



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:54 am BST

PDB ID : 4GSL
Title : Crystal structure of an Atg7-Atg3 crosslinked complex
Authors : Kaiser, S.E.; Mao, K.; Taherbhoy, A.M.; Yu, S.; Olszewski, J.L.; Duda, D.M.;
Kurinov, I.; Deng, A.; Fenn, T.D.; Klionsky, D.J.; Schulman, B.A.
Deposited on : 2012-08-27
Resolution : 2.70 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

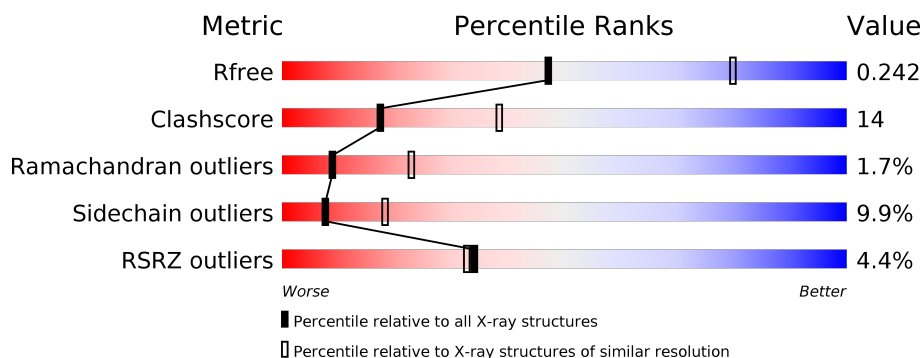
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	615	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>• •</div> </div> </div>
1	B	615	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• •</div> </div> </div>
2	C	312	<div> <div>6%</div> <div> <div></div> <div>34%</div> <div>21%</div> <div>• •</div> <div>40%</div> </div> </div>
2	D	312	<div> <div>6%</div> <div> <div></div> <div>34%</div> <div>21%</div> <div>•</div> <div>42%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12543 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 Ubiquitin-like modifier-activating enzyme ATG7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4767	3064	804	875	24			
1	B	592	Total	C	N	O	S	0	0	0
			4717	3031	795	867	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P38862
A	0	SER	-	EXPRESSION TAG	UNP P38862
B	-1	GLY	-	EXPRESSION TAG	UNP P38862
B	0	SER	-	EXPRESSION TAG	UNP P38862

- Molecule 2 is a protein called Autophagy-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	186	Total	C	N	O	S	0	0	0
			1534	993	246	288	7			
2	D	180	Total	C	N	O	S	0	0	0
			1480	958	239	277	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P40344
C	0	SER	-	EXPRESSION TAG	UNP P40344
C	41	ALA	CYS	ENGINEERED MUTATION	UNP P40344
C	76	ALA	CYS	ENGINEERED MUTATION	UNP P40344
C	83	ALA	CYS	ENGINEERED MUTATION	UNP P40344
D	-1	GLY	-	EXPRESSION TAG	UNP P40344
D	0	SER	-	EXPRESSION TAG	UNP P40344
D	41	ALA	CYS	ENGINEERED MUTATION	UNP P40344

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	76	ALA	CYS	ENGINEERED MUTATION	UNP P40344
D	83	ALA	CYS	ENGINEERED MUTATION	UNP P40344

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

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

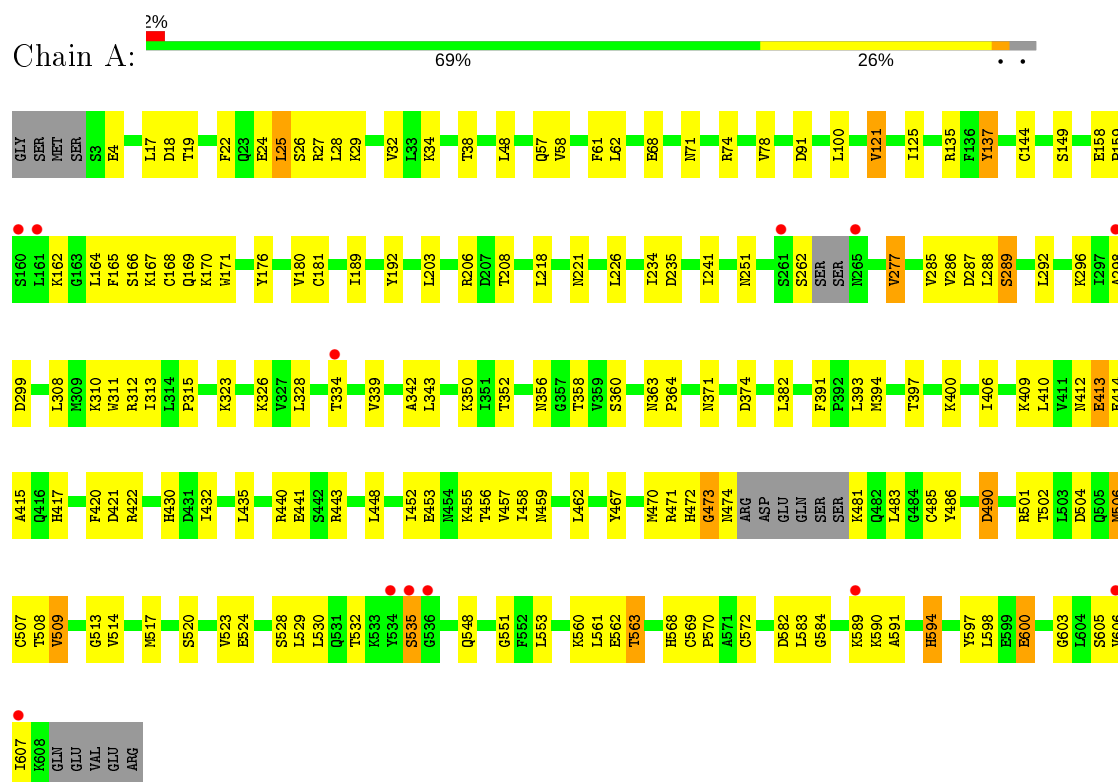
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total 19	O 19	0	0
4	B	19	Total 19	O 19	0	0
4	C	5	Total 5	O 5	0	0

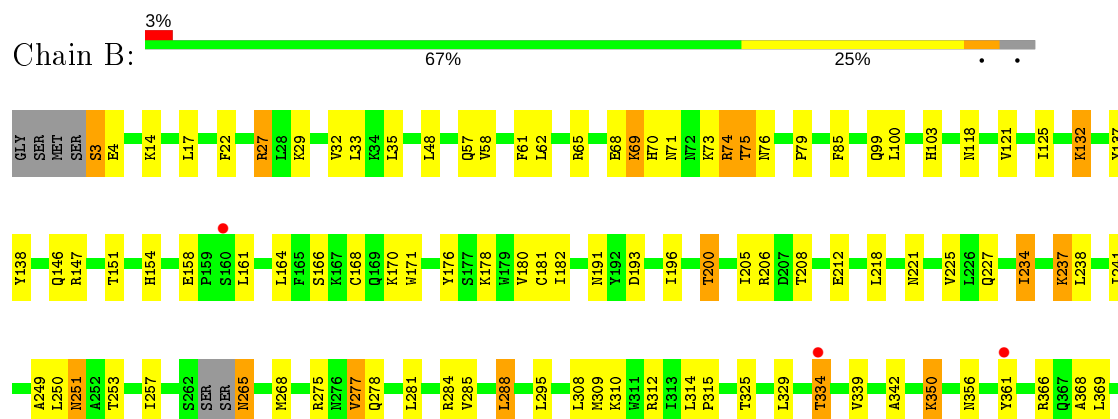
3 Residue-property plots [i](#)

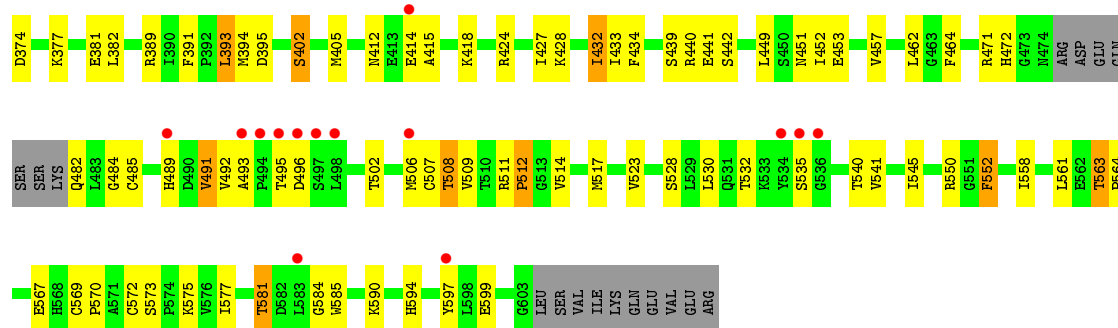
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Ubiquitin-like modifier-activating enzyme ATG7

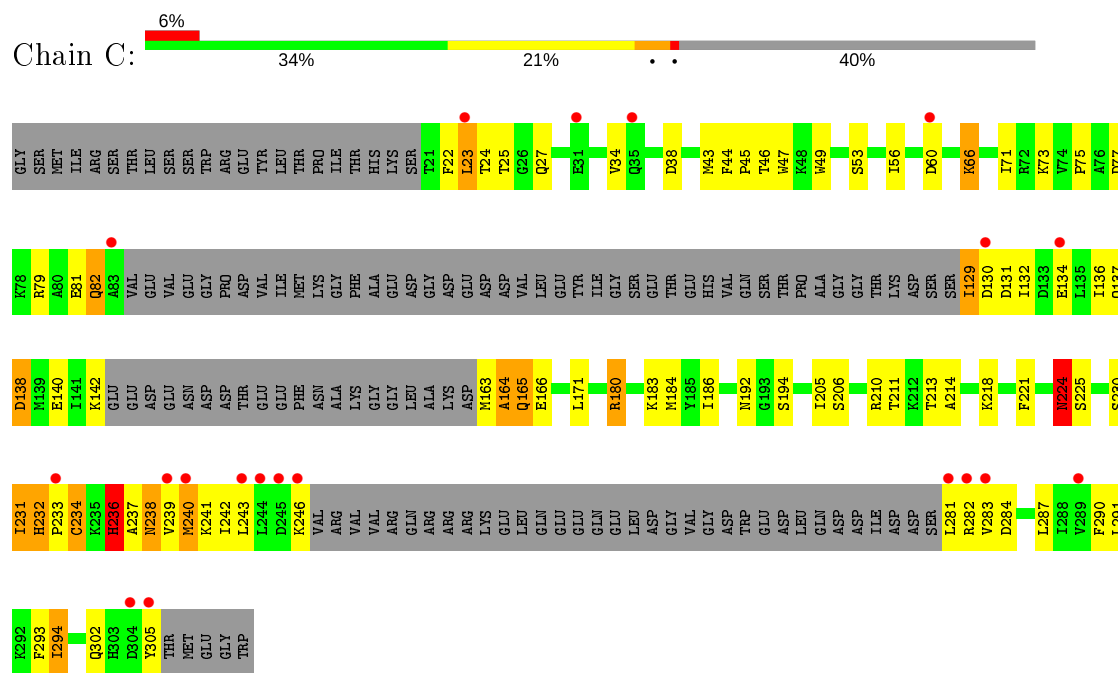


• Molecule 1: Ubiquitin-like modifier-activating enzyme ATG7

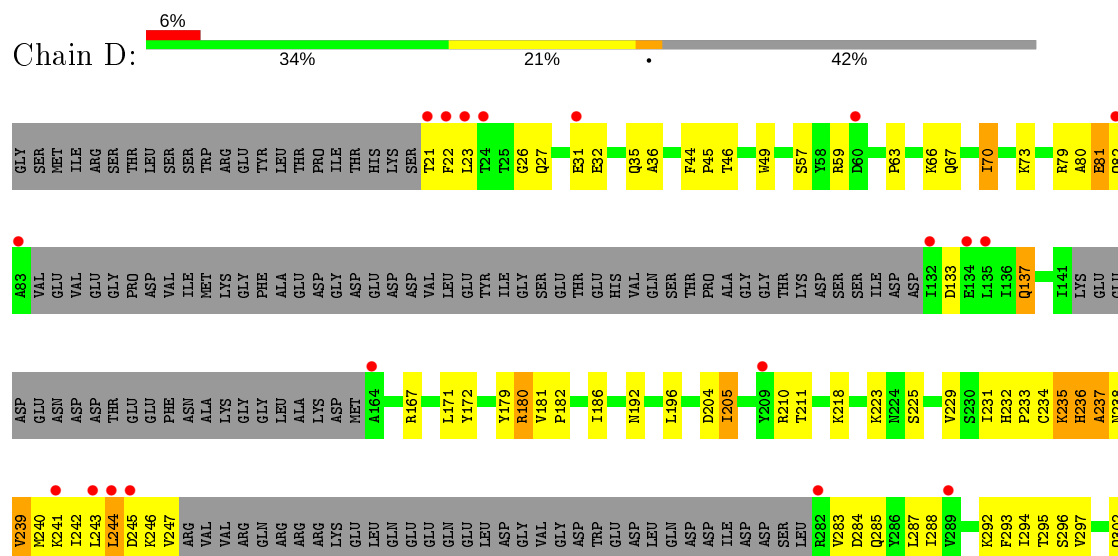




• Molecule 2: Autophagy-related protein 3



• Molecule 2: Autophagy-related protein 3



H3O3
DG04
TYR
THR
MET
GLU
GLY
TRP

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	281.56Å 125.08Å 71.08Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	37.07 – 2.70 37.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.07-2.70) 94.7 (37.35-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.193 , 0.246 0.184 , 0.242	Depositor DCC
R_{free} test set	1904 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12543	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/4869	0.61	0/6598
1	B	0.47	0/4819	0.60	0/6532
2	C	0.38	0/1570	0.63	0/2123
2	D	0.34	0/1515	0.55	0/2050
All	All	0.44	0/12773	0.60	0/17303

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
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	165	GLN	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	4767	0	4833	116	0
1	B	4717	0	4766	126	0
2	C	1534	0	1514	64	0
2	D	1480	0	1462	54	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	19	0	0	0	0
4	B	19	0	0	1	0
4	C	5	0	0	1	0
All	All	12543	0	12575	345	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 14.

All (345) 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)
2:C:237:ALA:HB2	2:C:240:MET:HB3	1.40	1.02
2:D:218:LYS:HG3	2:D:225:SER:HB3	1.43	1.01
1:B:502:THR:HB	1:B:508:THR:HG21	1.49	0.94
1:B:427:ILE:HG23	1:B:433:ILE:HD11	1.51	0.91
1:A:287:ASP:OD1	1:A:289:SER:OG	1.88	0.90
2:D:63:PRO:HG2	2:D:66:LYS:HB2	1.54	0.90
2:C:233:PRO:HA	2:C:234:CYS:O	1.72	0.89
1:A:413:GLU:HG3	1:A:414:GLU:N	1.92	0.83
1:B:491:VAL:O	1:B:550:ARG:NH1	2.11	0.83
1:B:414:GLU:HG3	1:B:418:LYS:HZ1	1.44	0.83
2:D:244:LEU:O	2:D:246:LYS:N	2.14	0.80
1:B:342:ALA:HB3	1:B:523:VAL:HG21	1.62	0.80
1:B:462:LEU:HD22	1:B:514:VAL:HG12	1.64	0.78
1:B:308:LEU:HD13	1:B:312:ARG:CZ	2.14	0.78
2:C:236:HIS:HA	2:C:239:VAL:HG22	1.65	0.77
2:D:243:LEU:O	2:D:246:LYS:HG2	1.84	0.77
2:D:179:TYR:O	2:D:181:VAL:N	2.18	0.77
2:C:205:ILE:O	2:C:210:ARG:NH1	2.17	0.77
2:C:231:ILE:HA	2:C:232:HIS:HB2	1.67	0.76
1:B:567:GLU:O	1:B:573:SER:HB2	1.87	0.75
2:C:282:ARG:HH11	2:C:282:ARG:HB2	1.52	0.75
2:D:22:PHE:O	2:D:26:GLY:N	2.17	0.74
2:D:237:ALA:HA	2:D:238:ASN:C	2.08	0.74
1:A:121:VAL:HG22	1:A:218:LEU:HD22	1.70	0.73
1:B:237:LYS:NZ	1:B:251:ASN:OD1	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:ASP:N	2:C:138:ASP:OD1	2.20	0.72
2:D:81:GLU:OE1	2:D:210:ARG:NH2	2.23	0.71
2:D:218:LYS:CG	2:D:225:SER:HB3	2.20	0.70
1:A:374:ASP:HB3	1:A:382:LEU:HD21	1.74	0.70
1:A:435:LEU:HD22	1:A:459:ASN:HD21	1.57	0.69
1:A:603:GLY:O	1:A:606:VAL:HG22	1.92	0.68
1:B:427:ILE:HG23	1:B:433:ILE:CD1	2.23	0.68
2:C:71:ILE:HG22	2:C:171:LEU:HB2	1.75	0.68
1:B:70:HIS:HE1	1:B:79:PRO:HB3	1.58	0.68
2:C:231:ILE:HA	2:C:232:HIS:CB	2.24	0.68
1:B:451:ASN:ND2	1:B:572:CYS:HB3	2.09	0.68
1:B:161:LEU:HD11	1:B:237:LYS:HG2	1.75	0.68
1:A:356:ASN:O	1:A:400:LYS:NZ	2.25	0.67
1:B:3:SER:CB	1:B:4:GLU:HA	2.26	0.66
1:A:462:LEU:HD22	1:A:514:VAL:HG12	1.77	0.65
2:C:282:ARG:NH1	2:C:282:ARG:HB2	2.12	0.65
2:D:240:MET:O	2:D:244:LEU:HB2	1.95	0.65
1:A:17:LEU:HD23	1:A:22:PHE:CZ	2.32	0.65
1:B:350:LYS:HD2	1:B:395:ASP:OD2	1.96	0.65
1:B:158:GLU:HG2	1:B:161:LEU:HD12	1.77	0.65
1:B:3:SER:HB2	1:B:4:GLU:HA	1.78	0.64
1:A:430:HIS:O	1:A:455:LYS:NZ	2.18	0.64
1:B:308:LEU:HD13	1:B:312:ARG:NH2	2.13	0.63
1:A:470:MET:HB2	1:A:548:GLN:HG2	1.81	0.63
1:A:158:GLU:OE2	1:A:251:ASN:ND2	2.31	0.63
1:A:159:PRO:O	1:A:162:LYS:HE2	1.98	0.63
1:B:310:LYS:O	1:B:315:PRO:HA	1.99	0.63
1:A:360:SER:H	1:A:363:ASN:ND2	1.96	0.62
1:B:277:VAL:HG22	2:C:192:ASN:OD1	1.99	0.62
2:D:59:ARG:H	2:D:67:GLN:HE22	1.47	0.62
1:A:159:PRO:HA	1:A:162:LYS:HE2	1.82	0.62
1:B:3:SER:HB2	1:B:4:GLU:CA	2.29	0.62
1:B:65:ARG:HG2	1:B:71:ASN:HD22	1.65	0.62
1:B:374:ASP:HB3	1:B:382:LEU:HD21	1.80	0.62
2:C:291:LEU:HD13	2:C:305:TYR:HB2	1.81	0.62
1:B:147:ARG:HE	1:B:268:MET:CE	2.13	0.61
2:C:130:ASP:HA	2:C:132:ILE:H	1.64	0.61
1:B:374:ASP:HA	1:B:377:LYS:HE3	1.83	0.61
1:A:17:LEU:HD11	1:A:62:LEU:HD12	1.83	0.60
1:A:391:PHE:HD2	1:A:394:MET:HE2	1.64	0.60
1:B:137:TYR:CD2	1:B:285:VAL:HG22	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PRO:O	1:A:162:LYS:HG2	2.01	0.60
1:B:439:SER:HB3	1:B:506:MET:HB2	1.83	0.60
1:B:285:VAL:HG23	2:C:136:ILE:HD11	1.83	0.60
1:B:325:THR:HG21	1:B:432:ILE:HG13	1.84	0.60
2:D:242:ILE:O	2:D:246:LYS:NZ	2.34	0.60
2:C:290:PHE:CE2	2:C:294:ILE:HD11	2.37	0.60
1:A:371:ASN:HB3	1:B:389:ARG:O	2.03	0.59
1:A:583:LEU:N	1:A:583:LEU:HD12	2.16	0.59
2:C:47:TRP:HE1	2:C:305:TYR:HB3	1.67	0.59
2:D:205:ILE:HD11	2:D:229:VAL:HG11	1.83	0.59
1:B:472:HIS:CE1	1:B:485:CYS:HB2	2.38	0.59
2:C:282:ARG:HH12	2:C:284:ASP:HB2	1.68	0.59
2:C:183:LYS:HG3	2:C:233:PRO:HD3	1.86	0.58
2:C:184:MET:SD	2:C:294:ILE:HD13	2.43	0.58
1:B:414:GLU:CG	1:B:418:LYS:HZ1	2.15	0.58
2:C:73:LYS:N	2:C:73:LYS:HD2	2.18	0.58
1:A:470:MET:CB	1:A:548:GLN:HG2	2.34	0.58
1:B:428:LYS:HG3	1:B:453:GLU:OE1	2.04	0.57
2:C:230:SER:C	2:C:231:ILE:HG12	2.25	0.57
1:A:502:THR:HB	1:A:508:THR:HG21	1.86	0.57
1:B:414:GLU:HG3	1:B:418:LYS:NZ	2.15	0.57
1:B:147:ARG:HE	1:B:268:MET:HE2	1.68	0.57
1:A:432:ILE:HD11	1:A:530:LEU:HD21	1.85	0.57
1:A:298:ALA:HA	1:B:361:TYR:HB3	1.86	0.57
2:C:282:ARG:NH1	2:C:284:ASP:OD2	2.37	0.57
1:A:582:ASP:HB2	1:A:583:LEU:HD12	1.86	0.57
1:A:78:VAL:HG13	1:A:176:TYR:O	2.04	0.57
2:C:38:ASP:OD2	2:C:66:LYS:NZ	2.38	0.57
2:D:180:ARG:H	2:D:180:ARG:HD3	1.70	0.56
1:A:17:LEU:HB3	1:A:22:PHE:CE2	2.40	0.56
1:B:118:ASN:ND2	1:B:178:LYS:HD2	2.21	0.56
2:D:73:LYS:N	2:D:73:LYS:HD2	2.20	0.56
1:A:435:LEU:HD13	1:A:457:VAL:HG13	1.87	0.56
2:C:233:PRO:HA	2:C:234:CYS:C	2.25	0.56
2:C:239:VAL:HA	2:C:242:ILE:HD12	1.88	0.56
1:B:161:LEU:CD1	1:B:237:LYS:HG2	2.36	0.56
2:D:133:ASP:O	2:D:137:GLN:NE2	2.39	0.56
2:C:130:ASP:CA	2:C:131:ASP:HB2	2.36	0.56
1:B:356:ASN:ND2	1:B:402:SER:HB2	2.21	0.55
1:A:137:TYR:CD2	1:A:285:VAL:HG22	2.41	0.55
1:B:329:LEU:HD23	1:B:434:PHE:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:LEU:HD23	2:C:23:LEU:H	1.71	0.55
2:D:234:CYS:O	2:D:235:LYS:HB2	2.06	0.55
1:B:594:HIS:O	1:B:597:TYR:HB3	2.06	0.55
1:B:552:PHE:CD1	1:B:552:PHE:N	2.75	0.55
2:D:235:LYS:O	2:D:237:ALA:N	2.38	0.55
1:A:472:HIS:CE1	1:A:485:CYS:HB2	2.41	0.55
2:D:218:LYS:HE3	2:D:225:SER:HB3	1.88	0.55
1:A:470:MET:HG3	1:A:470:MET:O	2.07	0.55
1:B:451:ASN:HD22	1:B:572:CYS:HB3	1.71	0.54
2:C:24:THR:O	2:C:241:LYS:NZ	2.28	0.54
1:A:326:LYS:HG2	1:A:350:LYS:HD2	1.89	0.54
2:C:129:ILE:N	2:C:131:ASP:OD2	2.40	0.54
1:B:158:GLU:CG	1:B:161:LEU:HD12	2.37	0.54
1:B:14:LYS:HB2	1:B:57:GLN:HE21	1.72	0.54
2:D:239:VAL:HG11	2:D:293:PHE:CD1	2.43	0.54
1:A:462:LEU:HD22	1:A:514:VAL:CG1	2.37	0.53
1:A:443:ARG:HD3	1:A:459:ASN:OD1	2.08	0.53
2:C:237:ALA:CB	2:C:240:MET:HB3	2.28	0.53
2:D:44:PHE:C	2:D:46:THR:H	2.12	0.53
2:D:36:ALA:HA	2:D:284:ASP:O	2.08	0.53
2:D:32:GLU:O	2:D:35:GLN:HB2	2.09	0.53
1:A:420:PHE:HD2	1:A:421:ASP:N	2.07	0.53
1:B:295:LEU:HD21	1:B:393:LEU:HD13	1.90	0.53
1:B:457:VAL:O	1:B:471:ARG:HA	2.09	0.53
2:C:43:MET:O	2:C:45:PRO:HD3	2.08	0.53
2:D:181:VAL:HB	2:D:182:PRO:HD2	1.90	0.53
1:A:435:LEU:HD22	1:A:459:ASN:ND2	2.23	0.53
2:D:59:ARG:H	2:D:67:GLN:NE2	2.07	0.53
1:A:311:TRP:HB3	2:D:211:THR:HB	1.90	0.53
1:A:443:ARG:NH1	1:A:459:ASN:OD1	2.41	0.52
1:B:312:ARG:HG3	2:C:211:THR:O	2.09	0.52
2:C:237:ALA:H	2:C:239:VAL:N	2.07	0.52
2:D:235:LYS:C	2:D:237:ALA:H	2.12	0.52
1:B:178:LYS:HE3	1:B:191:ASN:OD1	2.09	0.52
2:C:130:ASP:HA	2:C:131:ASP:HB2	1.90	0.52
1:B:492:VAL:HG23	1:B:493:ALA:O	2.09	0.52
1:A:62:LEU:HD11	1:A:125:ILE:HD11	1.91	0.52
1:B:484:GLY:HA3	1:B:563:THR:HG22	1.91	0.52
1:A:410:LEU:HD11	1:A:589:LYS:HG3	1.91	0.52
1:A:308:LEU:O	1:A:312:ARG:HB2	2.10	0.52
1:B:29:LYS:NZ	4:B:804:HOH:O	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ASN:ND2	1:A:415:ALA:HB3	2.25	0.51
1:A:342:ALA:HB3	1:A:523:VAL:HG21	1.91	0.51
2:C:237:ALA:HA	2:C:238:ASN:C	2.30	0.51
1:B:545:ILE:HG13	1:B:545:ILE:O	2.11	0.51
2:C:71:ILE:CG2	2:C:171:LEU:HB2	2.39	0.51
2:C:243:LEU:HA	2:C:246:LYS:HD2	1.93	0.51
2:D:171:LEU:HD22	2:D:186:ILE:HG22	1.92	0.51
2:D:218:LYS:HG3	2:D:225:SER:CB	2.29	0.51
1:B:334:THR:HG23	1:B:366:ARG:O	2.10	0.51
1:A:144:CYS:HA	1:A:221:ASN:OD1	2.11	0.51
1:A:277:VAL:HG22	2:D:192:ASN:OD1	2.11	0.50
1:B:441:GLU:H	1:B:441:GLU:CD	2.14	0.50
1:A:594:HIS:O	1:A:597:TYR:HB3	2.11	0.50
1:B:472:HIS:ND1	1:B:485:CYS:HB2	2.25	0.50
1:A:26:SER:O	1:A:28:LEU:N	2.44	0.50
1:A:591:ALA:HB1	1:A:598:LEU:HD22	1.93	0.50
1:B:314:LEU:HD22	1:B:541:VAL:HG22	1.94	0.50
2:D:70:ILE:HD13	2:D:172:TYR:CE2	2.47	0.50
2:D:44:PHE:O	2:D:46:THR:N	2.45	0.49
1:A:360:SER:H	1:A:363:ASN:HD22	1.59	0.49
1:A:568:HIS:HE1	1:A:607:ILE:HD11	1.74	0.49
1:A:483:LEU:O	1:A:563:THR:O	2.30	0.49
1:A:18:ASP:HB2	1:A:61:PHE:CE1	2.48	0.49
1:B:221:ASN:O	1:B:225:VAL:HG23	2.12	0.49
1:B:168:CYS:HB3	1:B:241:ILE:HG13	1.95	0.49
1:B:17:LEU:HD13	1:B:138:TYR:CE2	2.47	0.49
2:C:22:PHE:CD1	2:C:283:VAL:HG23	2.47	0.49
1:B:99:GLN:O	1:B:103:HIS:CD2	2.65	0.49
2:D:167:ARG:HD3	2:D:196:LEU:HD11	1.94	0.49
2:D:233:PRO:O	2:D:236:HIS:HB2	2.11	0.49
1:A:165:PHE:O	1:A:169:GLN:HG3	2.12	0.49
2:D:27:GLN:HB3	2:D:180:ARG:O	2.13	0.49
2:D:237:ALA:HB2	2:D:240:MET:HB2	1.94	0.49
2:D:231:ILE:HD13	2:D:297:VAL:HG11	1.95	0.49
1:B:489:HIS:CE1	1:B:563:THR:HG23	2.48	0.48
1:A:48:LEU:HD23	1:A:58:VAL:HG22	1.94	0.48
1:A:420:PHE:CD2	1:A:421:ASP:N	2.81	0.48
1:B:265:ASN:ND2	1:B:265:ASN:O	2.40	0.48
2:C:34:VAL:HG13	2:C:66:LYS:HG2	1.96	0.48
1:B:424:ARG:HB2	1:B:449:LEU:HD13	1.95	0.48
1:A:22:PHE:CD2	1:A:288:LEU:HD11	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG23	1:B:208:THR:HB	1.96	0.48
2:C:180:ARG:N	2:C:180:ARG:HD2	2.29	0.48
1:B:405:MET:HB3	1:B:441:GLU:HB2	1.96	0.48
1:B:278:GLN:N	1:B:278:GLN:OE1	2.47	0.48
1:A:600:GLU:HA	1:A:605:SER:OG	2.14	0.47
1:A:298:ALA:HB2	1:B:361:TYR:HD1	1.79	0.47
2:C:134:GLU:O	2:C:138:ASP:OD1	2.32	0.47
2:D:295:THR:HG21	2:D:303:HIS:CD2	2.49	0.47
1:A:506:MET:O	1:A:507:CYS:HB2	2.15	0.47
1:B:168:CYS:CB	1:B:241:ILE:HG13	2.45	0.47
1:B:489:HIS:ND1	1:B:563:THR:HG23	2.30	0.47
1:A:514:VAL:HG23	1:A:553:LEU:HD22	1.96	0.47
1:B:99:GLN:O	1:B:103:HIS:HD2	1.96	0.47
1:A:374:ASP:HB3	1:A:382:LEU:CD2	2.44	0.47
1:A:443:ARG:HD2	1:A:486:TYR:CE1	2.50	0.47
1:B:48:LEU:CD1	1:B:206:ARG:HD3	2.44	0.47
1:A:594:HIS:CD2	1:A:594:HIS:N	2.82	0.47
1:A:310:LYS:O	1:A:315:PRO:HA	2.15	0.46
1:B:374:ASP:HB3	1:B:382:LEU:CD2	2.44	0.46
1:B:61:PHE:CE1	2:C:73:LYS:NZ	2.75	0.46
1:A:374:ASP:CB	1:A:382:LEU:HD21	2.45	0.46
2:D:180:ARG:N	2:D:180:ARG:HD3	2.30	0.46
1:A:137:TYR:N	1:A:137:TYR:CD1	2.84	0.46
1:A:180:VAL:HG12	1:A:192:TYR:HB2	1.97	0.46
2:D:246:LYS:HA	2:D:246:LYS:HD3	1.54	0.46
2:D:49:TRP:CE3	2:D:66:LYS:HA	2.50	0.46
1:B:22:PHE:CD2	1:B:288:LEU:HD21	2.51	0.46
2:C:293:PHE:CD2	2:C:294:ILE:N	2.84	0.46
1:B:329:LEU:HD21	1:B:339:VAL:HG11	1.97	0.46
1:B:356:ASN:HB2	1:B:402:SER:HA	1.98	0.46
1:B:374:ASP:CB	1:B:382:LEU:HD21	2.44	0.46
1:B:569:CYS:O	1:B:573:SER:HB3	2.16	0.46
1:A:32:VAL:HG12	1:A:32:VAL:O	2.14	0.45
1:A:26:SER:O	1:A:29:LYS:N	2.42	0.45
1:B:27:ARG:HB3	1:B:27:ARG:CZ	2.45	0.45
2:C:27:GLN:HB3	2:C:180:ARG:CB	2.46	0.45
2:C:44:PHE:C	2:C:46:THR:H	2.20	0.45
1:B:285:VAL:CG2	2:C:136:ILE:HD11	2.45	0.45
1:A:502:THR:HB	1:A:508:THR:CG2	2.46	0.45
2:D:294:ILE:O	2:D:297:VAL:N	2.42	0.45
2:C:129:ILE:O	2:C:130:ASP:OD1	2.33	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:GLY:O	1:A:517:MET:HG3	2.16	0.45
1:B:412:ASN:HB3	1:B:415:ALA:HB3	1.98	0.45
1:A:167:LYS:HB3	1:A:189:ILE:HD12	1.99	0.45
2:C:56:ILE:HG23	2:C:221:PHE:O	2.17	0.45
1:A:394:MET:HE2	1:A:394:MET:HB2	1.87	0.45
1:A:412:ASN:ND2	1:A:415:ALA:CB	2.80	0.45
1:A:298:ALA:HB2	1:B:361:TYR:CD1	2.52	0.45
2:C:56:ILE:HA	2:C:221:PHE:O	2.16	0.45
2:D:287:LEU:HD23	2:D:287:LEU:HA	1.70	0.45
1:A:24:GLU:HG3	1:A:24:GLU:O	2.17	0.44
1:A:422:ARG:HA	1:A:422:ARG:HD2	1.87	0.44
1:B:234:ILE:O	1:B:253:THR:HA	2.17	0.44
2:D:288:ILE:N	2:D:288:ILE:HD12	2.32	0.44
2:C:49:TRP:CE3	2:C:66:LYS:HA	2.52	0.44
1:B:171:TRP:CZ3	1:B:181:CYS:HB3	2.53	0.44
2:C:214:ALA:HA	2:C:231:ILE:HD13	1.99	0.44
1:A:481:LYS:HE2	1:A:481:LYS:HB3	1.83	0.44
1:B:132:LYS:H	1:B:132:LYS:CD	2.31	0.44
1:B:308:LEU:O	1:B:312:ARG:HB2	2.18	0.44
1:B:325:THR:CG2	1:B:432:ILE:HG13	2.46	0.44
1:A:457:VAL:O	1:A:471:ARG:HA	2.17	0.44
1:A:569:CYS:HA	1:A:570:PRO:HD3	1.75	0.44
1:B:577:ILE:O	1:B:581:THR:HG23	2.18	0.44
1:A:520:SER:O	1:A:524:GLU:HG2	2.17	0.44
1:A:517:MET:SD	1:A:553:LEU:HD11	2.57	0.44
1:B:528:SER:O	1:B:540:THR:HG21	2.18	0.44
1:A:48:LEU:HD23	1:A:58:VAL:CG2	2.48	0.44
1:B:132:LYS:HE2	1:B:132:LYS:HB2	1.74	0.44
1:B:366:ARG:HH22	1:B:512:PRO:HD3	1.83	0.44
1:B:277:VAL:HG22	2:C:192:ASN:CG	2.37	0.44
2:C:232:HIS:O	2:C:234:CYS:HB2	2.18	0.44
1:A:203:LEU:HD22	1:A:226:LEU:HD22	1.99	0.44
1:A:509:VAL:HB	1:B:309:MET:HG3	2.00	0.44
1:B:275:ARG:HG2	1:B:281:LEU:HD23	1.99	0.44
2:D:80:ALA:HB2	2:D:204:ASP:HA	2.00	0.44
1:B:121:VAL:HG22	1:B:218:LEU:HD22	2.01	0.43
2:C:224:ASN:ND2	4:C:403:HOH:O	2.50	0.43
1:A:168:CYS:HB3	1:A:241:ILE:HG13	1.98	0.43
1:A:286:VAL:HG12	1:A:288:LEU:HG	2.01	0.43
1:B:374:ASP:CG	1:B:382:LEU:HD21	2.39	0.43
1:B:511:ARG:HA	1:B:512:PRO:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LEU:O	1:A:452:ILE:HG12	2.18	0.43
1:B:151:THR:HG21	1:B:227:GLN:OE1	2.18	0.43
1:B:74:ARG:HE	1:B:74:ARG:HB2	1.31	0.43
2:D:241:LYS:HG3	2:D:241:LYS:O	2.19	0.43
2:D:22:PHE:CE1	2:D:283:VAL:HB	2.53	0.43
1:A:17:LEU:CD2	1:A:22:PHE:CZ	3.01	0.43
1:A:363:ASN:HB2	1:A:364:PRO:HD3	2.01	0.43
1:B:58:VAL:HG23	1:B:208:THR:O	2.18	0.43
2:C:75:PRO:HG2	2:C:302:GLN:OE1	2.18	0.43
1:A:58:VAL:HG23	1:A:208:THR:O	2.19	0.43
1:B:62:LEU:HD11	1:B:125:ILE:HD11	2.01	0.43
1:A:313:ILE:HD13	1:B:464:PHE:CD1	2.54	0.43
1:A:58:VAL:HG23	1:A:208:THR:HB	2.00	0.43
1:B:257:ILE:O	1:B:257:ILE:HG22	2.18	0.43
2:C:27:GLN:HB3	2:C:180:ARG:HB3	2.00	0.43
1:A:19:THR:CG2	1:A:292:LEU:HD21	2.49	0.43
1:A:313:ILE:O	1:A:315:PRO:HD3	2.19	0.43
1:B:17:LEU:HD22	1:B:22:PHE:CZ	2.54	0.42
2:C:237:ALA:CA	2:C:238:ASN:C	2.87	0.42
2:D:232:HIS:HA	2:D:233:PRO:HD3	1.93	0.42
1:A:590:LYS:HE3	1:A:590:LYS:HB2	1.74	0.42
1:B:482:GLN:HA	1:B:482:GLN:OE1	2.19	0.42
1:B:511:ARG:O	1:B:514:VAL:HG23	2.19	0.42
1:B:75:THR:O	1:B:76:ASN:HB2	2.19	0.42
2:D:179:TYR:O	2:D:181:VAL:HG22	2.19	0.42
1:A:159:PRO:CA	1:A:162:LYS:HE2	2.48	0.42
1:A:420:PHE:C	1:A:420:PHE:CD2	2.93	0.42
1:B:391:PHE:HD2	1:B:394:MET:CE	2.32	0.42
1:A:441:GLU:CD	1:A:441:GLU:H	2.23	0.42
1:A:74:ARG:NH1	2:D:49:TRP:O	2.53	0.42
1:B:284:ARG:NH1	1:B:284:ARG:HG3	2.35	0.42
1:A:453:GLU:O	1:A:455:LYS:HG2	2.19	0.42
1:B:391:PHE:HB3	1:B:394:MET:CE	2.49	0.42
1:B:489:HIS:HE1	1:B:564:PRO:O	2.02	0.42
1:B:73:LYS:HE3	1:B:176:TYR:CD1	2.54	0.42
2:D:244:LEU:HD12	2:D:244:LEU:HA	1.92	0.42
1:B:369:LEU:HA	1:B:369:LEU:HD23	1.92	0.42
1:A:339:VAL:O	1:A:343:LEU:HG	2.20	0.42
1:B:3:SER:CB	1:B:4:GLU:CA	2.94	0.42
1:B:65:ARG:HG2	1:B:71:ASN:ND2	2.34	0.42
2:C:230:SER:O	2:C:231:ILE:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:THR:OG1	2:D:22:PHE:N	2.52	0.42
1:A:171:TRP:CZ3	1:A:181:CYS:HB3	2.55	0.42
1:A:467:TYR:CE2	1:A:551:GLY:HA3	2.55	0.42
1:B:249:ALA:O	1:B:250:LEU:HD23	2.19	0.42
1:B:205:ILE:HD12	1:B:238:LEU:HD11	2.02	0.41
1:A:17:LEU:HB3	1:A:22:PHE:CZ	2.55	0.41
1:A:171:TRP:CG	1:A:189:ILE:HG21	2.55	0.41
1:A:472:HIS:NE2	1:A:485:CYS:HB2	2.35	0.41
2:C:238:ASN:HB3	2:C:239:VAL:H	1.55	0.41
1:B:418:LYS:HZ2	1:B:418:LYS:HG3	1.71	0.41
2:C:287:LEU:HD23	2:C:287:LEU:HA	1.92	0.41
2:C:49:TRP:CD2	2:C:66:LYS:HG3	2.55	0.41
2:D:44:PHE:C	2:D:46:THR:N	2.72	0.41
1:A:25:LEU:HA	1:A:25:LEU:HD12	1.92	0.41
1:A:48:LEU:HD13	1:A:206:ARG:HD3	2.03	0.41
2:C:164:ALA:HA	2:C:165:GLN:HA	1.60	0.41
1:A:48:LEU:CD1	1:A:206:ARG:HD3	2.51	0.41
1:B:569:CYS:HA	1:B:570:PRO:HD3	1.88	0.41
1:A:328:LEU:HD12	1:A:352:THR:O	2.20	0.41
1:B:182:ILE:HD13	1:B:193:ASP:H	1.85	0.41
1:B:69:LYS:HB3	1:B:70:HIS:H	1.67	0.41
2:D:234:CYS:O	2:D:235:LYS:CB	2.66	0.41
1:A:583:LEU:N	1:A:583:LEU:CD1	2.83	0.40
1:B:85:PHE:N	1:B:85:PHE:CD1	2.89	0.40
2:C:137:GLN:O	2:C:140:GLU:HB3	2.21	0.40
1:A:583:LEU:H	1:A:583:LEU:HD12	1.86	0.40
1:A:568:HIS:CE1	1:A:607:ILE:HD11	2.55	0.40
1:B:132:LYS:CE	1:B:132:LYS:H	2.34	0.40
1:B:530:LEU:HA	1:B:530:LEU:HD23	1.94	0.40
1:A:473:GLY:O	1:A:474:ASN:HB2	2.21	0.40
1:A:529:LEU:HA	1:A:529:LEU:HD12	1.86	0.40
1:B:196:ILE:HG22	1:B:200:THR:OG1	2.21	0.40
2:C:163:MET:O	2:C:164:ALA:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	592/615 (96%)	551 (93%)	36 (6%)	5 (1%)	19	43
1	B	586/615 (95%)	559 (95%)	23 (4%)	4 (1%)	22	46
2	C	178/312 (57%)	157 (88%)	13 (7%)	8 (4%)	2	5
2	D	172/312 (55%)	156 (91%)	7 (4%)	9 (5%)	2	3
All	All	1528/1854 (82%)	1423 (93%)	79 (5%)	26 (2%)	9	23

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	232	HIS
2	D	180	ARG
2	D	245	ASP
1	A	27	ARG
1	A	473	GLY
1	B	584	GLY
2	C	164	ALA
2	C	231	ILE
2	C	234	CYS
2	D	239	VAL
1	A	490	ASP
2	C	224	ASN
2	C	236	HIS
2	D	82	GLN
2	D	223	LYS
2	D	236	HIS
1	B	368	ALA
2	D	237	ALA
1	A	535	SER
1	B	496	ASP
2	C	82	GLN
2	C	294	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	235	LYS
1	B	512	PRO
1	A	584	GLY
2	D	45	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	540/556 (97%)	490 (91%)	50 (9%)	9	21
1	B	533/556 (96%)	482 (90%)	51 (10%)	8	19
2	C	172/282 (61%)	147 (86%)	25 (14%)	3	8
2	D	166/282 (59%)	152 (92%)	14 (8%)	11	25
All	All	1411/1676 (84%)	1271 (90%)	140 (10%)	8	18

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	25	LEU
1	A	34	LYS
1	A	38	THR
1	A	57	GLN
1	A	68	GLU
1	A	71	ASN
1	A	91	ASP
1	A	100	LEU
1	A	121	VAL
1	A	135	ARG
1	A	137	TYR
1	A	149	SER
1	A	164	LEU
1	A	166	SER
1	A	170	LYS
1	A	234	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	ASP
1	A	262	SER
1	A	277	VAL
1	A	289	SER
1	A	296	LYS
1	A	299	ASP
1	A	323	LYS
1	A	334	THR
1	A	358	THR
1	A	393	LEU
1	A	397	THR
1	A	406	ILE
1	A	409	LYS
1	A	413	GLU
1	A	417	HIS
1	A	440	ARG
1	A	456	THR
1	A	458	ILE
1	A	490	ASP
1	A	501	ARG
1	A	504	ASP
1	A	506	MET
1	A	509	VAL
1	A	528	SER
1	A	532	THR
1	A	535	SER
1	A	560	LYS
1	A	561	LEU
1	A	562	GLU
1	A	563	THR
1	A	572	CYS
1	A	594	HIS
1	A	600	GLU
1	B	3	SER
1	B	27	ARG
1	B	32	VAL
1	B	33	LEU
1	B	35	LEU
1	B	68	GLU
1	B	69	LYS
1	B	74	ARG
1	B	75	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	100	LEU
1	B	132	LYS
1	B	146	GLN
1	B	154	HIS
1	B	164	LEU
1	B	166	SER
1	B	170	LYS
1	B	180	VAL
1	B	200	THR
1	B	212	GLU
1	B	234	ILE
1	B	237	LYS
1	B	251	ASN
1	B	265	ASN
1	B	277	VAL
1	B	288	LEU
1	B	334	THR
1	B	350	LYS
1	B	381	GLU
1	B	393	LEU
1	B	402	SER
1	B	432	ILE
1	B	440	ARG
1	B	442	SER
1	B	452	ILE
1	B	491	VAL
1	B	495	THR
1	B	507	CYS
1	B	508	THR
1	B	509	VAL
1	B	517	MET
1	B	532	THR
1	B	535	SER
1	B	552	PHE
1	B	558	ILE
1	B	561	LEU
1	B	563	THR
1	B	575	LYS
1	B	581	THR
1	B	585	TRP
1	B	590	LYS
1	B	599	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	23	LEU
2	C	25	THR
2	C	53	SER
2	C	60	ASP
2	C	66	LYS
2	C	77	ASP
2	C	79	ARG
2	C	81	GLU
2	C	82	GLN
2	C	129	ILE
2	C	138	ASP
2	C	142	LYS
2	C	166	GLU
2	C	180	ARG
2	C	186	ILE
2	C	194	SER
2	C	206	SER
2	C	213	THR
2	C	218	LYS
2	C	224	ASN
2	C	225	SER
2	C	236	HIS
2	C	238	ASN
2	C	240	MET
2	C	281	LEU
2	D	23	LEU
2	D	31	GLU
2	D	57	SER
2	D	70	ILE
2	D	79	ARG
2	D	81	GLU
2	D	137	GLN
2	D	205	ILE
2	D	244	LEU
2	D	247	VAL
2	D	285	GLN
2	D	292	LYS
2	D	296	SER
2	D	302	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	363	ASN
1	A	412	ASN
1	A	568	HIS
1	A	594	HIS
1	B	57	GLN
1	B	71	ASN
1	B	103	HIS
1	B	356	ASN
1	B	548	GLN
2	D	67	GLN
2	D	137	GLN
2	D	238	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	598/615 (97%)	-0.18	12 (2%) 65 67	27, 60, 102, 132	0
1	B	592/615 (96%)	-0.16	17 (2%) 51 52	25, 59, 110, 157	0
2	C	186/312 (59%)	0.32	20 (10%) 5 4	38, 91, 138, 174	0
2	D	180/312 (57%)	0.34	19 (10%) 6 4	43, 93, 145, 160	0
All	All	1556/1854 (83%)	-0.05	68 (4%) 34 33	25, 65, 126, 174	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	164	ALA	9.9
2	C	245	ASP	7.4
2	C	281	LEU	6.4
1	B	498	LEU	5.1
1	B	494	PRO	5.0
2	C	243	LEU	4.8
1	B	495	THR	4.7
2	D	60	ASP	4.3
1	B	414	GLU	4.1
2	D	31	GLU	4.0
1	B	160	SER	3.9
2	C	305	TYR	3.9
2	C	244	LEU	3.6
2	D	23	LEU	3.6
2	C	130	ASP	3.5
2	C	304	ASP	3.5
2	C	83	ALA	3.5
2	C	246	LYS	3.3
1	A	606	VAL	3.3
2	D	83	ALA	3.3
1	A	534	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	536	GLY	3.3
2	C	31	GLU	3.2
1	A	161	LEU	3.2
2	D	134	GLU	3.2
1	A	261	SER	3.2
2	D	24	THR	3.1
2	D	132	ILE	3.1
1	A	536	GLY	3.0
2	D	245	ASP	3.0
2	D	243	LEU	3.0
2	D	289	VAL	2.9
1	A	265	ASN	2.9
2	D	241	LYS	2.9
1	B	534	TYR	2.8
2	D	282	ARG	2.8
2	C	240	MET	2.7
2	D	135	LEU	2.7
1	B	535	SER	2.7
1	B	361	TYR	2.6
1	A	589	LYS	2.5
2	D	244	LEU	2.5
1	B	497	SER	2.5
2	C	282	ARG	2.5
2	C	35	GLN	2.5
1	B	583	LEU	2.4
2	D	82	GLN	2.4
1	A	607	ILE	2.4
2	D	209	TYR	2.4
2	C	134	GLU	2.3
2	C	283	VAL	2.3
1	B	496	ASP	2.3
1	B	506	MET	2.3
2	C	60	ASP	2.3
1	A	298	ALA	2.2
1	B	334	THR	2.2
2	C	289	VAL	2.2
1	B	493	ALA	2.2
2	C	23	LEU	2.1
1	A	160	SER	2.1
1	A	334	THR	2.1
2	D	21	THR	2.1
1	B	597	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	22	PHE	2.1
1	B	489	HIS	2.1
2	C	233	PRO	2.0
2	C	239	VAL	2.0
1	A	535	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
3	ZN	A	700	1/1	0.98	0.15	74,74,74,74	0
3	ZN	B	700	1/1	0.99	0.12	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.