Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 09:49 AM EDT

PDB ID	:	5ZGC
Title	:	Crystal Structure of SIRT3 in complex with H4K16bhb peptide
Authors	:	Li, H.; Zhang, X.
Deposited on	:	2018-03-08
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.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

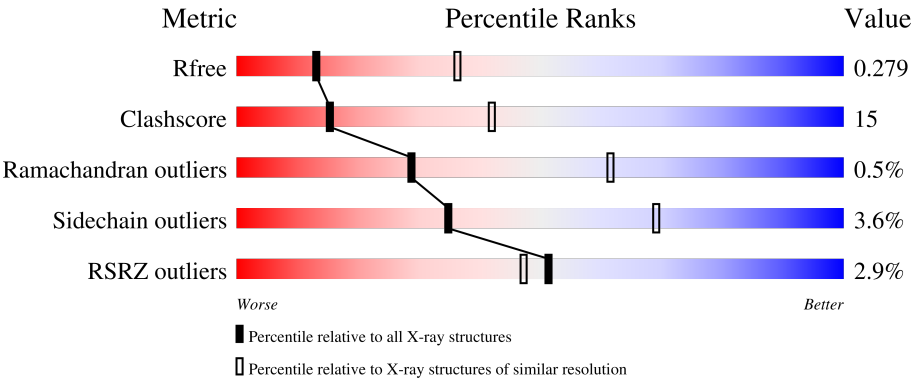
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 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	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 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	274	2% 77% 18%
1	B	274	2% 67% 27% 6%
1	C	274	% 74% 19%
1	D	274	7% 53% 39% 5%
1	E	274	2% 70% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	274	2% 52% 23% 23%
2	G	11	82% 9% 9%
2	H	11	45% 36% 18%
2	I	11	55% 9% 36%
2	J	11	27% 18% 55%
2	K	11	9% 18% 45% 36%
2	L	11	45% 55%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12436 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2072	1337	357	369	9			
1	B	258	Total	C	N	O	S	0	0	0
			2026	1308	348	361	9			
1	C	262	Total	C	N	O	S	0	0	0
			2066	1334	356	367	9			
1	D	260	Total	C	N	O	S	0	0	0
			2046	1320	352	365	9			
1	E	273	Total	C	N	O	S	0	0	0
			2144	1382	369	384	9			
1	F	212	Total	C	N	O	S	0	1	0
			1665	1071	289	300	5			

- Molecule 2 is a protein called Histone H4K16bhb peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	11	Total	C	N	O	0	0	0
			89	54	22	13			
2	H	9	Total	C	N	O	0	0	0
			73	43	19	11			
2	I	7	Total	C	N	O	0	0	0
			60	35	16	9			
2	J	5	Total	C	N	O	0	0	0
			45	27	11	7			
2	K	7	Total	C	N	O	0	0	0
			60	35	16	9			
2	L	5	Total	C	N	O	0	0	0
			24	14	5	5			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0

- Molecule 4 is water.

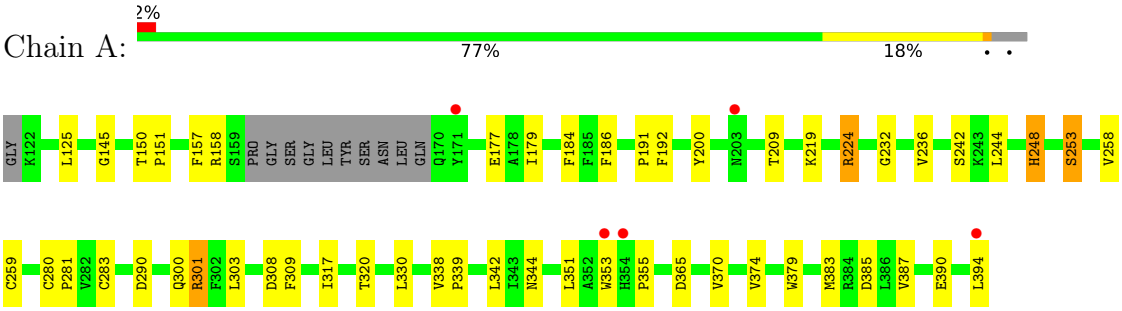
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	13	Total O 13 13	0	0
4	C	14	Total O 14 14	0	0
4	D	6	Total O 6 6	0	0
4	E	9	Total O 9 9	0	0
4	F	4	Total O 4 4	0	0
4	G	1	Total O 1 1	0	0
4	I	1	Total O 1 1	0	0

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.

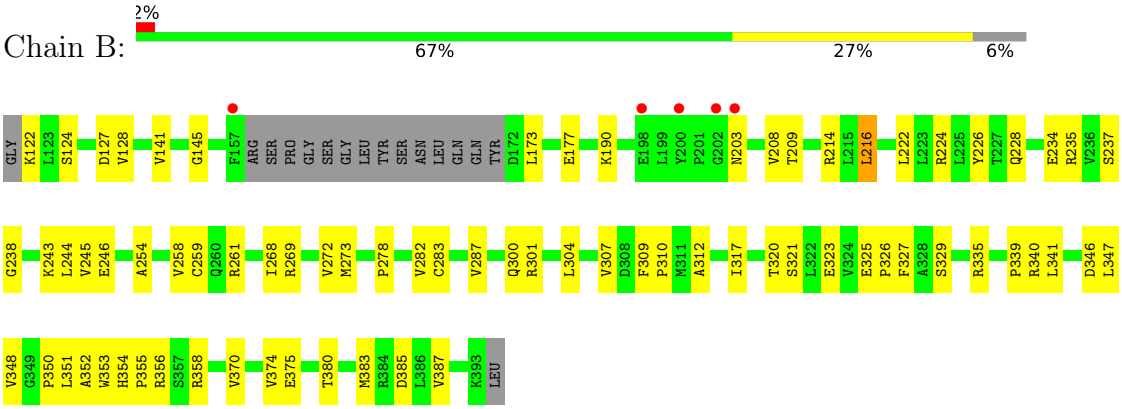
• Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial

Chain A:



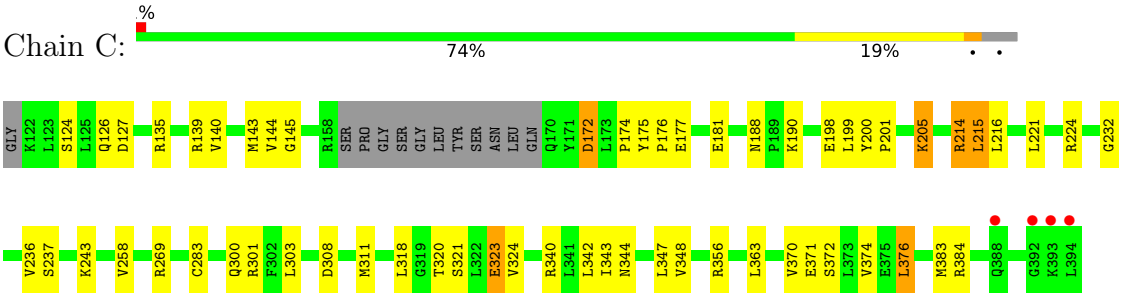
• Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial

Chain B:



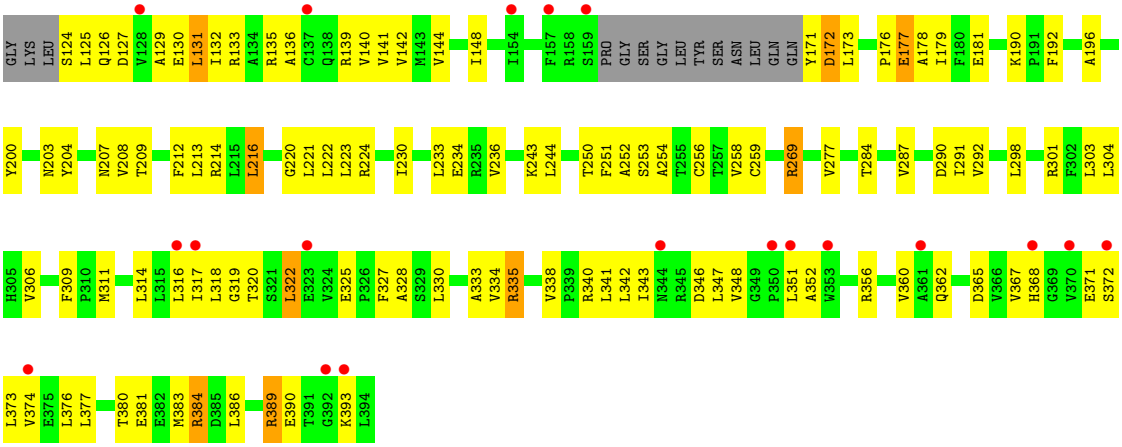
• Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial

Chain C:



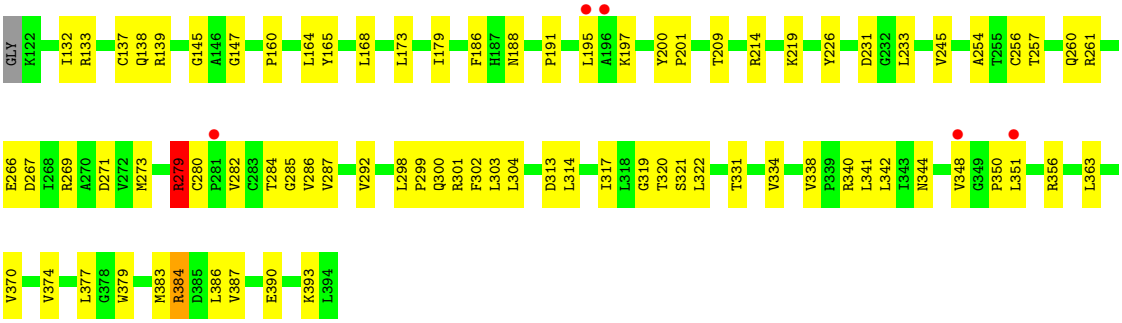
• Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial

Chain D:



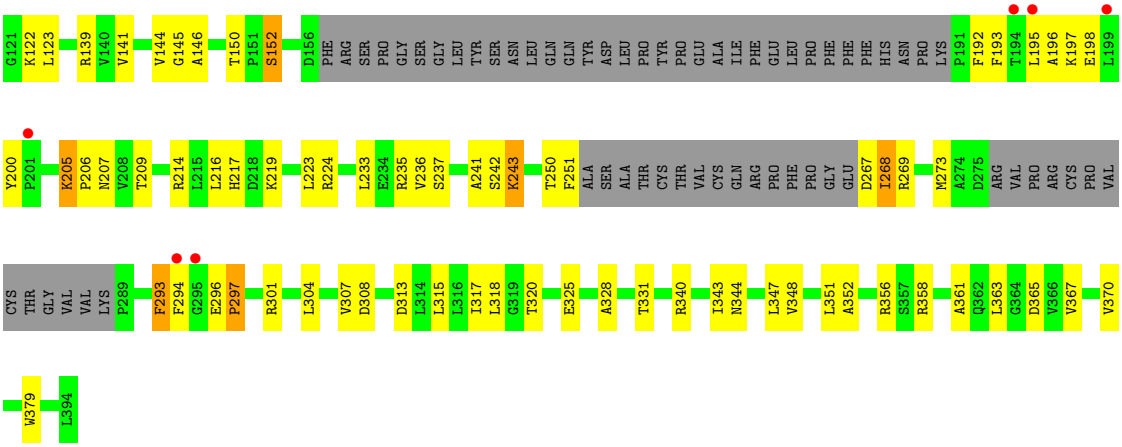
• Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial

Chain E:



• Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial

Chain F:



• Molecule 2: Histone H4K16bhb peptide

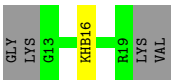
Chain G:

• Molecule 2: Histone H4K16bhb peptide

Chain H:

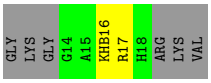
• Molecule 2: Histone H4K16bhb peptide

Chain I:



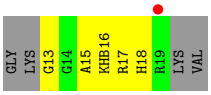
• Molecule 2: Histone H4K16bhb peptide

Chain J:



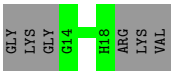
• Molecule 2: Histone H4K16bhb peptide

Chain K:



• Molecule 2: Histone H4K16bhb peptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	138.51Å 138.51Å 242.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.16 – 2.90 48.01 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.16-2.90) 99.6 (48.01-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14_3247	Depositor
R, R_{free}	0.224 , 0.280 0.224 , 0.279	Depositor DCC
R_{free} test set	2626 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12436	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

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

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	0.53	0/2124	0.74	2/2892 (0.1%)
1	B	0.51	0/2077	0.67	0/2829
1	C	0.58	0/2118	0.68	0/2884
1	D	0.47	0/2098	0.69	1/2858 (0.0%)
1	E	0.47	0/2199	0.68	1/2996 (0.0%)
1	F	0.46	0/1702	0.71	1/2309 (0.0%)
2	G	0.47	0/73	0.58	0/91
2	H	0.54	0/57	0.85	0/70
2	I	0.44	0/44	0.55	0/54
2	J	0.32	0/29	0.57	0/35
2	K	0.36	0/44	0.81	0/54
2	L	0.51	0/17	0.74	0/20
All	All	0.50	0/12582	0.69	5/17092 (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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	216	LEU	CA-CB-CG	6.80	130.93	115.30
1	A	125	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	F	216	LEU	CA-CB-CG	5.64	128.28	115.30
1	E	279	ARG	C-N-CA	5.57	135.62	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	LEU	CB-CG-CD2	-5.24	102.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	PHE	Peptide
1	A	200	TYR	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	2072	0	2091	33	0
1	B	2026	0	2045	66	0
1	C	2066	0	2086	44	1
1	D	2046	0	2059	126	0
1	E	2144	0	2160	66	0
1	F	1665	0	1698	48	1
2	G	89	0	81	2	0
2	H	73	0	59	8	0
2	I	60	0	43	0	0
2	J	45	0	27	0	0
2	K	60	0	43	4	0
2	L	24	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	13	0	0	0	0
4	B	13	0	0	1	0
4	C	14	0	0	0	0
4	D	6	0	0	0	0
4	E	9	0	0	0	0
4	F	4	0	0	0	0
4	G	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
All	All	12436	0	12403	368	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 15.

All (368) 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:129:ALA:CB	1:D:376:LEU:HD22	1.94	0.97
1:D:334:VAL:HB	1:D:338:VAL:HG21	1.45	0.96
1:B:268:ILE:HD11	1:B:287:VAL:HG12	1.52	0.92
1:D:129:ALA:HB3	1:D:376:LEU:CD2	2.01	0.91
1:E:279:ARG:HD3	1:E:284:THR:O	1.71	0.89
1:D:129:ALA:HB3	1:D:376:LEU:HD22	1.52	0.88
1:D:341:LEU:CD1	1:D:343:ILE:HD11	2.04	0.88
1:A:301:ARG:HH12	1:B:300:GLN:NE2	1.71	0.88
1:E:279:ARG:CD	1:E:284:THR:O	2.22	0.87
1:F:224:ARG:NH1	1:F:308:ASP:OD2	2.07	0.86
1:D:322:LEU:HD12	1:D:328:ALA:HA	1.58	0.86
1:F:347:LEU:HB2	1:F:363:LEU:HD21	1.58	0.86
1:E:139:ARG:NH2	1:F:313:ASP:OD2	2.09	0.85
1:D:320:THR:HG22	1:D:322:LEU:H	1.42	0.83
1:E:313:ASP:OD2	1:F:139:ARG:NH1	2.11	0.82
1:F:293:PHE:HD1	1:F:294:PHE:H	1.29	0.80
1:B:222:LEU:O	1:B:243:LYS:HE2	1.81	0.80
1:D:341:LEU:HD23	1:D:360:VAL:HB	1.63	0.80
1:D:220:GLY:O	1:D:221:LEU:HD12	1.83	0.79
1:D:148:ILE:HD12	1:D:319:GLY:HA3	1.65	0.78
1:D:148:ILE:CD1	1:D:319:GLY:HA3	2.14	0.78
1:E:137:CYS:SG	1:E:314:LEU:HD23	2.24	0.77
1:E:132:ILE:HD11	1:E:314:LEU:HD21	1.67	0.76
1:C:321:SER:OG	1:C:323:GLU:OE2	2.03	0.75
1:F:268:ILE:HG13	1:F:269:ARG:H	1.52	0.75
1:B:321:SER:OG	1:B:323:GLU:OE1	2.01	0.75
1:D:373:LEU:O	1:D:377:LEU:HD23	1.88	0.74
1:D:129:ALA:CB	1:D:376:LEU:CD2	2.63	0.74
1:D:325:GLU:HG3	1:D:328:ALA:HB3	1.70	0.73
1:D:346:ASP:OD1	1:D:348:VAL:HG13	1.89	0.72
1:B:321:SER:HA	1:B:348:VAL:HG21	1.72	0.72
1:D:144:VAL:HG13	1:D:148:ILE:HG12	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:HG3	1:B:326:PRO:HA	1.73	0.71
1:D:208:VAL:HG21	1:D:367:VAL:HG23	1.73	0.71
1:D:340:ARG:HH22	1:D:356:ARG:CZ	2.03	0.71
1:D:173:LEU:HD21	1:D:179:ILE:HB	1.73	0.70
1:D:381:GLU:HA	1:D:384:ARG:CZ	2.21	0.70
1:E:266:GLU:N	1:E:266:GLU:OE2	2.21	0.70
1:D:148:ILE:HD12	1:D:148:ILE:N	2.07	0.70
1:D:341:LEU:HD13	1:D:343:ILE:HD11	1.71	0.69
1:C:140:VAL:HG12	1:C:221:LEU:O	1.92	0.69
1:A:253:SER:HB2	1:A:290:ASP:OD2	1.93	0.69
1:C:144:VAL:HG12	1:C:318:LEU:HB2	1.75	0.69
1:E:279:ARG:CD	1:E:284:THR:C	2.62	0.69
1:E:292:VAL:HG21	1:E:299:PRO:HD3	1.75	0.68
1:E:321:SER:HA	1:E:348:VAL:HG21	1.76	0.68
1:B:350:PRO:HD3	2:H:19:ARG:HH12	1.59	0.67
1:F:152:SER:OG	1:F:205:LYS:O	2.13	0.66
1:A:303:LEU:HD22	1:B:307:VAL:HG21	1.77	0.66
1:E:279:ARG:HD2	1:E:284:THR:O	1.93	0.66
1:B:346:ASP:HB2	1:B:348:VAL:HG13	1.77	0.66
1:E:138:GLN:HE21	1:F:139:ARG:HE	1.44	0.66
1:E:322:LEU:HD23	1:E:350:PRO:HD2	1.77	0.66
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.09	0.65
1:D:148:ILE:HD12	1:D:148:ILE:H	1.61	0.65
1:A:179:ILE:HD11	1:A:192:PHE:HA	1.77	0.65
1:B:235:ARG:HD2	1:B:244:LEU:HD21	1.78	0.65
1:D:177:GLU:OE1	1:D:177:GLU:N	2.22	0.65
1:D:303:LEU:O	1:D:306:VAL:HG12	1.97	0.65
1:F:268:ILE:HG13	1:F:269:ARG:N	2.12	0.65
1:A:186:PHE:CD2	1:C:300:GLN:HG3	2.32	0.64
1:D:309:PHE:HE2	1:D:330:LEU:HB3	1.62	0.64
1:A:224:ARG:HD2	1:A:308:ASP:OD2	1.97	0.64
1:D:258:VAL:HG22	1:E:304:LEU:HD21	1.80	0.64
1:F:325:GLU:HG3	1:F:328:ALA:HB3	1.79	0.64
1:B:190:LYS:NZ	1:E:267:ASP:OD1	2.32	0.63
1:D:390:GLU:OE1	1:D:393:LYS:HD3	1.99	0.63
1:F:209:THR:HG22	1:F:370:VAL:HG21	1.81	0.62
1:A:370:VAL:O	1:A:374:VAL:HG23	1.99	0.62
1:D:141:VAL:HG11	1:D:309:PHE:CE1	2.35	0.62
1:A:374:VAL:HG11	1:A:383:MET:HG3	1.80	0.62
1:F:296:GLU:HG3	1:F:297:PRO:HD2	1.80	0.62
1:E:138:GLN:NE2	1:F:139:ARG:HE	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:ARG:HH22	2:K:13:GLY:HA3	1.65	0.62
1:B:254:ALA:CB	1:B:268:ILE:HD12	2.30	0.61
1:E:186:PHE:HE1	1:E:257:THR:HB	1.65	0.61
1:C:188:ASN:HD21	1:C:190:LYS:HB2	1.66	0.61
1:C:139:ARG:NH2	1:C:311:MET:HE3	2.15	0.61
1:A:353:TRP:O	1:A:355:PRO:HD3	2.00	0.60
1:D:250:THR:HG23	1:D:252:ALA:H	1.66	0.60
1:A:209:THR:HG23	1:A:370:VAL:HG21	1.82	0.60
1:B:128:VAL:HG11	1:B:341:LEU:HD22	1.82	0.60
1:D:341:LEU:HD13	1:D:343:ILE:CD1	2.32	0.59
1:E:279:ARG:HD3	1:E:284:THR:C	2.21	0.59
1:E:209:THR:HG23	1:E:370:VAL:HG21	1.83	0.59
1:F:331:THR:O	1:F:340:ARG:NH1	2.35	0.59
1:A:390:GLU:O	1:A:394:LEU:HD12	2.02	0.59
1:E:137:CYS:HB3	1:E:314:LEU:HD23	1.84	0.59
1:F:219:LYS:HD2	1:F:379:TRP:CZ2	2.37	0.59
1:C:139:ARG:NH2	1:C:311:MET:CE	2.65	0.59
1:B:177:GLU:HG2	2:H:18:HIS:CE1	2.38	0.59
1:F:348:VAL:HA	1:F:352:ALA:HB2	1.85	0.59
1:D:127:ASP:O	1:D:131:LEU:HD12	2.03	0.58
1:B:209:THR:HG22	1:B:370:VAL:HG21	1.83	0.58
1:A:383:MET:O	1:A:387:VAL:HG23	2.03	0.58
1:D:214:ARG:NH1	1:D:390:GLU:OE2	2.35	0.58
1:D:384:ARG:H	1:D:384:ARG:HD3	1.66	0.58
1:E:254:ALA:HB1	1:E:287:VAL:HG12	1.85	0.58
1:D:316:LEU:HB3	1:D:318:LEU:HD11	1.86	0.58
1:E:298:LEU:HD23	1:E:302:PHE:CD1	2.39	0.58
1:A:301:ARG:HH12	1:B:300:GLN:HE21	1.52	0.57
1:D:140:VAL:HG22	1:D:314:LEU:HB3	1.84	0.57
1:D:126:GLN:HA	1:D:376:LEU:HD21	1.86	0.57
1:F:340:ARG:CZ	1:F:356:ARG:HD2	2.33	0.57
1:F:145:GLY:HA3	1:F:320:THR:HB	1.84	0.57
1:C:318:LEU:HD23	1:C:343:ILE:HB	1.86	0.57
1:D:230:ILE:HD12	1:D:291:ILE:HD12	1.87	0.57
1:D:142:VAL:HG11	1:D:213:LEU:HD21	1.86	0.57
1:F:269:ARG:O	1:F:273:MET:HG2	2.05	0.57
1:C:340:ARG:NH2	1:C:356:ARG:HG3	2.20	0.56
1:C:321:SER:HA	1:C:348:VAL:HG21	1.86	0.56
1:E:179:ILE:HG21	1:E:195:LEU:HD23	1.88	0.56
1:E:219:LYS:HD2	1:E:379:TRP:CZ2	2.40	0.56
1:D:244:LEU:O	1:D:301:ARG:NH2	2.32	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ARG:O	1:D:338:VAL:HG22	2.06	0.56
1:F:152:SER:HB2	1:F:207:ASN:HD22	1.71	0.56
1:D:148:ILE:CD1	1:D:148:ILE:H	2.18	0.56
1:B:310:PRO:O	1:B:335:ARG:NH1	2.39	0.56
1:D:213:LEU:HA	1:D:216:LEU:HD13	1.88	0.56
1:D:341:LEU:HD11	1:D:343:ILE:HD11	1.86	0.56
1:F:193:PHE:O	1:F:197:LYS:HG3	2.05	0.55
1:E:137:CYS:CB	1:E:314:LEU:HD23	2.35	0.55
1:E:226:TYR:HA	1:E:245:VAL:HG13	1.89	0.55
1:E:340:ARG:NH2	1:E:356:ARG:HD3	2.22	0.55
1:D:148:ILE:HG23	1:D:209:THR:HB	1.88	0.55
1:E:256:CYS:HB3	1:E:260:GLN:H	1.72	0.54
1:C:139:ARG:HH21	1:C:311:MET:HE3	1.71	0.54
1:D:127:ASP:O	1:D:130:GLU:HB3	2.06	0.54
1:B:268:ILE:HG23	1:B:278:PRO:HG3	1.89	0.54
1:B:269:ARG:O	1:B:272:VAL:HG12	2.08	0.54
1:C:232:GLY:O	1:C:236:VAL:HG23	2.08	0.54
1:E:351:LEU:HD22	1:E:351:LEU:H	1.72	0.54
1:D:130:GLU:HA	1:D:133:ARG:HH12	1.73	0.54
1:D:139:ARG:HB3	1:D:223:LEU:HD22	1.88	0.54
1:A:232:GLY:O	1:A:236:VAL:HG23	2.08	0.53
1:E:344:ASN:O	1:E:363:LEU:HA	2.09	0.53
1:B:141:VAL:HG23	1:B:312:ALA:HB2	1.89	0.53
1:F:193:PHE:HA	1:F:196:ALA:HB3	1.89	0.53
1:B:350:PRO:CD	2:H:19:ARG:HH12	2.22	0.53
1:D:212:PHE:CE2	1:D:216:LEU:HD11	2.44	0.53
1:B:383:MET:O	1:B:387:VAL:HG23	2.09	0.53
1:F:304:LEU:O	1:F:307:VAL:HG12	2.09	0.53
1:D:213:LEU:HA	1:D:216:LEU:CD1	2.39	0.52
1:E:164:LEU:HD21	1:E:195:LEU:HD13	1.90	0.52
1:B:261:ARG:NH2	1:B:282:VAL:HG11	2.24	0.52
1:D:342:LEU:HD12	1:D:351:LEU:HD22	1.90	0.52
1:E:342:LEU:HD11	1:E:348:VAL:HG12	1.90	0.52
1:F:144:VAL:HG12	1:F:318:LEU:HB2	1.91	0.52
1:B:177:GLU:HG2	2:H:18:HIS:HE1	1.74	0.52
1:C:342:LEU:HD11	1:C:344:ASN:HB2	1.91	0.52
1:B:347:LEU:HG	1:B:352:ALA:HB2	1.91	0.52
1:C:188:ASN:ND2	1:C:190:LYS:H	2.08	0.52
1:D:140:VAL:HB	1:D:221:LEU:O	2.10	0.52
1:F:195:LEU:HA	1:F:198:GLU:HB3	1.91	0.52
1:D:129:ALA:HB2	1:D:376:LEU:HD22	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ILE:O	1:D:207:ASN:ND2	2.41	0.52
1:D:309:PHE:HD2	1:D:333:ALA:HB3	1.75	0.52
1:E:173:LEU:HD21	1:E:179:ILE:HG13	1.93	0.51
1:F:224:ARG:HG3	1:F:243:LYS:O	2.11	0.51
1:C:175:TYR:HB2	1:C:176:PRO:HD2	1.92	0.51
1:F:320:THR:O	1:F:344:ASN:ND2	2.43	0.51
1:A:385:ASP:OD2	1:D:135:ARG:NH2	2.42	0.51
1:D:371:GLU:O	1:D:374:VAL:HG12	2.10	0.51
1:B:141:VAL:CG2	1:B:312:ALA:HB2	2.41	0.51
1:B:325:GLU:CG	1:B:326:PRO:HA	2.41	0.51
1:C:124:SER:N	1:C:127:ASP:OD2	2.32	0.51
1:A:301:ARG:HH22	1:B:300:GLN:HE22	1.59	0.51
1:C:372:SER:O	1:C:376:LEU:HD12	2.11	0.50
1:D:176:PRO:O	1:D:178:ALA:N	2.44	0.50
1:D:256:CYS:HA	1:D:287:VAL:HA	1.93	0.50
1:B:301:ARG:O	1:B:304:LEU:HB2	2.11	0.50
1:D:148:ILE:HD11	1:D:318:LEU:C	2.32	0.50
1:C:214:ARG:HD2	1:C:214:ARG:C	2.32	0.50
1:E:280:CYS:O	1:E:284:THR:N	2.37	0.50
1:C:214:ARG:NH1	1:C:237:SER:O	2.45	0.50
1:D:327:PHE:HA	1:D:330:LEU:CD2	2.41	0.50
1:E:342:LEU:CD2	1:E:344:ASN:HB2	2.42	0.50
1:F:365:ASP:OD1	1:F:367:VAL:N	2.45	0.50
1:D:124:SER:HA	1:D:127:ASP:OD2	2.12	0.50
1:D:148:ILE:CD1	1:D:148:ILE:N	2.75	0.50
1:D:203:ASN:HB3	1:D:204:TYR:HD1	1.77	0.50
1:F:217:HIS:CE1	1:F:243:LYS:HD2	2.47	0.49
1:E:322:LEU:HD21	1:E:331:THR:HG21	1.94	0.49
1:D:320:THR:HG22	1:D:322:LEU:HD22	1.93	0.49
1:E:279:ARG:HG2	1:E:285:GLY:C	2.32	0.49
1:C:224:ARG:NE	1:C:308:ASP:OD2	2.30	0.49
1:D:269:ARG:CZ	1:D:269:ARG:HB3	2.37	0.49
1:D:334:VAL:CB	1:D:338:VAL:HG21	2.31	0.49
1:C:371:GLU:O	1:C:374:VAL:HG22	2.13	0.49
1:D:346:ASP:OD1	1:D:347:LEU:N	2.46	0.49
1:D:131:LEU:HB3	1:D:136:ALA:HB3	1.95	0.49
1:E:279:ARG:HD2	1:E:284:THR:C	2.32	0.49
1:D:377:LEU:HD22	1:D:377:LEU:N	2.28	0.49
1:B:145:GLY:HA3	1:B:320:THR:HB	1.95	0.48
1:F:315:LEU:HD23	1:F:340:ARG:HB3	1.94	0.48
1:F:250:THR:OG1	1:F:251:PHE:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLY:HA3	1:C:320:THR:HB	1.95	0.48
1:B:385:ASP:OD2	1:C:135:ARG:NE	2.42	0.48
1:F:340:ARG:NH2	1:F:351:LEU:HD22	2.29	0.48
1:D:341:LEU:HD23	1:D:360:VAL:CB	2.40	0.48
1:D:132:ILE:HG12	1:D:377:LEU:HD11	1.95	0.47
1:D:212:PHE:O	1:D:216:LEU:HD12	2.14	0.47
1:C:198:GLU:C	1:C:200:TYR:H	2.18	0.47
1:D:327:PHE:HA	1:D:330:LEU:HD23	1.96	0.47
1:B:269:ARG:O	1:B:273:MET:HG2	2.15	0.47
1:D:133:ARG:HB2	1:D:133:ARG:CZ	2.44	0.47
1:B:259:CYS:SG	1:B:261:ARG:HG3	2.54	0.47
1:C:224:ARG:HG2	1:C:243:LYS:O	2.15	0.47
1:D:381:GLU:OE1	1:D:384:ARG:NH2	2.39	0.47
1:E:261:ARG:HD3	1:E:282:VAL:HG11	1.96	0.47
1:F:340:ARG:NH2	1:F:351:LEU:CD2	2.77	0.47
1:B:224:ARG:CD	1:B:245:VAL:HG23	2.45	0.47
1:B:228:GLN:HG3	1:B:327:PHE:CE2	2.49	0.47
1:F:123:LEU:HD11	1:F:358:ARG:HG2	1.97	0.47
2:K:15:ALA:O	2:K:17:ARG:N	2.48	0.47
1:D:347:LEU:HD23	1:D:352:ALA:HB2	1.97	0.46
1:F:224:ARG:NH1	1:F:308:ASP:CG	2.67	0.46
1:F:235:ARG:CZ	1:F:241:ALA:HB2	2.45	0.46
1:A:374:VAL:HG13	1:A:379:TRP:HB2	1.96	0.46
1:D:253:SER:HB2	1:D:290:ASP:OD2	2.16	0.46
1:A:301:ARG:NH1	1:B:300:GLN:NE2	2.52	0.46
1:D:365:ASP:O	1:D:368:HIS:HB3	2.16	0.46
1:A:258:VAL:CG2	1:A:283:CYS:SG	3.04	0.46
1:C:205:LYS:HD2	1:C:205:LYS:O	2.15	0.46
1:D:330:LEU:N	1:D:330:LEU:HD22	2.31	0.46
1:C:214:ARG:CG	1:C:214:ARG:NH1	2.72	0.46
1:A:342:LEU:HD11	1:A:344:ASN:HB2	1.98	0.46
1:B:234:GLU:O	1:B:237:SER:OG	2.33	0.46
1:D:317:ILE:C	1:D:318:LEU:HD12	2.36	0.46
1:D:330:LEU:HD22	1:D:330:LEU:H	1.80	0.46
1:C:200:TYR:CD1	1:C:201:PRO:HD2	2.51	0.46
1:F:193:PHE:HA	1:F:196:ALA:CB	2.45	0.46
1:C:214:ARG:HH11	1:C:214:ARG:HG2	1.80	0.45
1:C:215:LEU:HD23	1:C:383:MET:SD	2.56	0.45
1:D:200:TYR:O	1:D:203:ASN:HB2	2.16	0.45
1:D:384:ARG:HG2	1:D:384:ARG:HH11	1.82	0.45
1:B:374:VAL:HG11	1:B:383:MET:HG3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:GLY:O	1:D:221:LEU:CD1	2.60	0.45
1:E:147:GLY:N	1:E:319:GLY:O	2.39	0.45
1:F:206:PRO:HG3	1:F:236:VAL:HG13	1.98	0.45
1:B:375:GLU:HA	1:B:380:THR:HG23	1.98	0.45
1:D:125:LEU:HD13	1:D:341:LEU:HD21	1.99	0.45
1:E:320:THR:HG23	1:E:322:LEU:HD13	1.98	0.45
1:D:171:TYR:O	1:D:172:ASP:HB2	2.17	0.45
1:D:251:PHE:HE1	1:D:291:ILE:CG1	2.30	0.45
1:E:197:LYS:HE2	1:E:273:MET:CE	2.47	0.45
1:E:383:MET:O	1:E:387:VAL:HG12	2.17	0.45
1:B:224:ARG:HD2	1:B:245:VAL:CG2	2.46	0.45
1:D:212:PHE:CZ	1:D:216:LEU:HD11	2.52	0.45
1:A:300:GLN:NE2	1:B:301:ARG:HH12	2.15	0.44
1:B:317:ILE:HD13	1:B:351:LEU:HD11	1.98	0.44
1:A:179:ILE:CD1	1:A:192:PHE:HA	2.45	0.44
1:D:343:ILE:HG13	1:D:362:GLN:HB3	1.99	0.44
1:B:224:ARG:HG3	1:B:243:LYS:O	2.17	0.44
1:E:334:VAL:HB	1:E:338:VAL:HG21	1.98	0.44
1:F:233:LEU:HA	1:F:236:VAL:HG12	1.99	0.44
1:E:145:GLY:HA3	1:E:320:THR:HB	2.00	0.44
1:B:173:LEU:HA	1:B:173:LEU:HD12	1.79	0.44
1:D:284:THR:HG22	1:D:284:THR:O	2.18	0.44
1:E:279:ARG:HD3	1:E:285:GLY:HA2	2.00	0.44
1:C:190:LYS:HD3	1:C:190:LYS:HA	1.77	0.44
1:C:214:ARG:HH11	1:C:214:ARG:HG3	1.82	0.44
1:D:254:ALA:HB1	1:D:287:VAL:HG22	2.00	0.44
1:D:335:ARG:HA	1:D:335:ARG:HD2	1.67	0.44
1:D:346:ASP:CG	1:D:348:VAL:HG13	2.38	0.44
1:A:248:HIS:HD2	2:G:16:KHB:O2	2.01	0.44
1:E:384:ARG:HA	1:E:387:VAL:HG12	2.00	0.44
1:B:258:VAL:HG23	1:D:301:ARG:HA	2.00	0.43
1:C:139:ARG:NH2	1:C:311:MET:HE1	2.32	0.43
1:D:325:GLU:CG	1:D:328:ALA:HB3	2.45	0.43
1:D:373:LEU:O	1:D:377:LEU:CD2	2.61	0.43
1:B:353:TRP:O	1:B:355:PRO:HD3	2.18	0.43
1:C:269:ARG:HA	1:C:269:ARG:HD2	1.61	0.43
1:D:190:LYS:HE3	1:D:277:VAL:HG23	1.99	0.43
1:D:316:LEU:HB3	1:D:318:LEU:CD1	2.49	0.43
1:B:208:VAL:HG13	1:B:383:MET:CE	2.48	0.43
1:E:257:THR:HG23	1:E:286:VAL:O	2.18	0.43
1:E:317:ILE:HD13	1:E:351:LEU:HD21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:GLU:O	1:C:181:GLU:HG3	2.17	0.43
1:D:380:THR:O	1:D:384:ARG:HD3	2.17	0.43
1:E:334:VAL:HB	1:E:338:VAL:CG2	2.49	0.43
1:C:214:ARG:NH1	1:C:214:ARG:HG3	2.32	0.43
1:D:314:LEU:HD21	1:D:316:LEU:HD21	2.00	0.43
1:A:177:GLU:HG2	2:G:18:HIS:HE1	1.83	0.43
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.91	0.43
1:D:133:ARG:HB2	1:D:133:ARG:NH1	2.33	0.43
1:E:233:LEU:HD23	1:E:233:LEU:HA	1.86	0.43
1:F:217:HIS:ND1	1:F:243:LYS:HD2	2.34	0.43
1:D:320:THR:CG2	1:D:322:LEU:H	2.23	0.43
1:D:222:LEU:O	1:D:243:LYS:HE3	2.19	0.43
1:D:234:GLU:HB2	1:D:244:LEU:HD21	2.00	0.43
1:C:370:VAL:O	1:C:374:VAL:HG13	2.19	0.43
1:D:179:ILE:HD11	1:D:192:PHE:HA	2.00	0.43
1:B:301:ARG:O	1:B:301:ARG:HG2	2.18	0.42
1:D:139:ARG:HD3	1:D:311:MET:O	2.19	0.42
1:D:177:GLU:O	1:D:181:GLU:HG3	2.18	0.42
1:E:300:GLN:O	1:E:303:LEU:HB2	2.18	0.42
1:A:219:LYS:HE3	1:A:379:TRP:CE2	2.54	0.42
1:C:323:GLU:HG2	1:C:324:VAL:HG23	2.00	0.42
1:C:347:LEU:HB2	1:C:363:LEU:HD11	2.01	0.42
1:D:292:VAL:HG11	1:D:298:LEU:HD23	2.02	0.42
1:A:186:PHE:CE2	1:C:300:GLN:HG3	2.54	0.42
1:A:280:CYS:HA	1:A:281:PRO:HD3	1.88	0.42
1:B:214:ARG:NH1	1:B:238:GLY:HA3	2.34	0.42
1:E:201:PRO:O	1:E:269:ARG:NH1	2.53	0.42
1:A:184:PHE:HE2	1:A:191:PRO:HG2	1.84	0.42
1:B:329:SER:HB3	2:H:12:LYS:HG3	2.00	0.42
1:D:309:PHE:CE2	1:D:330:LEU:HB3	2.49	0.42
1:E:188:ASN:ND2	1:E:191:PRO:HD3	2.34	0.42
1:B:340:ARG:NE	1:B:356:ARG:HD2	2.35	0.42
1:D:142:VAL:HG11	1:D:213:LEU:CD2	2.49	0.42
1:E:374:VAL:HG11	1:E:383:MET:HG3	2.02	0.42
1:F:344:ASN:O	1:F:363:LEU:HA	2.20	0.42
1:D:347:LEU:HD23	1:D:347:LEU:O	2.20	0.42
1:E:164:LEU:O	1:E:168:LEU:HG	2.19	0.42
1:A:317:ILE:HD13	1:A:351:LEU:HD11	2.02	0.42
1:B:353:TRP:HZ3	2:H:19:ARG:NH2	2.18	0.42
1:D:176:PRO:C	1:D:178:ALA:H	2.23	0.42
1:E:334:VAL:HG23	1:E:356:ARG:NH2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:ILE:O	1:F:318:LEU:HD23	2.20	0.42
1:B:246:GLU:OE2	4:B:501:HOH:O	2.22	0.41
1:D:234:GLU:H	1:D:234:GLU:CD	2.24	0.41
1:F:146:ALA:O	1:F:150:THR:HG23	2.20	0.41
1:B:261:ARG:CZ	1:B:282:VAL:HG11	2.50	0.41
1:B:346:ASP:HB2	1:B:348:VAL:CG1	2.47	0.41
1:D:132:ILE:CG1	1:D:377:LEU:HD11	2.50	0.41
1:D:258:VAL:O	1:E:301:ARG:NH1	2.49	0.41
1:D:381:GLU:HA	1:D:384:ARG:NH1	2.35	0.41
1:E:132:ILE:CD1	1:E:314:LEU:HD21	2.42	0.41
1:F:361:ALA:HB1	1:F:363:LEU:HD11	2.02	0.41
2:K:17:ARG:HB3	2:K:18:HIS:H	1.69	0.41
1:B:254:ALA:HB1	1:B:268:ILE:HD12	2.03	0.41
1:E:133:ARG:HD2	1:E:377:LEU:HA	2.02	0.41
1:A:145:GLY:HA3	1:A:320:THR:HB	2.02	0.41
1:B:350:PRO:HD3	2:H:19:ARG:NH1	2.32	0.41
1:C:214:ARG:HD2	1:C:214:ARG:O	2.20	0.41
1:E:197:LYS:HD3	1:E:197:LYS:C	2.41	0.41
1:F:214:ARG:HD3	1:F:237:SER:O	2.20	0.41
2:K:17:ARG:HB3	2:K:17:ARG:HE	1.41	0.41
1:A:150:THR:OG1	1:A:151:PRO:HD3	2.20	0.41
1:B:124:SER:O	1:B:127:ASP:HB2	2.20	0.41
1:B:370:VAL:O	1:B:374:VAL:HG23	2.20	0.41
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.85	0.41
1:F:340:ARG:NH2	1:F:356:ARG:HD2	2.36	0.41
1:B:254:ALA:HB2	1:B:268:ILE:HD12	2.03	0.41
1:D:196:ALA:HA	1:D:251:PHE:HE2	1.84	0.41
1:D:309:PHE:CE2	1:D:330:LEU:HD12	2.55	0.41
1:F:318:LEU:HD22	1:F:343:ILE:HB	2.02	0.41
1:A:338:VAL:HA	1:A:339:PRO:HD3	1.97	0.41
1:B:353:TRP:CZ3	2:H:19:ARG:NH2	2.89	0.41
1:D:233:LEU:HA	1:D:236:VAL:HG23	2.03	0.41
1:D:377:LEU:HD13	1:D:377:LEU:HA	1.87	0.41
1:D:386:LEU:O	1:D:389:ARG:HG2	2.21	0.41
1:E:160:PRO:HA	1:E:165:TYR:CG	2.55	0.41
1:B:226:TYR:CE1	1:B:309:PHE:HE1	2.39	0.40
1:B:339:PRO:HA	1:B:358:ARG:O	2.22	0.40
1:D:304:LEU:HD23	1:D:304:LEU:HA	1.83	0.40
1:D:365:ASP:OD1	1:D:367:VAL:HG12	2.20	0.40
1:E:214:ARG:HG2	1:E:386:LEU:HD21	2.03	0.40
1:B:375:GLU:HB2	1:B:380:THR:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:MET:HE2	1:D:383:MET:HB2	1.73	0.40
1:A:309:PHE:CE2	1:A:330:LEU:HB3	2.57	0.40
1:E:304:LEU:HD23	1:E:304:LEU:HA	1.96	0.40
1:E:390:GLU:HA	1:E:393:LYS:HB2	2.03	0.40
1:F:141:VAL:CG2	1:F:223:LEU:HD23	2.52	0.40
1:B:258:VAL:HG13	1:B:283:CYS:SG	2.62	0.40
1:C:126:GLN:HA	1:C:376:LEU:HD22	2.04	0.40
1:D:173:LEU:CD2	1:D:179:ILE:HB	2.48	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:C:258:VAL:O	1:F:301:ARG:NH2[5_444]	1.96	0.24

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	259/274 (94%)	246 (95%)	13 (5%)	0	100	100
1	B	254/274 (93%)	239 (94%)	15 (6%)	0	100	100
1	C	258/274 (94%)	241 (93%)	14 (5%)	3 (1%)	13	40
1	D	256/274 (93%)	232 (91%)	21 (8%)	3 (1%)	13	40
1	E	271/274 (99%)	256 (94%)	15 (6%)	0	100	100
1	F	205/274 (75%)	190 (93%)	14 (7%)	1 (0%)	29	61
2	G	8/11 (73%)	8 (100%)	0	0	100	100
2	H	6/11 (54%)	6 (100%)	0	0	100	100
2	I	4/11 (36%)	4 (100%)	0	0	100	100
2	J	2/11 (18%)	2 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	K	4/11 (36%)	2 (50%)	2 (50%)	0	100 100
2	L	2/11 (18%)	2 (100%)	0	0	100 100
All	All	1529/1710 (89%)	1428 (93%)	94 (6%)	7 (0%)	29 61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	172	ASP
1	C	174	PRO
1	D	177	GLU
1	D	322	LEU
1	C	199	LEU
1	F	268	ILE
1	C	172	ASP

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	229/237 (97%)	221 (96%)	8 (4%)	36 70
1	B	224/237 (94%)	220 (98%)	4 (2%)	59 85
1	C	228/237 (96%)	217 (95%)	11 (5%)	25 58
1	D	226/237 (95%)	218 (96%)	8 (4%)	36 70
1	E	237/237 (100%)	231 (98%)	6 (2%)	47 78
1	F	183/237 (77%)	173 (94%)	10 (6%)	21 53
2	G	6/6 (100%)	6 (100%)	0	100 100
2	H	4/6 (67%)	4 (100%)	0	100 100
2	I	3/6 (50%)	3 (100%)	0	100 100
2	J	2/6 (33%)	1 (50%)	1 (50%)	0 0
2	K	3/6 (50%)	3 (100%)	0	100 100
All	All	1345/1452 (93%)	1297 (96%)	48 (4%)	35 69

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	224	ARG
1	A	242	SER
1	A	248	HIS
1	A	253	SER
1	A	259	CYS
1	A	301	ARG
1	A	365	ASP
1	B	122	LYS
1	B	203	ASN
1	B	216	LEU
1	B	354	HIS
1	C	143	MET
1	C	172	ASP
1	C	205	LYS
1	C	214	ARG
1	C	215	LEU
1	C	216	LEU
1	C	283	CYS
1	C	301	ARG
1	C	323	GLU
1	C	376	LEU
1	C	384	ARG
1	D	131	LEU
1	D	224	ARG
1	D	259	CYS
1	D	269	ARG
1	D	335	ARG
1	D	372	SER
1	D	384	ARG
1	D	389	ARG
1	E	200	TYR
1	E	231	ASP
1	E	271	ASP
1	E	279	ARG
1	E	341	LEU
1	E	384	ARG
1	F	122	LYS
1	F	152	SER
1	F	192	PHE
1	F	200	TYR
1	F	205	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	242	SER
1	F	243	LYS
1	F	267	ASP
1	F	293	PHE
1	F	297	PRO
2	J	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	248	HIS
1	A	300	GLN
1	B	300	GLN
1	C	188	ASN
1	D	228	GLN
1	D	248	HIS
1	D	354	HIS
1	E	138	GLN
2	G	18	HIS
2	H	18	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	KHB	G	16	2	13,14,15	1.71	2 (15%)	10,16,18	1.00	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	KHB	L	16	2	3,4,15	1.04	0	2,4,18	0.91	0
2	KHB	K	16	2	13,14,15	1.77	1 (7%)	10,16,18	0.86	0
2	KHB	J	16	2	13,14,15	1.60	1 (7%)	10,16,18	1.56	2 (20%)
2	KHB	I	16	2	13,14,15	1.68	2 (15%)	10,16,18	1.57	4 (40%)
2	KHB	H	16	2	13,14,15	1.63	2 (15%)	10,16,18	1.46	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KHB	G	16	2	-	0/13/14/16	-
2	KHB	L	16	2	-	0/0/2/16	-
2	KHB	K	16	2	-	4/13/14/16	-
2	KHB	J	16	2	-	0/13/14/16	-
2	KHB	I	16	2	-	3/13/14/16	-
2	KHB	H	16	2	-	2/13/14/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	16	KHB	C1-NZ	5.54	1.46	1.33
2	I	16	KHB	C1-NZ	5.29	1.45	1.33
2	G	16	KHB	C1-NZ	5.13	1.45	1.33
2	J	16	KHB	C1-NZ	4.99	1.44	1.33
2	H	16	KHB	C1-NZ	4.52	1.43	1.33
2	H	16	KHB	CA-N	-2.65	1.40	1.48
2	I	16	KHB	CA-N	-2.27	1.41	1.48
2	G	16	KHB	CA-N	-2.16	1.41	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	16	KHB	C2-C1-NZ	3.12	120.29	115.97
2	J	16	KHB	CE-NZ-C1	-3.04	117.19	122.84
2	H	16	KHB	C2-C1-NZ	2.94	120.04	115.97
2	I	16	KHB	CE-NZ-C1	-2.56	118.09	122.84
2	I	16	KHB	O1-C1-C2	-2.36	118.04	121.50
2	I	16	KHB	C4-C3-C2	-2.21	107.30	111.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	16	KHB	C2-C1-NZ	2.21	119.03	115.97
2	H	16	KHB	O1-C1-NZ	-2.20	118.87	123.01
2	G	16	KHB	C2-C1-NZ	2.11	118.89	115.97

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	16	KHB	O-C-CA-CB
2	I	16	KHB	C1-C2-C3-C4
2	I	16	KHB	C1-C2-C3-O2
2	K	16	KHB	O-C-CA-CB
2	K	16	KHB	C1-C2-C3-C4
2	H	16	KHB	CG-CD-CE-NZ
2	K	16	KHB	C1-C2-C3-O2
2	H	16	KHB	N-CA-CB-CG
2	K	16	KHB	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	16	KHB	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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	263/274 (95%)	-0.24	5 (1%) 66 65	36, 52, 90, 109	0
1	B	258/274 (94%)	-0.16	5 (1%) 66 65	38, 56, 106, 121	0
1	C	262/274 (95%)	-0.08	4 (1%) 73 73	44, 61, 86, 129	0
1	D	260/274 (94%)	0.42	19 (7%) 15 11	51, 93, 136, 170	0
1	E	273/274 (99%)	-0.02	5 (1%) 68 67	51, 74, 116, 138	0
1	F	212/274 (77%)	0.05	6 (2%) 53 49	49, 71, 116, 131	0
2	G	10/11 (90%)	-0.20	0 100 100	41, 62, 83, 103	0
2	H	8/11 (72%)	-0.56	0 100 100	46, 51, 73, 80	0
2	I	6/11 (54%)	0.04	0 100 100	62, 69, 75, 85	0
2	J	4/11 (36%)	0.37	0 100 100	74, 77, 78, 85	0
2	K	6/11 (54%)	1.36	1 (16%) 1 1	102, 111, 128, 139	0
2	L	4/11 (36%)	-0.20	0 100 100	66, 84, 87, 92	0
All	All	1566/1710 (91%)	-0.01	45 (2%) 51 47	36, 67, 117, 170	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	351	LEU	7.9
1	D	350	PRO	5.1
1	F	295	GLY	4.7
1	E	196	ALA	4.4
1	D	128	VAL	4.2
1	F	194	THR	4.1
1	F	294	PHE	4.0
1	D	353	TRP	3.9
1	B	157	PHE	3.7
1	C	394	LEU	3.7
1	D	372	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	344	ASN	3.2
1	F	195	LEU	3.1
1	D	157	PHE	3.1
2	K	19	ARG	3.0
1	D	137	CYS	3.0
1	A	203	ASN	2.9
1	C	388	GLN	2.8
1	D	393	LYS	2.8
1	E	281	PRO	2.7
1	C	392	GLY	2.7
1	D	368	HIS	2.6
1	F	201	PRO	2.6
1	E	351	LEU	2.5
1	A	353	TRP	2.4
1	E	195	LEU	2.4
1	D	361	ALA	2.4
1	B	200	TYR	2.4
1	A	354	HIS	2.3
1	D	392	GLY	2.3
1	D	316	LEU	2.3
1	D	323	GLU	2.3
1	D	317	ILE	2.3
1	C	393	LYS	2.3
1	E	348	VAL	2.2
1	F	199	LEU	2.2
1	D	154	ILE	2.2
1	B	203	ASN	2.2
1	B	198	GLU	2.2
1	D	370	VAL	2.2
1	A	394	LEU	2.1
1	D	374	VAL	2.1
1	A	171	TYR	2.1
1	D	159	SER	2.1
1	B	202	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KHB	K	16	15/16	0.90	0.23	70,78,94,102	0
2	KHB	L	16	5/16	0.90	0.17	85,86,87,88	0
2	KHB	J	16	15/16	0.94	0.18	62,70,75,77	0
2	KHB	H	16	15/16	0.96	0.21	43,51,54,57	0
2	KHB	G	16	15/16	0.97	0.17	33,42,50,51	0
2	KHB	I	16	15/16	0.98	0.19	45,51,59,60	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	E	401	1/1	0.73	0.25	179,179,179,179	0
3	ZN	D	401	1/1	0.98	0.17	57,57,57,57	0
3	ZN	B	401	1/1	0.99	0.12	92,92,92,92	0
3	ZN	C	401	1/1	0.99	0.15	52,52,52,52	0
3	ZN	A	401	1/1	1.00	0.17	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.