.15	0.46
1:B:127:TRP:CE2	1:B:336:GLU:HB2	2.51	0.46
1:B:143:ASP:OD2	1:B:147:ARG:NE	2.43	0.46
1:B:391:VAL:HG23	1:B:392:TYR:CD1	2.51	0.46
1:C:215:GLN:HE22	1:C:387:LEU:N	2.09	0.46
1:B:173:ASP:O	1:B:174:ALA:C	2.53	0.46
1:C:243:TYR:CZ	1:C:247:LEU:HD11	2.51	0.46
1:A:101:MSE:HE3	1:A:322:PHE:CE1	2.50	0.46
1:B:235:ARG:HG3	2:B:475:HOH:O	2.15	0.46
1:D:234:VAL:HG23	1:D:237:ALA:H	1.80	0.46
1:A:163:ASN:ND2	1:A:163:ASN:C	2.66	0.46
1:C:90:SER:HB3	1:C:96:GLU:HA	1.98	0.46
1:D:163:ASN:ND2	1:D:166:LEU:HD23	2.31	0.46
1:C:126:ASP:O	1:C:127:TRP:CD1	2.61	0.46
1:B:204:TRP:CH2	1:B:280:MSE:HE2	2.51	0.45
1:C:129:LEU:HG	1:C:343:TYR:CD1	2.50	0.45
1:D:350:ARG:HD3	1:D:354:GLU:OE1	2.16	0.45
1:C:85:GLN:N	1:C:85:GLN:NE2	2.57	0.45
1:A:281:SER:OG	1:A:373:VAL:HG13	2.16	0.45
1:A:94:ARG:HH11	1:A:94:ARG:HG2	1.80	0.45
1:B:419:ARG:O	1:B:423:GLU:HG3	2.17	0.45
1:B:348:VAL:HG11	1:B:363:THR:CG2	2.44	0.45
1:A:138:LEU:HD21	2:A:445:HOH:O	2.17	0.45
1:D:102:VAL:HG22	1:D:103:ASN:H	1.80	0.45
1:B:350:ARG:HD2	2:B:447:HOH:O	2.16	0.45
1:D:243:TYR:CZ	1:D:303:ALA:HB2	2.51	0.45
1:A:285:ALA:HB2	1:A:373:VAL:HG21	1.99	0.45
1:C:163:ASN:C	1:C:163:ASN:ND2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ARG:HD2	1:C:392:TYR:CE2	2.52	0.45
1:D:329:VAL:C	1:D:331:LYS:H	2.20	0.45
1:D:358:ASP:O	1:D:359:MSE:CE	2.54	0.45
1:A:127:TRP:CZ2	1:A:336:GLU:HB2	2.52	0.45
1:C:241:ILE:HG23	1:C:418:VAL:HG11	1.99	0.45
1:D:177:THR:O	1:D:177:THR:CG2	2.65	0.45
1:C:55:SER:HB2	1:C:56:PRO:HD3	1.98	0.45
1:D:111:TRP:HE3	1:D:117:THR:HG21	1.82	0.45
1:A:197:VAL:HG22	1:A:276:VAL:HB	1.99	0.44
1:B:175:ILE:HG13	1:B:181:GLN:HB3	1.99	0.44
1:B:382:GLU:N	1:B:382:GLU:OE1	2.39	0.44
1:A:163:ASN:HD22	1:A:164:ARG:N	2.15	0.44
1:C:125:ASP:C	1:C:126:ASP:O	2.54	0.44
1:D:167:LEU:HD12	1:D:167:LEU:HA	1.78	0.44
1:A:399:GLN:HE21	1:A:399:GLN:HB3	1.61	0.44
1:B:173:ASP:O	1:B:174:ALA:O	2.36	0.44
1:B:175:ILE:HG13	1:B:182:LEU:N	2.33	0.44
1:B:376:ALA:HA	1:B:379:LEU:HD22	2.00	0.44
1:C:94:ARG:HG2	1:C:94:ARG:HH11	1.82	0.44
1:D:255:ASP:C	1:D:256:LYS:HG2	2.38	0.44
1:A:55:SER:N	1:A:56:PRO:CD	2.80	0.43
1:D:202:ASN:HB2	1:D:258:GLN:O	2.18	0.43
1:D:58:TYR:O	1:D:62:VAL:HG23	2.18	0.43
1:B:197:VAL:O	1:B:197:VAL:HG23	2.17	0.43
1:D:82:ASP:HA	1:D:85:GLN:NE2	2.34	0.43
1:A:158:TRP:CH2	1:A:208:LYS:HG3	2.53	0.43
1:C:235:ARG:CD	1:C:235:ARG:H	2.31	0.43
1:A:192:LYS:HD3	1:A:192:LYS:HA	1.82	0.43
1:C:127:TRP:CE3	1:C:336:GLU:HG3	2.54	0.43
1:A:315:ARG:CZ	1:A:317:TYR:OH	2.66	0.43
1:C:363:THR:HG23	2:C:480:HOH:O	2.18	0.43
1:C:45:HIS:NE2	1:C:79:ASN:ND2	2.65	0.43
1:C:82:ASP:HA	1:C:85:GLN:NE2	2.33	0.43
1:D:387:LEU:HD11	1:D:392:TYR:CE1	2.53	0.43
1:D:91:ARG:CZ	1:D:116:ALA:HA	2.48	0.43
1:A:129:LEU:HG	1:A:343:TYR:CD1	2.53	0.43
1:B:195:ALA:O	1:B:274:ALA:HA	2.19	0.43
1:D:293:GLY:HA3	2:D:456:HOH:O	2.18	0.43
1:D:315:ARG:CZ	1:D:385:GLN:NE2	2.82	0.43
1:D:104:LEU:HB3	1:D:318:THR:HB	2.01	0.43
1:D:376:ALA:HA	1:D:379:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ASP:OD1	1:D:127:TRP:HD1	2.02	0.43
1:D:215:GLN:HA	1:D:218:LEU:HB2	2.01	0.43
1:A:351:PHE:HB3	1:A:359:MSE:HE3	1.99	0.43
1:A:319:LEU:N	1:A:319:LEU:HD12	2.34	0.42
1:A:69:ASN:ND2	1:A:337:LYS:HD3	2.34	0.42
1:C:36:ASP:N	1:C:36:ASP:OD1	2.52	0.42
1:B:172:VAL:CG1	1:B:173:ASP:H	2.26	0.42
1:C:312:THR:HA	1:C:384:SER:O	2.20	0.42
1:D:126:ASP:OD1	1:D:127:TRP:CD1	2.72	0.42
1:D:334:GLN:HG2	2:D:467:HOH:O	2.19	0.42
1:B:164:ARG:NH1	1:B:164:ARG:HG3	2.34	0.42
1:B:47:GLN:HA	1:B:79:ASN:O	2.19	0.42
1:C:46:THR:HG22	1:C:47:GLN:N	2.34	0.42
1:A:163:ASN:OD1	1:A:166:LEU:HD22	2.19	0.42
1:B:121:LYS:N	1:B:122:PRO:CD	2.82	0.42
1:B:357:ARG:HG2	1:B:359:MSE:HE1	2.01	0.42
1:B:379:LEU:O	1:B:382:GLU:OE1	2.38	0.42
1:C:290:LYS:HZ3	1:C:290:LYS:HB3	1.83	0.42
1:C:163:ASN:HD22	1:C:164:ARG:N	2.18	0.42
1:A:315:ARG:HD3	2:A:442:HOH:O	2.20	0.42
1:A:374:GLY:O	1:A:378:ARG:HG3	2.19	0.42
1:B:178:THR:HB	1:B:303:ALA:HA	2.00	0.42
1:C:100:VAL:HB	1:C:323:TRP:HB2	2.01	0.42
1:B:391:VAL:HG23	1:B:392:TYR:CE1	2.55	0.42
1:C:127:TRP:HZ3	1:C:336:GLU:HA	1.82	0.42
1:D:229:THR:CG2	1:D:231:ASP:HB2	2.50	0.42
1:D:52:ALA:HA	1:D:53:PRO:HD3	1.94	0.42
1:B:180:ASP:O	1:B:184:ALA:N	2.53	0.42
1:B:203:ASP:C	1:B:203:ASP:OD1	2.59	0.42
1:B:368:THR:HG22	1:B:378:ARG:NH2	2.35	0.42
1:A:204:TRP:O	1:A:208:LYS:HG2	2.20	0.41
1:B:41:THR:HB	1:B:73:LYS:HB3	2.01	0.41
1:C:129:LEU:HA	1:C:129:LEU:HD12	1.79	0.41
1:D:169:ARG:HG3	1:D:169:ARG:NH1	2.27	0.41
1:D:96:GLU:HG3	1:D:96:GLU:H	1.34	0.41
1:B:179:GLY:C	1:B:181:GLN:N	2.73	0.41
1:B:171:GLY:O	1:B:188:LYS:HE2	2.20	0.41
1:D:243:TYR:CD1	1:D:303:ALA:HB2	2.55	0.41
1:D:330:ARG:O	1:D:331:LYS:HB3	2.21	0.41
1:B:373:VAL:O	1:B:377:GLN:HG3	2.19	0.41
1:C:218:LEU:HD22	1:C:222:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:HA	1:B:73:LYS:HD3	1.95	0.41
1:D:102:VAL:CG2	1:D:103:ASN:N	2.82	0.41
1:D:80:GLY:O	1:D:82:ASP:N	2.47	0.41
1:B:154:PHE:CD1	1:B:359:MSE:HE1	2.56	0.41
1:C:163:ASN:HD21	1:C:165:ALA:HB3	1.86	0.41
1:C:64:ARG:O	1:C:64:ARG:HD3	2.21	0.41
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.93	0.41
1:B:47:GLN:HG3	1:B:83:LEU:HD13	2.01	0.41
1:C:38:ASP:O	1:C:41:THR:HB	2.21	0.41
1:A:45:HIS:HB2	1:A:97:ALA:HB3	2.03	0.41
1:C:120:VAL:HG22	1:C:151:PHE:CE1	2.55	0.41
1:C:166:LEU:N	1:C:166:LEU:HD22	2.36	0.41
1:C:399:GLN:HB2	2:C:9:HOH:O	2.20	0.41
1:D:121:LYS:N	1:D:122:PRO:HD2	2.34	0.41
1:A:414:SER:OG	1:A:417:ARG:HG3	2.21	0.41
1:B:102:VAL:HG22	1:B:103:ASN:N	2.35	0.41
1:B:124:LEU:HD13	1:B:130:ARG:HG3	2.02	0.41
1:D:344:ARG:O	1:D:345:PRO:C	2.59	0.41
1:C:163:ASN:ND2	1:C:166:LEU:HD23	2.36	0.41
1:C:46:THR:HG23	1:C:101:MSE:SE	2.70	0.41
1:D:320:ILE:HG13	2:D:445:HOH:O	2.21	0.41
1:A:100:VAL:HB	1:A:323:TRP:HB2	2.02	0.40
1:A:120:VAL:HG13	1:A:151:PHE:CE1	2.57	0.40
1:A:182:LEU:HD23	1:A:247:LEU:HD22	2.02	0.40
1:A:40:ASP:O	1:A:73:LYS:NZ	2.43	0.40
1:C:195:ALA:O	1:C:274:ALA:HA	2.21	0.40
1:C:327:ASN:HA	1:C:327:ASN:HD22	1.69	0.40
1:D:46:THR:HG22	1:D:47:GLN:H	1.85	0.40
1:C:296:GLU:HA	2:C:453:HOH:O	2.21	0.40
1:C:83:LEU:HD22	1:C:102:VAL:CG1	2.51	0.40
1:D:178:THR:OG1	1:D:181:GLN:HG3	2.20	0.40
1:D:300:TRP:HA	1:D:301:PRO:HD3	1.93	0.40
1:A:47:GLN:HA	1:A:79:ASN:O	2.21	0.40
1:B:84:ALA:HB1	1:B:107:LYS:HG2	2.02	0.40
1:C:104:LEU:HD11	1:C:109:LEU:CD1	2.51	0.40
1:C:324:ILE:HD13	1:C:335:VAL:HG11	2.04	0.40
1:A:387:LEU:O	1:A:389:PRO:HD3	2.21	0.40
1:B:55:SER:HB2	1:B:56:PRO:HD3	2.03	0.40
1:D:169:ARG:CG	1:D:169:ARG:NH1	2.84	0.40
1:D:199:VAL:HA	1:D:265:MSE:SE	2.72	0.40
1:A:94:ARG:HH22	1:B:94:ARG:HH21	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:TRP:CZ3	1:B:150:ALA:HB3	2.56	0.40
1:D:255:ASP:O	1:D:256:LYS:HG2	2.21	0.40
1:D:379:LEU:HA	1:D:379:LEU:HD12	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/405 (96%)	371 (95%)	15 (4%)	3 (1%)	19	23
1	B	388/405 (96%)	361 (93%)	20 (5%)	7 (2%)	8	7
1	C	392/405 (97%)	369 (94%)	18 (5%)	5 (1%)	12	12
1	D	389/405 (96%)	366 (94%)	17 (4%)	6 (2%)	10	10
All	All	1558/1620 (96%)	1467 (94%)	70 (4%)	21 (1%)	12	12

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	196	PRO
1	B	180	ASP
1	C	127	TRP
1	C	310	GLY
1	D	310	GLY
1	D	331	LYS
1	B	179	GLY
1	B	196	PRO
1	C	196	PRO
1	C	320	ILE
1	D	126	ASP

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Mol	Chain	Res	Type
1	D	196	PRO
1	D	390	ASP
1	B	174	ALA
1	C	128	GLY
1	D	382	GLU
1	B	181	GLN
1	B	371	PRO
1	B	369	GLY
1	A	371	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	305/314 (97%)	278 (91%)	27 (9%)	9 11
1	B	302/314 (96%)	268 (89%)	34 (11%)	6 6
1	C	306/314 (98%)	263 (86%)	43 (14%)	3 3
1	D	305/314 (97%)	276 (90%)	29 (10%)	8 10
All	All	1218/1256 (97%)	1085 (89%)	133 (11%)	6 7

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	42	LEU
1	A	64	ARG
1	A	73	LYS
1	A	85	GLN
1	A	94	ARG
1	A	109	LEU
1	A	117	THR
1	A	129	LEU
1	A	130	ARG
1	A	134	LEU
1	A	159	PRO

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Mol	Chain	Res	Type
1	A	163	ASN
1	A	209	LEU
1	A	210	LEU
1	A	239	LEU
1	A	264	SER
1	A	284	LEU
1	A	289	GLU
1	A	304	ASP
1	A	330	ARG
1	A	353	THR
1	A	379	LEU
1	A	390	ASP
1	A	411	ARG
1	A	419	ARG
1	A	422	LEU
1	B	41	THR
1	B	42	LEU
1	B	64	ARG
1	B	77	LEU
1	B	85	GLN
1	B	96	GLU
1	B	103	ASN
1	B	107	LYS
1	B	109	LEU
1	B	117	THR
1	B	124	LEU
1	B	138	LEU
1	B	159	PRO
1	B	164	ARG
1	B	166	LEU
1	B	173	ASP
1	B	175	ILE
1	B	177	THR
1	B	178	THR
1	B	187	ARG
1	B	207	GLN
1	B	208	LYS
1	B	209	LEU
1	B	210	LEU
1	B	239	LEU
1	B	267	THR
1	B	286	LYS

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Mol	Chain	Res	Type
1	B	309	ASP
1	B	333	GLU
1	B	357	ARG
1	B	379	LEU
1	B	391	VAL
1	B	411	ARG
1	B	422	LEU
1	C	36	ASP
1	C	40	ASP
1	C	42	LEU
1	C	64	ARG
1	C	69	ASN
1	C	85	GLN
1	C	102	VAL
1	C	103	ASN
1	C	109	LEU
1	C	117	THR
1	C	120	VAL
1	C	124	LEU
1	C	127	TRP
1	C	129	LEU
1	C	130	ARG
1	C	134	LEU
1	C	157	ASN
1	C	163	ASN
1	C	172	VAL
1	C	173	ASP
1	C	202	ASN
1	C	207	GLN
1	C	208	LYS
1	C	209	LEU
1	C	210	LEU
1	C	220	GLN
1	C	224	ARG
1	C	235	ARG
1	C	238	ARG
1	C	258	GLN
1	C	284	LEU
1	C	289	GLU
1	C	339	LEU
1	C	362	ARG
1	C	363	THR

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Mol	Chain	Res	Type
1	C	379	LEU
1	C	382	GLU
1	C	383	VAL
1	C	387	LEU
1	C	391	VAL
1	C	399	GLN
1	C	422	LEU
1	C	424	SER
1	D	42	LEU
1	D	46	THR
1	D	64	ARG
1	D	75	LYS
1	D	77	LEU
1	D	85	GLN
1	D	96	GLU
1	D	126	ASP
1	D	129	LEU
1	D	134	LEU
1	D	159	PRO
1	D	167	LEU
1	D	207	GLN
1	D	208	LYS
1	D	210	LEU
1	D	221	ASP
1	D	281	SER
1	D	304	ASP
1	D	336	GLU
1	D	339	LEU
1	D	350	ARG
1	D	357	ARG
1	D	363	THR
1	D	368	THR
1	D	379	LEU
1	D	383	VAL
1	D	385	GLN
1	D	399	GLN
1	D	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN

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Mol	Chain	Res	Type
1	A	85	GLN
1	A	163	ASN
1	A	215	GLN
1	A	268	GLN
1	A	334	GLN
1	A	399	GLN
1	B	79	ASN
1	B	85	GLN
1	B	103	ASN
1	B	207	GLN
1	B	215	GLN
1	B	334	GLN
1	C	69	ASN
1	C	79	ASN
1	C	85	GLN
1	C	103	ASN
1	C	163	ASN
1	C	202	ASN
1	C	207	GLN
1	C	215	GLN
1	C	258	GLN
1	C	268	GLN
1	C	327	ASN
1	D	45	HIS
1	D	69	ASN
1	D	85	GLN
1	D	207	GLN
1	D	220	GLN
1	D	225	HIS
1	D	268	GLN
1	D	308	HIS
1	D	385	GLN
1	D	399	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	386/405 (95%)	-0.23	0 100 100	21, 34, 48, 65	0
1	B	385/405 (95%)	-0.02	6 (1%) 72 77	24, 40, 58, 66	0
1	C	389/405 (96%)	-0.06	5 (1%) 77 81	25, 37, 55, 66	0
1	D	386/405 (95%)	-0.07	3 (0%) 86 89	23, 37, 54, 67	0
All	All	1546/1620 (95%)	-0.09	14 (0%) 84 88	21, 37, 55, 67	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	ASP	7.0
1	C	310	GLY	4.3
1	D	310	GLY	4.0
1	D	169	ARG	2.6
1	B	307	ALA	2.4
1	B	235	ARG	2.3
1	C	36	ASP	2.3
1	C	38	ASP	2.2
1	B	172	VAL	2.1
1	B	178	THR	2.1
1	B	174	ALA	2.1
1	D	223	ALA	2.0
1	C	175	ILE	2.0
1	C	381	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.