



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 PM UTC

PDB ID : 4GSL / pdb_00004gsl
Title : Crystal structure of an Atg7-Atg3 crosslinked complex
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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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

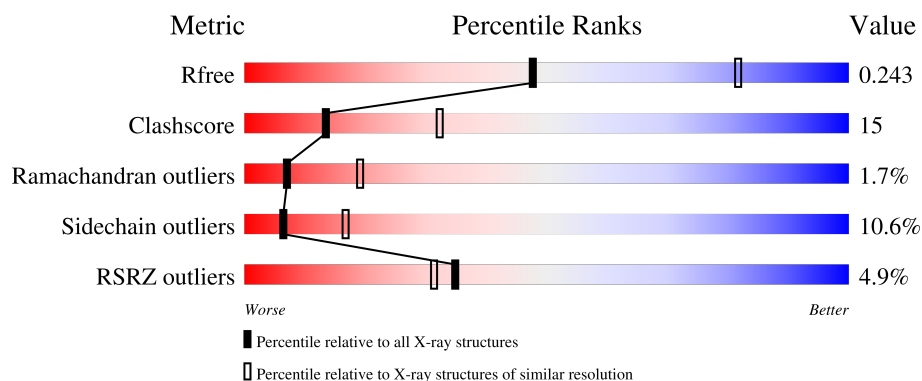
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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 $\leq 5\%$. 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	4% 67% 27% . .
1	B	615	3% 65% 27% 5% .
2	C	312	6% 32% 23% . . 40%
2	D	312	5% 33% 21% . 42%

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

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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 (CCD ID: 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

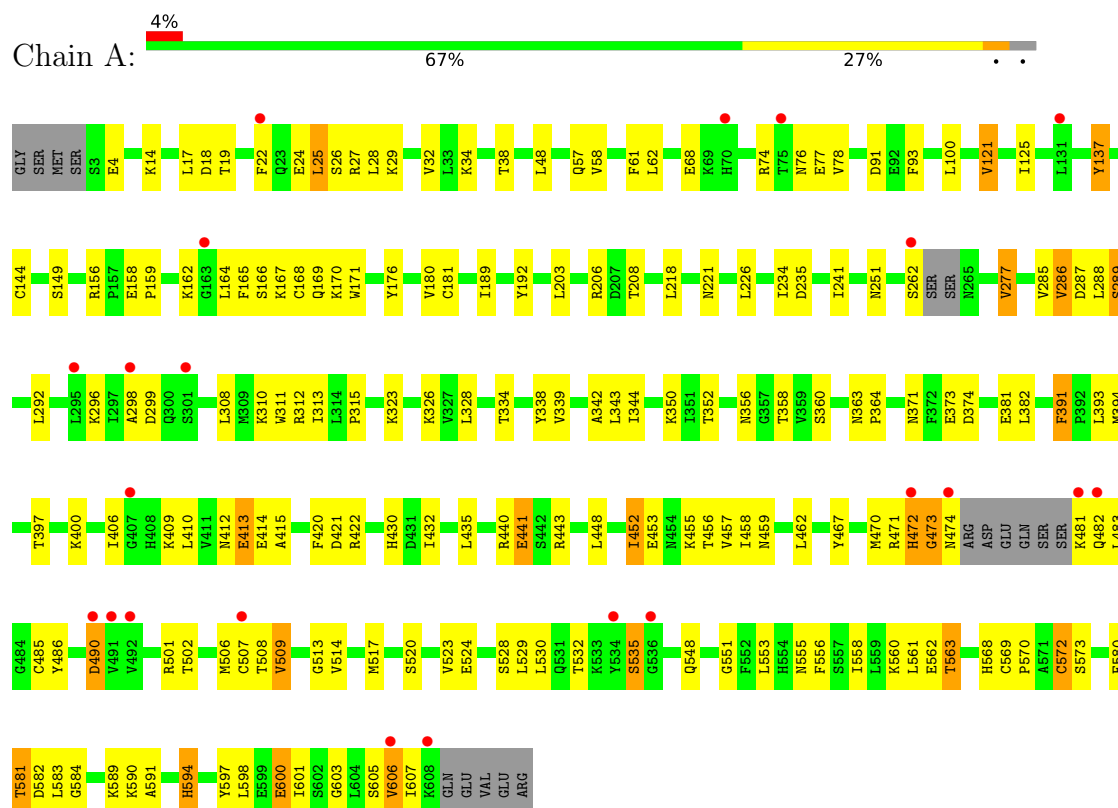
- Molecule 4 is water.

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

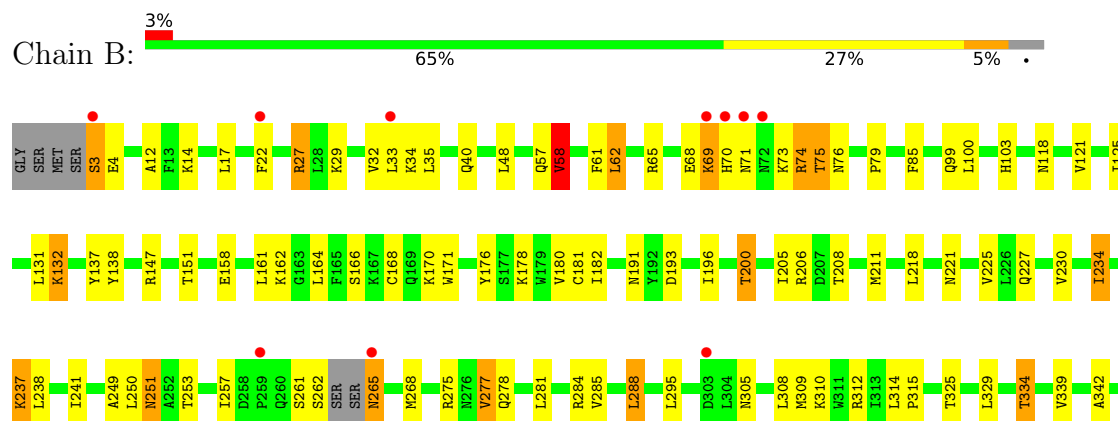
3 Residue-property plots [i](#)

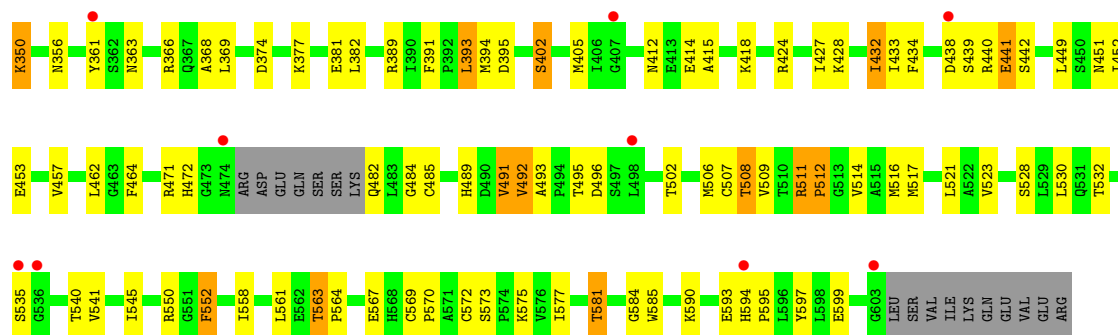
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

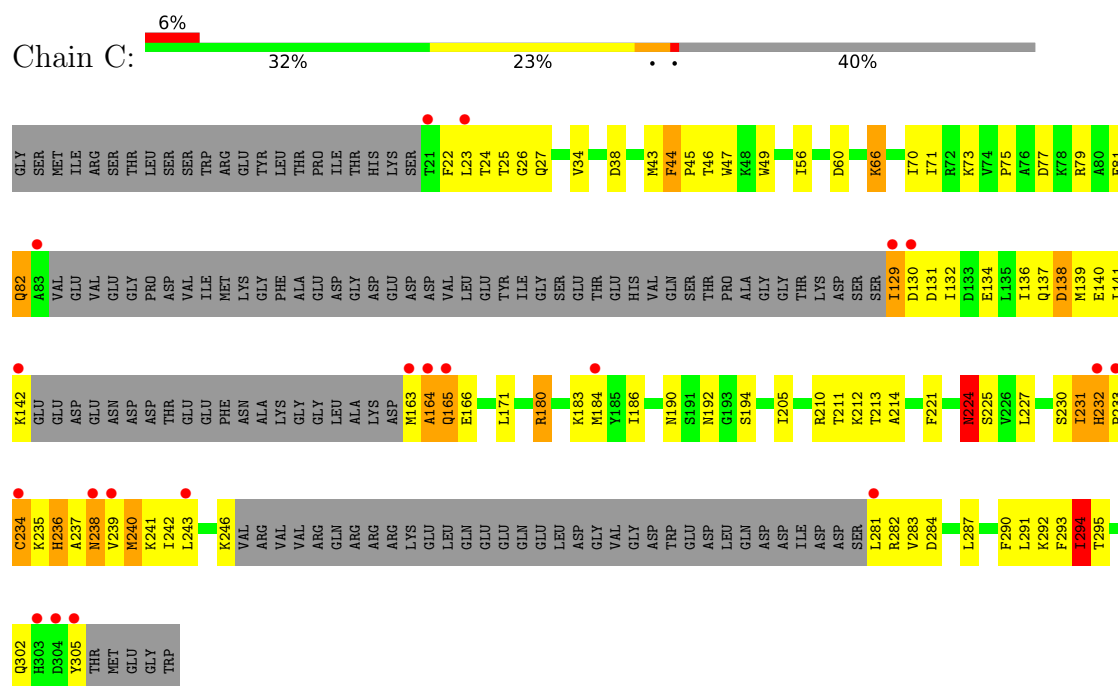


• Molecule 1: Ubiquitin-like modifier-activating enzyme ATG7

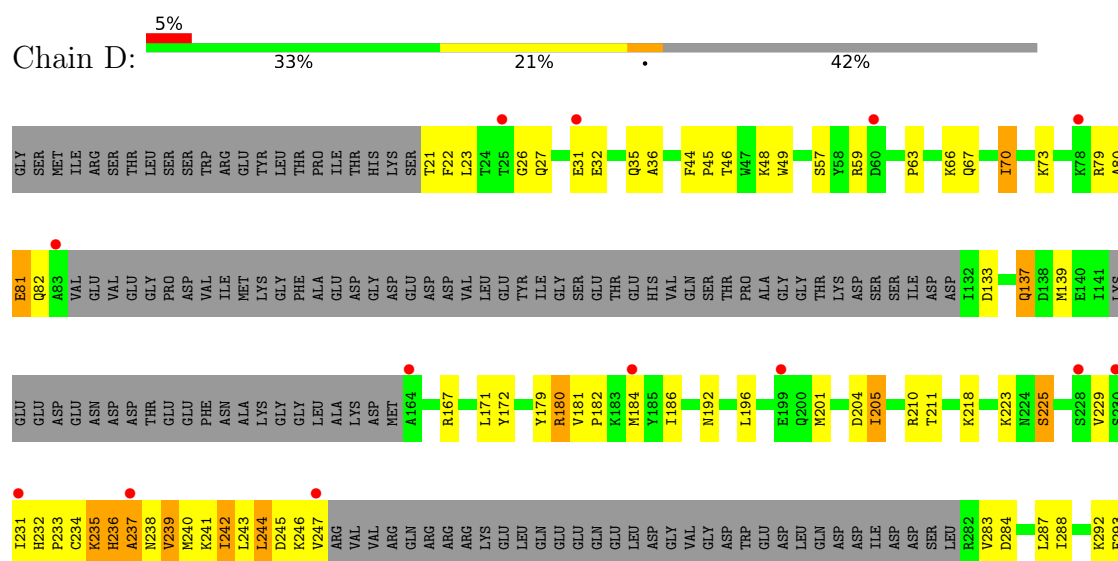




• Molecule 2: Autophagy-related protein 3



• Molecule 2: Autophagy-related protein 3



I294	Q302	H303	E304	TYR	THR	MET	GLU	GLY	TRP
T295									
S296									
V297									

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 37.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.07-2.70) 94.7 (37.07-2.70)	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 0.188 , 0.243	Depositor DCC
R_{free} test set	1904 reflections (2.59%)	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 , 61.3	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

5.1 Standard geometry

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	0.56	0/4869	0.91	6/6598 (0.1%)
1	B	0.57	0/4819	0.90	13/6532 (0.2%)
2	C	0.46	0/1570	0.97	7/2123 (0.3%)
2	D	0.42	0/1515	0.87	2/2050 (0.1%)
All	All	0.54	0/12773	0.91	28/17303 (0.2%)

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.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	225	SER	N-CA-C	7.84	120.98	109.69
1	A	391	PHE	CA-C-N	7.73	127.78	119.28
1	A	391	PHE	C-N-CA	7.73	127.78	119.28
1	A	472	HIS	CB-CA-C	-7.61	106.11	117.07
1	B	58	VAL	CB-CA-C	-7.38	103.65	110.88
1	B	34	LYS	N-CA-C	7.33	121.48	112.54
2	C	166	GLU	N-CA-C	-6.96	100.69	110.50
2	C	225	SER	N-CA-C	6.75	120.60	110.14
1	B	511	ARG	CA-C-N	6.67	128.18	119.84
1	B	511	ARG	C-N-CA	6.67	128.18	119.84
2	C	26	GLY	N-CA-C	-6.25	106.29	115.72
1	A	472	HIS	CA-C-O	6.20	121.54	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	LEU	N-CA-C	6.15	118.50	111.11
2	C	44	PHE	CA-C-N	6.15	127.53	119.84
2	C	44	PHE	C-N-CA	6.15	127.53	119.84
1	B	363	ASN	CA-C-N	-5.83	113.62	119.56
1	B	363	ASN	C-N-CA	-5.83	113.62	119.56
1	B	230	VAL	CA-C-N	5.73	125.58	119.28
1	B	230	VAL	C-N-CA	5.73	125.58	119.28
2	C	141	ILE	CB-CA-C	-5.45	103.43	110.84
1	B	162	LYS	N-CA-C	5.36	118.99	112.23
1	A	452	ILE	N-CA-C	5.29	116.65	110.62
1	B	40	GLN	CA-C-N	5.26	125.20	119.78
1	B	40	GLN	C-N-CA	5.26	125.20	119.78
2	D	242	ILE	CB-CA-C	-5.15	105.23	111.87
2	C	235	LYS	CB-CA-C	-5.12	110.69	116.63
1	A	76	ASN	N-CA-C	5.10	119.35	113.38
1	B	12	ALA	N-CA-C	5.07	116.89	111.36

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 ⓘ

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	125	0
1	B	4717	0	4766	133	0
2	C	1534	0	1514	70	0
2	D	1480	0	1462	60	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	369	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 15.

All (369) 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:B:147:ARG:HE	1:B:268:MET:HE3	1.38	0.89
2:D:184:MET:HE2	2:D:294:ILE:HG21	1.59	0.85
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	1.46	0.81
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
2:D:237:ALA:HA	2:D:238:ASN:C	2.08	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:438:ASP:HB2	1:B:506:MET:HE3	1.76	0.66
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:HB2	2:C:282:ARG:NH1	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
2:C:230:SER:C	2:C:231:ILE:HG12	2.25	0.61
2:C:24:THR:O	2:C:241:LYS:NZ	2.28	0.61
2:D:201:MET:HE3	2:D:229:VAL:HG23	1.82	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
2:C:233:PRO:HA	2:C:234:CYS:C	2.25	0.60
1:A:17:LEU:HD11	1:A:62:LEU:HD12	1.83	0.60
1:B:137:TYR:CD2	1:B:285:VAL:HG22	2.37	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:147:ARG:HE	1:B:268:MET:CE	2.13	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
2:C:73:LYS:N	2:C:73:LYS:HD2	2.18	0.58
2:D:44:PHE:C	2:D:46:THR:H	2.12	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:D:235:LYS:C	2:D:237:ALA:H	2.12	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:A:298:ALA:HA	1:B:361:TYR:HB3	1.86	0.57
1:A:432:ILE:HD11	1:A:530:LEU:HD21	1.85	0.57
2:C:282:ARG:NH1	2:C:284:ASP:OD2	2.37	0.57
1:A:78:VAL:HG13	1:A:176:TYR:O	2.04	0.57
1:A:582:ASP:HB2	1:A:583:LEU:HD12	1.86	0.57
2:C:38:ASP:OD2	2:C:66:LYS:NZ	2.38	0.57
1:B:414:GLU:CG	1:B:418:LYS:HZ1	2.16	0.56
2:D:180:ARG:HD3	2:D:180:ARG:H	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:HD2	2:D:73:LYS:N	2.20	0.56
1:A:435:LEU:HD13	1:A:457:VAL:HG13	1.87	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:C:237:ALA:HA	2:C:238:ASN:C	2.30	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
2:C:23:LEU:H	2:C:23:LEU:HD23	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:441:GLU:H	1:B:441:GLU:CD	2.14	0.55
1:B:552:PHE:N	1:B:552:PHE:CD1	2.75	0.55
2:D:235:LYS:O	2:D:237:ALA:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:171:LEU:HD22	2:C:184:MET:HE3	1.88	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:32:GLU:O	2:D:35:GLN:HB2	2.09	0.53
2:D:36:ALA:HA	2:D:284:ASP:O	2.08	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
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:A:391:PHE:HD2	1:A:394:MET:HE2	1.75	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:545:ILE:O	1:B:545:ILE:HG13	2.11	0.50
1:A:594:HIS:O	1:A:597:TYR:HB3	2.11	0.50
2:C:44:PHE:C	2:C:46:THR:H	2.20	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:168:CYS:HB3	1:B:241:ILE:HG13	1.95	0.49
1:B:221:ASN:O	1:B:225:VAL:HG23	2.12	0.49
1:B:277:VAL:HG22	2:C:192:ASN:CG	2.37	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:O	1:B:265:ASN:ND2	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:B:374:ASP:CG	1:B:382:LEU:HD21	2.39	0.48
1:A:22:PHE:CD2	1:A:288:LEU:HD11	2.49	0.48
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:298:ALA:HB2	1:B:361:TYR:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:GLU:HA	1:A:605:SER:OG	2.14	0.47
2:C:134:GLU:O	2:C:138:ASP:OD1	2.32	0.47
2:C:237:ALA:CA	2:C:238:ASN:C	2.87	0.47
2:D:295:THR:HG21	2:D:303:HIS:CD2	2.49	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:374:ASP:HB3	1:A:382:LEU:CD2	2.44	0.47
1:A:420:PHE:CD2	1:A:420:PHE:C	2.93	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:441:GLU:CD	1:A:441:GLU:H	2.23	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:61:PHE:CE1	2:C:73:LYS:NZ	2.75	0.46
1:B:374:ASP:HB3	1:B:382:LEU:CD2	2.44	0.46
1:A:93:PHE:CE2	2:D:139:MET:HE1	2.50	0.46
1:A:374:ASP:CB	1:A:382:LEU:HD21	2.45	0.46
2:D:180:ARG:HD3	2:D:180:ARG:N	2.30	0.46
2:D:44:PHE:C	2:D:46:THR:N	2.72	0.46
1:A:517:MET:HE2	1:B:521:LEU:HD23	1.97	0.46
1:A:137:TYR:CD1	1:A:137:TYR:N	2.84	0.46
1:A:180:VAL:HG12	1:A:192:TYR:HB2	1.97	0.46
2:D:49:TRP:CE3	2:D:66:LYS:HA	2.50	0.46
2:D:246:LYS:HD3	2:D:246:LYS:HA	1.54	0.46
1:A:506:MET:O	1:A:507:CYS:HB2	2.15	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
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

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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:298:ALA:HB2	1:B:361:TYR:CD1	2.52	0.45
1:A:412:ASN:ND2	1:A:415:ALA:CB	2.80	0.45
2:C:56:ILE:HA	2:C:221:PHE:O	2.16	0.45
2:D:237:ALA:CA	2:D:238:ASN:C	2.85	0.45
2:D:287:LEU:HD23	2:D:287:LEU:HA	1.70	0.45
1:A:24:GLU:O	1:A:24:GLU:HG3	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:HD12	2:D:288:ILE:N	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
1:B:391:PHE:HD2	1:B:394:MET:HE1	1.81	0.44
2:C:214:ALA:HA	2:C:231:ILE:HD13	1.99	0.44
1:A:481:LYS:HB3	1:A:481:LYS:HE2	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:517:MET:SD	1:A:553:LEU:HD11	2.57	0.44
1:A:520:SER:O	1:A:524:GLU:HG2	2.17	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:HB2	1:B:132:LYS:HE2	1.74	0.44
1:B:366:ARG:HH22	1:B:512:PRO:HD3	1.83	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:593:GLU:C	1:B:595:PRO:HD3	2.43	0.43
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:511:ARG:HA	1:B:512:PRO:HD2	1.84	0.43

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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:74:ARG:HE	1:B:74:ARG:HB2	1.31	0.43
1:B:151:THR:HG21	1:B:227:GLN:OE1	2.18	0.43
2:D:22:PHE:CE1	2:D:283:VAL:HB	2.53	0.43
2:D:241:LYS:O	2:D:241:LYS:HG3	2.19	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:A:572:CYS:O	1:A:573:SER:C	2.62	0.43
1:B:62:LEU:HD11	1:B:125:ILE:HD11	2.01	0.43
1:A:58:VAL:HG23	1:A:208:THR:HB	2.00	0.43
1:A:313:ILE:HD13	1:B:464:PHE:CD1	2.54	0.43
1:A:555:ASN:O	1:A:556:PHE:C	2.62	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
2:C:211:THR:C	2:C:212:LYS:HG3	2.44	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
2:C:190:ASN:OD1	2:C:190:ASN:C	2.62	0.43
1:B:17:LEU:HD22	1:B:22:PHE:CZ	2.54	0.42
2:D:232:HIS:HA	2:D:233:PRO:HD3	1.93	0.42
1:A:394:MET:HE2	1:A:394:MET:HB2	1.68	0.42
1:A:590:LYS:HE3	1:A:590:LYS:HB2	1.74	0.42
1:B:75:THR:O	1:B:76:ASN:HB2	2.19	0.42
1:B:511:ARG:O	1:B:514:VAL:HG23	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:B:391:PHE:HD2	1:B:394:MET:CE	2.32	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
2:C:129:ILE:C	2:C:131:ASP:HB2	2.44	0.42
1:A:453:GLU:O	1:A:455:LYS:HG2	2.19	0.42
1:B:73:LYS:HE3	1:B:176:TYR:CD1	2.54	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
2:D:244:LEU:HD12	2:D:244:LEU:HA	1.92	0.42
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.92	0.42
1:A:339:VAL:O	1:A:343:LEU:HG	2.20	0.42
1:A:159:PRO:C	1:A:162:LYS:HE2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:237:LYS:HZ3	1:B:237:LYS:HG3	1.78	0.42
2:C:139:MET:HB3	2:C:139:MET:HE2	1.57	0.42
2:C:230:SER:O	2:C:231:ILE:HG12	2.20	0.42
2:D:21:THR:OG1	2:D:22:PHE:N	2.52	0.42
2:D:235:LYS:C	2:D:237:ALA:N	2.77	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
2:C:49:TRP:CD2	2:C:66:LYS:HG3	2.55	0.41
2:C:287:LEU:HD23	2:C:287:LEU:HA	1.92	0.41
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.92	0.41
1:B:394:MET:HE2	1:B:394:MET:HB2	1.86	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
2:C:44:PHE:C	2:C:46:THR:N	2.79	0.41
1:A:328:LEU:HD12	1:A:352:THR:O	2.20	0.41
1:B:69:LYS:HB3	1:B:70:HIS:H	1.67	0.41
1:B:182:ILE:HD13	1:B:193:ASP:H	1.85	0.41
1:B:482:GLN:OE1	1:B:482:GLN:HA	2.19	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:CD1	1:B:85:PHE:N	2.89	0.40
1:A:412:ASN:O	1:A:413:GLU:C	2.64	0.40
2:C:137:GLN:O	2:C:140:GLU:HB3	2.21	0.40
1:A:277:VAL:HG22	2:D:192:ASN:CG	2.46	0.40
1:A:338:TYR:O	1:B:516:MET:HE1	2.22	0.40
1:A:568:HIS:CE1	1:A:607:ILE:HD11	2.55	0.40
1:A:583:LEU:HD12	1:A:583:LEU:H	1.86	0.40
1:B:132:LYS:H	1:B:132:LYS:CE	2.34	0.40
1:B:530:LEU:HD23	1:B:530:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:PHE:O	1:A:581:THR:C	2.65	0.40
1:B:196:ILE:HG22	1:B:200:THR:OG1	2.21	0.40
1:B:261:SER:O	1:B:262:SER:C	2.64	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 [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	592/615 (96%)	551 (93%)	36 (6%)	5 (1%)	16	37
1	B	586/615 (95%)	559 (95%)	23 (4%)	4 (1%)	18	41
2	C	178/312 (57%)	157 (88%)	13 (7%)	8 (4%)	2	4
2	D	172/312 (55%)	156 (91%)	7 (4%)	9 (5%)	1	3
All	All	1528/1854 (82%)	1423 (93%)	79 (5%)	26 (2%)	7	19

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

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Mol	Chain	Res	Type
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
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%)	482 (89%)	58 (11%)	6	16
1	B	533/556 (96%)	479 (90%)	54 (10%)	7	18
2	C	172/282 (61%)	149 (87%)	23 (13%)	4	9
2	D	166/282 (59%)	152 (92%)	14 (8%)	10	26
All	All	1411/1676 (84%)	1262 (89%)	149 (11%)	6	17

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	14	LYS
1	A	25	LEU
1	A	34	LYS
1	A	38	THR
1	A	57	GLN

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Mol	Chain	Res	Type
1	A	68	GLU
1	A	77	GLU
1	A	91	ASP
1	A	100	LEU
1	A	121	VAL
1	A	137	TYR
1	A	149	SER
1	A	156	ARG
1	A	164	LEU
1	A	166	SER
1	A	170	LYS
1	A	234	ILE
1	A	235	ASP
1	A	262	SER
1	A	277	VAL
1	A	286	VAL
1	A	289	SER
1	A	296	LYS
1	A	299	ASP
1	A	323	LYS
1	A	334	THR
1	A	344	ILE
1	A	358	THR
1	A	373	GLU
1	A	381	GLU
1	A	393	LEU
1	A	397	THR
1	A	406	ILE
1	A	409	LYS
1	A	413	GLU
1	A	440	ARG
1	A	441	GLU
1	A	456	THR
1	A	458	ILE
1	A	482	GLN
1	A	490	ASP
1	A	501	ARG
1	A	509	VAL
1	A	528	SER
1	A	532	THR
1	A	535	SER
1	A	558	ILE

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Mol	Chain	Res	Type
1	A	560	LYS
1	A	561	LEU
1	A	562	GLU
1	A	563	THR
1	A	572	CYS
1	A	581	THR
1	A	594	HIS
1	A	600	GLU
1	A	601	ILE
1	A	606	VAL
1	B	3	SER
1	B	27	ARG
1	B	32	VAL
1	B	33	LEU
1	B	35	LEU
1	B	58	VAL
1	B	62	LEU
1	B	68	GLU
1	B	69	LYS
1	B	74	ARG
1	B	75	THR
1	B	100	LEU
1	B	132	LYS
1	B	164	LEU
1	B	166	SER
1	B	170	LYS
1	B	180	VAL
1	B	200	THR
1	B	211	MET
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	305	ASN
1	B	334	THR
1	B	350	LYS
1	B	381	GLU
1	B	393	LEU
1	B	402	SER
1	B	432	ILE

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Mol	Chain	Res	Type
1	B	440	ARG
1	B	441	GLU
1	B	442	SER
1	B	452	ILE
1	B	491	VAL
1	B	492	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
2	C	25	THR
2	C	60	ASP
2	C	66	LYS
2	C	70	ILE
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	180	ARG
2	C	186	ILE
2	C	194	SER
2	C	213	THR
2	C	224	ASN
2	C	227	LEU
2	C	238	ASN
2	C	240	MET
2	C	281	LEU

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Mol	Chain	Res	Type
2	C	292	LYS
2	C	294	ILE
2	C	295	THR
2	D	23	LEU
2	D	31	GLU
2	D	48	LYS
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	292	LYS
2	D	296	SER
2	D	302	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	191	ASN
1	A	213	ASN
1	A	363	ASN
1	A	412	ASN
1	A	489	HIS
1	A	568	HIS
1	A	594	HIS
1	B	45	ASN
1	B	57	GLN
1	B	71	ASN
1	B	103	HIS
1	B	300	GLN
1	B	356	ASN
1	B	371	ASN
1	B	416	GLN
1	B	451	ASN
1	B	548	GLN
2	C	42	HIS
2	C	224	ASN
2	C	238	ASN

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Mol	Chain	Res	Type
2	D	67	GLN
2	D	137	GLN
2	D	238	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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, 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%)	-0.03	22 (3%) 45 41	27, 60, 102, 132	0
1	B	592/615 (96%)	-0.06	19 (3%) 50 46	25, 59, 110, 157	0
2	C	186/312 (59%)	0.62	20 (10%) 11 9	38, 91, 138, 174	0
2	D	180/312 (57%)	0.62	15 (8%) 17 14	43, 93, 145, 160	0
All	All	1556/1854 (83%)	0.11	76 (4%) 35 31	25, 65, 126, 174	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	247	VAL	5.6
2	D	164	ALA	5.4
1	B	72	ASN	5.0
2	D	83	ALA	4.4
1	A	491	VAL	4.0
2	C	305	TYR	3.8
2	D	231	ILE	3.8
2	C	281	LEU	3.6
2	D	184	MET	3.5
1	B	474	ASN	3.4
2	C	304	ASP	3.4
2	C	163	MET	3.3
2	C	165	GLN	3.3
2	C	83	ALA	3.2
2	C	129	ILE	3.2
1	B	70	HIS	3.2
1	A	262	SER	3.2
1	A	407	GLY	3.1
1	A	70	HIS	3.1
2	C	164	ALA	3.1
1	B	535	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	507	CYS	3.0
2	D	31	GLU	3.0
1	A	536	GLY	2.9
1	A	481	LYS	2.9
1	B	536	GLY	2.8
1	B	3	SER	2.7
2	C	232	HIS	2.7
1	B	71	ASN	2.7
2	C	303	HIS	2.7
1	A	298	ALA	2.7
2	C	239	VAL	2.7
1	A	534	TYR	2.6
1	A	131	LEU	2.6
1	A	474	ASN	2.6
2	D	237	ALA	2.6
1	B	603	GLY	2.6
1	B	498	LEU	2.6
1	A	301	SER	2.5
2	D	304	ASP	2.5
2	D	199	GLU	2.5
1	A	482	GLN	2.5
1	B	265	ASN	2.5
2	C	142	LYS	2.4
1	B	407	GLY	2.4
2	C	243	LEU	2.4
1	A	606	VAL	2.4
1	A	492	VAL	2.4
2	D	230	SER	2.3
1	A	163	GLY	2.3
1	A	75	THR	2.3
1	B	594	HIS	2.3
2	C	233	PRO	2.3
1	A	22	PHE	2.3
1	A	472	HIS	2.3
2	D	25	THR	2.3
1	B	33	LEU	2.3
1	A	608	LYS	2.3
1	A	490	ASP	2.3
2	C	130	ASP	2.3
1	B	69	LYS	2.2
1	B	438	ASP	2.2
2	D	78	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	184	MET	2.2
2	C	21	THR	2.2
1	B	361	TYR	2.2
2	D	296	SER	2.2
2	C	238	ASN	2.2
2	C	234	CYS	2.1
2	C	23	LEU	2.1
1	B	22	PHE	2.1
2	D	60	ASP	2.1
1	B	259	PRO	2.1
1	B	303	ASP	2.0
2	D	228	SER	2.0
1	A	295	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	ZN	A	700	1/1	0.99	0.05	74,74,74,74	0
3	ZN	B	700	1/1	1.00	0.03	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.