Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2017 – 04:38 PM EDT

PDB ID	:	4YCV
Title	:	Crystal structure of cladosporin in complex with plasmodium lysyl-tRNA synthetase
Authors	:	Fang, P.; Wang, J.; Guo, M.
Deposited on	:	unknown
Resolution	:	3.41 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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 3.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.257
Clashscore		15
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		3.0%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
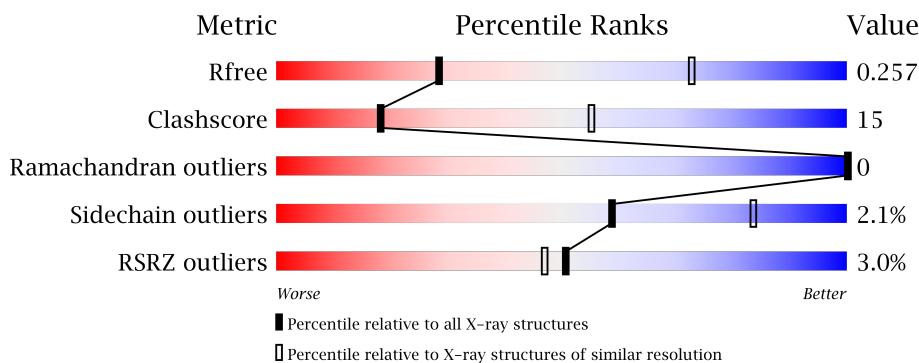
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	516	.% 62% 31% · 6%
1	B	516	2% 67% 25% · 6%
1	C	516	5% 62% 31% · 6%
1	D	516	3% 64% 27% · 7%

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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15261 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 Lysine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total 3852	C 2487	N 639	O 709	S 17	0	0	0
1	B	486	Total 3830	C 2472	N 637	O 704	S 17	0	0	0
1	C	485	Total 3752	C 2420	N 621	O 694	S 17	0	0	0
1	D	479	Total 3736	C 2413	N 620	O 686	S 17	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP W7JP72
A	584	GLY	-	expression tag	UNP W7JP72
A	585	GLY	-	expression tag	UNP W7JP72
A	586	HIS	-	expression tag	UNP W7JP72
A	587	HIS	-	expression tag	UNP W7JP72
A	588	HIS	-	expression tag	UNP W7JP72
A	589	HIS	-	expression tag	UNP W7JP72
A	590	HIS	-	expression tag	UNP W7JP72
A	591	HIS	-	expression tag	UNP W7JP72
B	76	MET	-	initiating methionine	UNP W7JP72
B	584	GLY	-	expression tag	UNP W7JP72
B	585	GLY	-	expression tag	UNP W7JP72
B	586	HIS	-	expression tag	UNP W7JP72
B	587	HIS	-	expression tag	UNP W7JP72
B	588	HIS	-	expression tag	UNP W7JP72
B	589	HIS	-	expression tag	UNP W7JP72
B	590	HIS	-	expression tag	UNP W7JP72
B	591	HIS	-	expression tag	UNP W7JP72
C	76	MET	-	initiating methionine	UNP W7JP72
C	584	GLY	-	expression tag	UNP W7JP72
C	585	GLY	-	expression tag	UNP W7JP72

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Chain	Residue	Modelled	Actual	Comment	Reference
C	586	HIS	-	expression tag	UNP W7JP72
C	587	HIS	-	expression tag	UNP W7JP72
C	588	HIS	-	expression tag	UNP W7JP72
C	589	HIS	-	expression tag	UNP W7JP72
C	590	HIS	-	expression tag	UNP W7JP72
C	591	HIS	-	expression tag	UNP W7JP72
D	76	MET	-	initiating methionine	UNP W7JP72
D	584	GLY	-	expression tag	UNP W7JP72
D	585	GLY	-	expression tag	UNP W7JP72
D	586	HIS	-	expression tag	UNP W7JP72
D	587	HIS	-	expression tag	UNP W7JP72
D	588	HIS	-	expression tag	UNP W7JP72
D	589	HIS	-	expression tag	UNP W7JP72
D	590	HIS	-	expression tag	UNP W7JP72
D	591	HIS	-	expression tag	UNP W7JP72

• Molecule 2 is cladosporin (three-letter code: KRS) (formula: $C_{16}H_{20}O_5$).
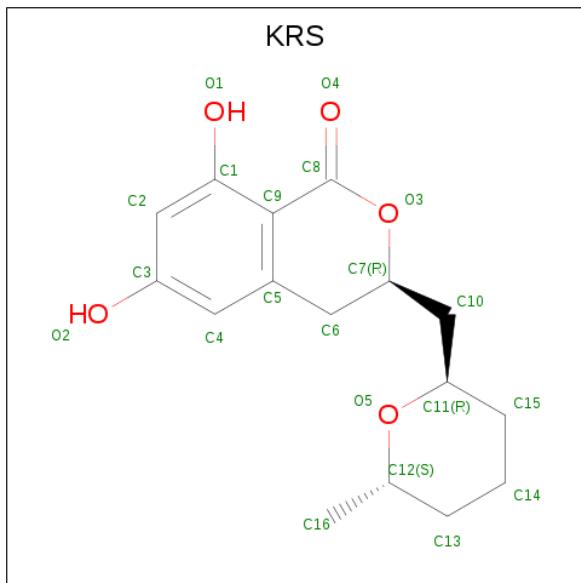
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 21	C 16	O 5	0	0
2	B	1	Total 21	C 16	O 5	0	0
2	C	1	Total 21	C 16	O 5	0	0
2	D	1	Total 21	C 16	O 5	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	1	Total 1	O 1	0	0
3	C	1	Total 1	O 1	0	0
3	D	2	Total 2	O 2	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: Lysine–tRNA ligase
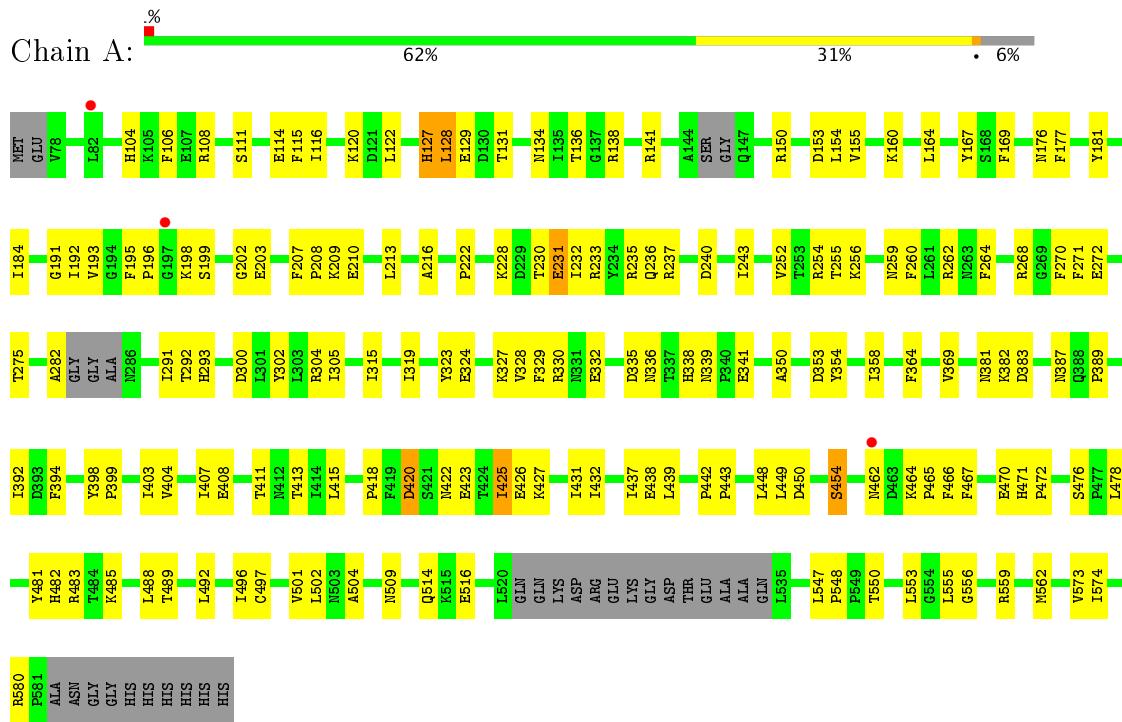
- Molecule 1: Lysine–tRNA ligase
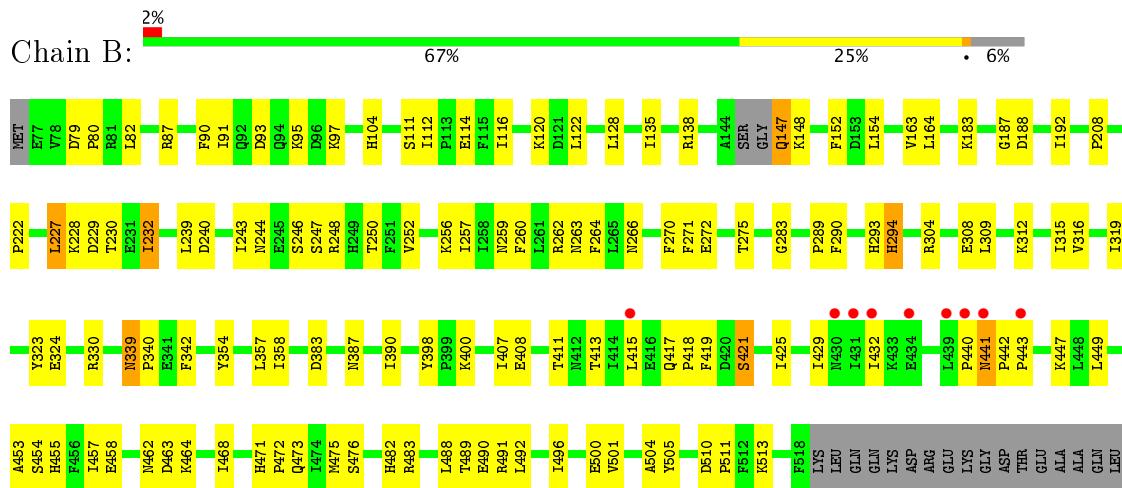
• Molecule 1: Lysine–tRNA ligase
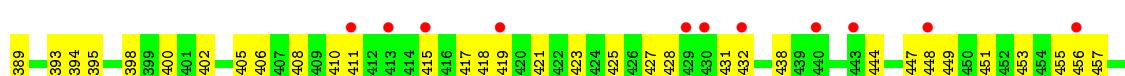
• Molecule 1: Lysine–tRNA ligase
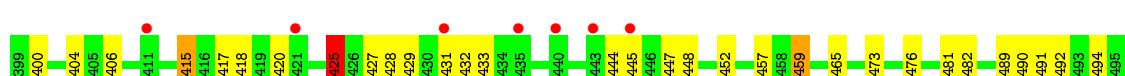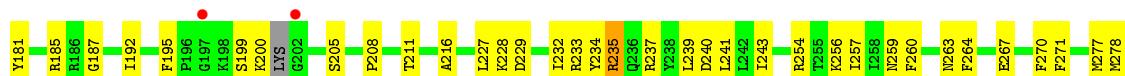
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.63Å 112.10Å 170.79Å 90.00° 99.30° 90.00°	Depositor
Resolution (Å)	49.90 – 3.41	Depositor
	49.90 – 3.41	EDS
% Data completeness	95.6 (49.90-3.41)	Depositor
(in resolution range)	95.6 (49.90-3.41)	EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.257	Depositor
	0.230 , 0.257	DCC
R_{free} test set	1706 reflections (4.94%)	DCC
Wilson B-factor (Å^2)	62.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	15261	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.35	0/3948	0.60	1/5354 (0.0%)
1	B	0.33	0/3927	0.59	0/5332
1	C	0.32	0/3846	0.59	0/5237
1	D	0.35	0/3829	0.61	2/5205 (0.0%)
All	All	0.34	0/15550	0.60	3/21128 (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
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	425	ILE	CG1-CB-CG2	-7.78	94.28	111.40
1	A	128	LEU	CA-CB-CG	5.84	128.74	115.30
1	D	555	LEU	CA-CB-CG	5.47	127.88	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	420	ASP	Peptide
1	B	417	GLN	Peptide
1	B	418	PRO	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	3852	0	3688	118	0
1	B	3830	0	3659	108	0
1	C	3752	0	3496	132	0
1	D	3736	0	3525	107	0
2	A	21	0	18	1	0
2	B	21	0	18	0	0
2	C	21	0	18	3	0
2	D	21	0	18	4	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
All	All	15261	0	14440	446	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 (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:THR:O	1:C:464:LYS:NZ	1.73	1.20
1:D:504:ALA:HB2	1:D:553:LEU:HD13	1.45	0.95
1:C:395:THR:O	1:C:464:LYS:CE	2.14	0.95
1:C:480:LYS:HA	1:C:508:LEU:HB2	1.48	0.95
1:A:104:HIS:HD2	1:B:483:ARG:HG2	1.36	0.91
1:D:502:LEU:HG	1:D:553:LEU:HD11	1.51	0.91
1:B:441:ASN:HD22	1:B:441:ASN:N	1.69	0.91
1:C:339:ASN:HD22	1:C:340:PRO:N	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ASN:C	1:C:339:ASN:HD22	1.83	0.82
1:D:429:ILE:O	1:D:432:ILE:HG13	1.82	0.79
1:A:233:ARG:HG3	1:A:240:ASP:HB2	1.66	0.78
1:C:143:SER:HB2	1:C:151:PHE:HB2	1.64	0.78
1:B:440:PRO:C	1:B:441:ASN:HD22	1.88	0.77
1:D:547:LEU:HD12	1:D:548:PRO:HD2	1.66	0.76
1:A:271:PHE:HZ	1:B:252:VAL:HA	1.48	0.76
1:D:288:ARG:HB3	1:D:331:ASN:HB3	1.68	0.76
1:B:90:PHE:HZ	1:B:183:LYS:HG3	1.51	0.74
1:C:235:ARG:NH2	1:C:580:ARG:O	2.21	0.73
1:C:262:ARG:NH1	1:C:272:GLU:OE1	2.21	0.73
1:C:338:HIS:HB3	2:C:601:KRS:C2	2.18	0.73
1:C:141:ARG:NH2	1:C:143:SER:OG	2.22	0.73
1:A:350:ALA:HA	1:A:550:THR:HG22	1.69	0.73
1:A:104:HIS:CD2	1:B:483:ARG:HG2	2.23	0.73
1:A:470:GLU:HB3	1:A:488:LEU:HD23	1.71	0.72
1:C:438:GLU:O	1:C:451:GLN:NE2	2.23	0.72
1:A:335:ASP:OD1	1:A:336:ASN:N	2.23	0.72
1:A:128:LEU:HD21	1:A:131:THR:HG23	1.71	0.71
1:A:192:ILE:HG23	1:A:208:PRO:HB3	1.71	0.71
1:A:353:ASP:OD2	1:A:483:ARG:NH2	2.24	0.71
1:C:339:ASN:ND2	1:C:341:GLU:H	1.87	0.71
1:A:264:PHE:O	1:A:268:ARG:NH1	2.25	0.70
1:D:185:ARG:HH21	1:D:185:ARG:HG2	1.57	0.70
1:D:192:ILE:HG23	1:D:208:PRO:HB3	1.72	0.70
1:D:295:ASN:O	1:D:298:ASP:N	2.25	0.69
1:C:406:GLU:HG2	1:C:457:ILE:HG13	1.73	0.69
1:B:90:PHE:CZ	1:B:183:LYS:HG3	2.28	0.68
1:D:235:ARG:NH2	1:D:580:ARG:O	2.25	0.68
1:D:476:SER:OG	1:D:491:ARG:NH1	2.22	0.68
1:B:259:ASN:O	1:B:263:ASN:ND2	2.26	0.68
1:D:233:ARG:HG3	1:D:240:ASP:HB2	1.75	0.68
1:C:235:ARG:NH1	1:C:579:MET:SD	2.68	0.67
1:A:315:ILE:HG21	1:A:550:THR:HG21	1.77	0.67
1:B:441:ASN:ND2	1:B:441:ASN:N	2.43	0.67
1:C:462:ASN:O	1:C:464:LYS:HG3	1.95	0.66
1:C:141:ARG:HB3	1:C:153:ASP:HB2	1.78	0.66
1:A:235:ARG:NH2	1:A:580:ARG:O	2.19	0.66
1:D:294:HIS:ND1	1:D:294:HIS:O	2.28	0.66
1:D:553:LEU:HD12	1:D:554:GLY:H	1.61	0.65
1:B:387:ASN:HD22	1:B:387:ASN:N	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:O	1:A:387:ASN:HB2	1.97	0.65
1:A:252:VAL:HA	1:B:271:PHE:HZ	1.61	0.65
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.61	0.64
1:A:181:TYR:HA	1:A:184:ILE:HD12	1.79	0.64
1:C:237:ARG:NH1	1:C:240:ASP:OD2	2.29	0.64
1:D:425:ILE:HG22	1:D:429:ILE:CD1	2.28	0.64
1:D:354:TYR:CD2	1:D:490:GLU:HB3	2.33	0.64
1:C:268:ARG:HH11	1:C:268:ARG:HG2	1.62	0.64
1:D:108:ARG:NH2	1:D:111:SER:HB2	2.13	0.64
1:B:510:ASP:OD2	1:B:513:LYS:NZ	2.27	0.63
1:B:411:THR:HG23	1:B:413:THR:H	1.63	0.63
1:D:553:LEU:HD12	1:D:554:GLY:N	2.13	0.63
1:C:580:ARG:HB2	1:D:297:LEU:HD11	1.81	0.63
1:C:295:ASN:HB2	1:D:331:ASN:HD21	1.63	0.63
1:A:381:ASN:HD22	1:A:389:PRO:HB3	1.65	0.62
1:B:339:ASN:HD22	1:B:574:ILE:HD12	1.65	0.62
1:C:335:ASP:CG	1:C:336:ASN:H	2.00	0.62
1:D:354:TYR:HB2	1:D:492:LEU:HD21	1.82	0.62
1:D:278:MET:HG2	1:D:303:LEU:HD23	1.81	0.62
1:C:166:ASN:HB3	1:C:169:PHE:HD2	1.64	0.62
1:B:87:ARG:NH1	1:B:188:ASP:OD1	2.29	0.62
1:A:449:LEU:HD13	1:A:472:PRO:HG2	1.82	0.61
1:A:381:ASN:ND2	1:A:389:PRO:HB3	2.15	0.61
1:D:167:TYR:O	1:D:172:HIS:NE2	2.27	0.61
1:B:227:LEU:HD22	1:B:232:ILE:HD11	1.83	0.61
1:A:256:LYS:HA	1:A:259:ASN:HB2	1.82	0.60
1:D:482:HIS:HA	1:D:490:GLU:HG3	1.82	0.60
1:D:254:ARG:NH1	1:D:573:VAL:O	2.34	0.60
1:A:407:ILE:O	1:A:411:THR:HG22	2.00	0.60
1:A:262:ARG:NH1	1:A:272:GLU:OE1	2.35	0.60
1:B:152:PHE:HB2	1:B:163:VAL:HB	1.84	0.59
1:B:398:TYR:O	1:B:400:LYS:NZ	2.24	0.59
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.83	0.59
1:C:263:ASN:HA	1:C:266:ASN:HB2	1.84	0.59
1:C:339:ASN:HB3	1:C:570:ILE:HD13	1.85	0.59
1:C:408:GLU:OE2	1:C:415:LEU:N	2.35	0.59
1:C:290:PHE:HD1	1:C:329:PHE:HB3	1.67	0.59
1:C:421:SER:OG	1:C:423:GLU:OE1	2.20	0.59
1:A:271:PHE:CZ	1:B:252:VAL:HA	2.35	0.59
1:A:399:PRO:HD3	1:A:464:LYS:HE3	1.85	0.59
1:A:437:ILE:HG22	1:A:438:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:O	1:B:91:ILE:HG12	2.03	0.58
1:D:556:GLY:O	1:D:560:ILE:HD12	2.02	0.58
1:A:167:TYR:HD1	1:A:177:PHE:CD2	2.22	0.58
1:A:176:ASN:OD1	1:A:177:PHE:N	2.37	0.58
1:A:260:PHE:O	1:A:264:PHE:HB2	2.03	0.58
1:B:419:PHE:HE2	1:B:449:LEU:HD21	1.69	0.58
1:C:444:THR:OG1	1:C:447:LYS:HD3	2.04	0.58
1:C:453:ALA:O	1:C:457:ILE:HG22	2.02	0.58
1:D:347:PHE:CE2	1:D:553:LEU:HD23	2.39	0.58
1:B:354:TYR:CE2	1:B:490:GLU:HB3	2.38	0.58
1:C:379:SER:O	1:C:566:ASN:ND2	2.36	0.57
1:A:237:ARG:NH2	1:A:574:ILE:O	2.37	0.57
1:C:152:PHE:HB2	1:C:163:VAL:HB	1.85	0.57
1:C:421:SER:O	1:C:425:ILE:HD13	2.04	0.57
1:D:406:GLU:HG2	1:D:457:ILE:HG21	1.86	0.57
1:D:398:TYR:O	1:D:400:LYS:NZ	2.36	0.57
1:A:255:THR:HG21	1:B:272:GLU:O	2.05	0.57
1:C:547:LEU:HD12	1:C:548:PRO:HD2	1.86	0.57
1:A:358:ILE:HG13	1:A:492:LEU:HD22	1.87	0.57
1:B:354:TYR:CD2	1:B:490:GLU:HB3	2.40	0.56
1:B:472:PRO:HD2	1:B:475:MET:HE3	1.88	0.56
1:D:304:ARG:HH12	1:D:324:GLU:CD	2.07	0.56
1:D:444:THR:OG1	1:D:447:LYS:HG3	2.06	0.56
1:A:282:ALA:HB1	1:A:305:ILE:HD11	1.87	0.56
1:B:262:ARG:NH1	1:B:272:GLU:OE1	2.38	0.56
1:A:339:ASN:ND2	1:A:341:GLU:O	2.37	0.56
1:A:476:SER:HB2	1:A:489:THR:HG21	1.88	0.56
1:C:137:GLY:HA3	1:C:154:LEU:HD21	1.88	0.56
1:C:355:ASN:N	1:C:355:ASN:OD1	2.38	0.56
1:B:358:ILE:HG13	1:B:492:LEU:HD22	1.88	0.56
1:C:84:PHE:HE1	1:C:218:LEU:HD23	1.70	0.55
1:A:232:ILE:O	1:A:236:GLN:N	2.35	0.55
1:B:87:ARG:HH12	1:B:188:ASP:CG	2.09	0.55
1:C:142:VAL:HG23	1:C:152:PHE:CE1	2.41	0.55
1:C:192:ILE:HG23	1:C:208:PRO:HB3	1.88	0.55
1:C:341:GLU:OE1	1:D:277:MET:N	2.29	0.55
1:B:230:THR:HG22	1:B:232:ILE:N	2.22	0.55
1:B:339:ASN:OD1	1:B:340:PRO:HD2	2.05	0.55
1:B:491:ARG:HG3	1:B:505:TYR:HB3	1.89	0.55
1:C:380:TYR:HA	1:C:566:ASN:ND2	2.22	0.55
1:A:327:LYS:HD2	1:A:341:GLU:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:TYR:HB2	1:A:492:LEU:HD23	1.89	0.55
1:C:502:LEU:HB3	1:C:555:LEU:HD23	1.88	0.55
1:C:150:ARG:NH2	1:C:182:ASP:OD1	2.40	0.54
1:D:420:ASP:HA	1:D:445:ALA:HB2	1.89	0.54
1:D:465:PRO:HB2	1:D:494:MET:HE3	1.89	0.54
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.87	0.54
1:D:257:ILE:HG12	1:D:372:LEU:HD11	1.89	0.54
1:A:482:HIS:HB3	1:A:485:LYS:O	2.07	0.54
1:B:561:THR:O	1:B:565:THR:OG1	2.20	0.54
1:A:122:LEU:HB2	1:A:198:LYS:HD2	1.89	0.54
1:C:94:GLN:HG2	1:C:99:ILE:HD12	1.90	0.54
1:A:230:THR:O	1:A:231:GLU:HB3	2.07	0.54
1:B:266:ASN:OD1	1:B:323:TYR:OH	2.18	0.54
1:B:476:SER:HB3	1:B:491:ARG:HH11	1.73	0.54
1:C:268:ARG:NH1	1:C:268:ARG:HG2	2.22	0.54
1:C:338:HIS:HB3	2:C:601:KRS:C1	2.38	0.54
1:D:427:LYS:O	1:D:431:ILE:HG13	2.07	0.54
1:C:104:HIS:HE1	1:D:481:TYR:O	1.91	0.54
1:A:128:LEU:HD21	1:A:131:THR:CG2	2.39	0.53
1:C:339:ASN:ND2	1:C:339:ASN:C	2.57	0.53
1:C:339:ASN:HD22	1:C:341:GLU:H	1.54	0.53
1:D:425:ILE:HG22	1:D:429:ILE:HD11	1.90	0.53
1:D:256:LYS:HA	1:D:259:ASN:HB2	1.90	0.53
1:D:128:LEU:O	1:D:195:PHE:HB2	2.09	0.53
1:D:420:ASP:O	1:D:425:ILE:HD13	2.09	0.53
1:D:111:SER:HB3	1:D:114:GLU:OE2	2.09	0.53
1:C:292:THR:HB	1:D:292:THR:HB	1.90	0.53
1:D:335:ASP:OD1	1:D:338:HIS:HB2	2.09	0.53
1:A:335:ASP:HB3	1:A:338:HIS:HB2	1.90	0.53
1:A:403:ILE:HG21	1:A:471:HIS:HA	1.91	0.53
1:D:239:LEU:O	1:D:243:ILE:HG12	2.09	0.53
1:B:111:SER:OG	1:B:114:GLU:HG3	2.09	0.52
1:B:270:PHE:HB3	1:B:323:TYR:CD1	2.44	0.52
1:B:468:ILE:HG22	1:B:471:HIS:HE1	1.74	0.52
1:C:109:THR:HG23	1:C:134:ASN:HB2	1.90	0.52
1:D:459:ASN:OD1	1:D:459:ASN:N	2.42	0.52
1:B:339:ASN:HD22	1:B:574:ILE:CD1	2.22	0.52
1:D:170:HIS:CD2	1:D:170:HIS:O	2.63	0.52
1:A:481:TYR:CE2	1:B:104:HIS:HE1	2.28	0.52
1:C:465:PRO:HB3	1:C:496:ILE:HG12	1.91	0.52
1:D:473:GLN:HA	1:D:489:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:LYS:O	1:C:431:ILE:HG13	2.09	0.52
1:D:125:GLY:N	1:D:199:SER:O	2.36	0.52
1:D:232:ILE:HG13	1:D:233:ARG:N	2.25	0.52
1:A:213:LEU:HD21	1:A:216:ALA:HB2	1.92	0.51
1:D:425:ILE:HG22	1:D:429:ILE:HD12	1.92	0.51
1:B:222:PRO:HG2	1:B:243:ILE:HD13	1.92	0.51
1:D:290:PHE:O	1:D:302:TYR:HA	2.09	0.51
1:D:304:ARG:NH1	1:D:324:GLU:OE2	2.37	0.51
1:C:353:ASP:N	1:C:353:ASP:OD1	2.44	0.51
1:D:102:TYR:HE1	1:D:216:ALA:H	1.57	0.51
1:B:472:PRO:HA	1:B:488:LEU:HA	1.93	0.51
1:C:299:LEU:HD23	1:C:301:LEU:HD21	1.91	0.51
1:A:514:GLN:HG3	1:A:516:GLU:H	1.76	0.51
1:B:468:ILE:HG22	1:B:471:HIS:CE1	2.45	0.51
1:C:509:ASN:N	1:C:509:ASN:OD1	2.41	0.51
1:C:288:ARG:HG3	1:C:331:ASN:HB3	1.93	0.51
1:C:338:HIS:CD2	1:C:559:ARG:NH2	2.78	0.51
1:C:81:ARG:O	1:C:85:GLU:HG3	2.11	0.51
1:B:339:ASN:ND2	1:B:574:ILE:CD1	2.74	0.51
1:D:199:SER:OG	1:D:200:LYS:N	2.44	0.51
1:C:381:ASN:HA	1:C:389:PRO:HA	1.91	0.50
1:A:252:VAL:HA	1:B:271:PHE:CZ	2.45	0.50
1:A:328:VAL:HG12	1:A:329:PHE:N	2.25	0.50
1:C:145:SER:HB3	1:C:146:GLY:HA3	1.94	0.50
1:C:494:MET:HB3	1:C:502:LEU:HG	1.92	0.50
1:C:556:GLY:O	1:C:559:ARG:N	2.45	0.50
1:A:275:THR:HB	1:A:324:GLU:OE1	2.12	0.50
1:B:454:SER:HA	1:B:458:GLU:HG3	1.93	0.49
1:B:471:HIS:O	1:B:489:THR:OG1	2.24	0.49
1:A:464:LYS:HB2	1:A:465:PRO:HD2	1.94	0.49
1:C:134:ASN:OD1	1:C:193:VAL:HG22	2.12	0.49
1:D:383:ASP:O	1:D:387:ASN:HB2	2.12	0.49
1:D:305:ILE:HG22	1:D:329:PHE:O	2.12	0.49
1:D:270:PHE:HB3	1:D:323:TYR:CD1	2.48	0.49
1:D:465:PRO:HB3	1:D:496:ILE:HG12	1.95	0.49
1:A:111:SER:OG	1:A:114:GLU:HG3	2.12	0.49
1:A:481:TYR:O	1:B:104:HIS:NE2	2.26	0.49
1:B:315:ILE:HD13	1:B:319:ILE:O	2.13	0.49
1:C:312:LYS:HD2	1:C:539:PHE:CE2	2.47	0.49
1:D:138:ARG:NH1	1:D:187:GLY:O	2.46	0.49
1:D:232:ILE:HA	1:D:235:ARG:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG21	1:A:394:PHE:CG	2.47	0.49
1:C:467:PHE:HB3	1:C:469:VAL:HG23	1.94	0.49
1:B:312:LYS:HE3	1:B:539:PHE:CZ	2.48	0.49
1:B:239:LEU:O	1:B:243:ILE:HD12	2.13	0.49
1:C:338:HIS:CD2	1:C:559:ARG:HH21	2.31	0.49
1:C:103:PRO:HD2	1:C:214:LEU:HA	1.95	0.48
1:C:290:PHE:HE2	1:D:294:HIS:HA	1.77	0.48
1:B:387:ASN:ND2	1:B:387:ASN:N	2.61	0.48
1:C:365:PHE:HE2	1:C:502:LEU:HD23	1.78	0.48
1:A:382:LYS:HE2	1:A:497:CYS:SG	2.54	0.48
1:D:432:ILE:HD12	1:D:433:LYS:N	2.28	0.48
1:A:415:LEU:HD23	1:A:427:LYS:HG2	1.94	0.48
1:C:314:LEU:HD11	1:D:575:LEU:HD13	1.95	0.48
1:C:252:VAL:HA	1:D:271:PHE:CZ	2.48	0.48
1:A:392:ILE:HG23	1:A:464:LYS:HA	1.94	0.48
1:A:403:ILE:O	1:A:407:ILE:HG13	2.13	0.48
1:A:559:ARG:O	1:A:562:MET:HB2	2.14	0.48
1:B:247:SER:O	1:B:250:THR:HB	2.14	0.48
1:A:254:ARG:NH1	1:A:573:VAL:O	2.47	0.48
1:B:408:GLU:HG2	1:B:415:LEU:H	1.79	0.48
1:B:496:ILE:HD12	1:B:501:VAL:HG21	1.95	0.48
1:D:237:ARG:O	1:D:241:LEU:HD12	2.13	0.48
1:D:291:ILE:HG12	1:D:302:TYR:CE1	2.49	0.48
1:A:422:ASN:O	1:A:425:ILE:HB	2.14	0.47
1:C:109:THR:CG2	1:C:134:ASN:HD22	2.28	0.47
1:D:185:ARG:HG2	1:D:185:ARG:NH2	2.27	0.47
1:D:509:ASN:N	1:D:509:ASN:OD1	2.40	0.47
1:A:233:ARG:HG3	1:A:240:ASP:CB	2.41	0.47
1:A:450:ASP:O	1:A:454:SER:OG	2.26	0.47
1:C:154:LEU:HB2	1:C:163:VAL:HG23	1.96	0.47
1:B:390:ILE:HD12	1:B:462:ASN:HB3	1.96	0.47
1:D:234:TYR:CE2	1:D:571:LYS:HB2	2.49	0.47
1:C:193:VAL:HB	1:C:210:GLU:HG2	1.96	0.47
1:A:293:HIS:ND1	1:A:300:ASP:OD1	2.39	0.47
1:C:419:PHE:O	1:C:425:ILE:HD11	2.14	0.47
1:C:358:ILE:HG13	1:C:492:LEU:HD22	1.96	0.47
1:C:410:VAL:HG22	1:C:411:THR:H	1.79	0.47
1:A:127:HIS:HB3	1:A:195:PHE:HE1	1.79	0.47
1:B:122:LEU:HD21	1:B:128:LEU:HD11	1.96	0.47
1:B:138:ARG:NH1	1:B:187:GLY:O	2.48	0.47
1:D:263:ASN:O	1:D:267:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:THR:O	1:D:448:LEU:HB2	2.15	0.47
1:D:556:GLY:H	2:D:601:KRS:H20	1.80	0.47
1:A:556:GLY:O	1:A:559:ARG:N	2.47	0.47
1:B:419:PHE:CE2	1:B:449:LEU:HD21	2.49	0.46
1:A:136:THR:HG22	1:A:191:GLY:HA2	1.96	0.46
1:A:465:PRO:HB3	1:A:496:ILE:HG12	1.97	0.46
1:B:228:LYS:HA	1:B:229:ASP:HA	1.61	0.46
1:B:383:ASP:HB2	1:B:387:ASN:HB3	1.97	0.46
1:A:411:THR:HG23	1:A:413:THR:HG22	1.97	0.46
1:B:275:THR:OG1	1:B:304:ARG:NH1	2.47	0.46
1:B:87:ARG:HA	1:B:90:PHE:HB3	1.97	0.46
1:A:478:LEU:HA	1:A:478:LEU:HD23	1.72	0.46
1:B:93:ASP:O	1:B:97:LYS:HG3	2.15	0.46
1:D:144:ALA:O	1:D:146:GLY:N	2.48	0.46
1:D:305:ILE:HB	1:D:330:ARG:HD3	1.98	0.46
1:D:417:GLN:HA	1:D:418:PRO:C	2.36	0.46
1:C:335:ASP:OD2	1:C:336:ASN:N	2.48	0.46
1:D:170:HIS:CE1	1:D:177:PHE:HA	2.51	0.46
1:C:484:THR:OG1	1:C:485:LYS:N	2.49	0.46
1:C:491:ARG:HA	1:C:505:TYR:HB3	1.97	0.46
1:D:139:ILE:HG23	1:D:152:PHE:HB3	1.98	0.46
1:A:141:ARG:HB3	1:A:153:ASP:HB2	1.97	0.46
1:A:106:PHE:CZ	1:A:134:ASN:HB3	2.51	0.46
1:B:112:ILE:HG12	1:B:135:ILE:HD11	1.97	0.46
1:C:335:ASP:CG	1:C:336:ASN:N	2.68	0.46
1:C:402:SER:HB2	1:C:405:GLU:HG2	1.96	0.46
1:A:252:VAL:O	1:A:256:LYS:HG2	2.16	0.46
1:A:315:ILE:HA	1:A:319:ILE:O	2.16	0.46
1:C:166:ASN:HB3	1:C:169:PHE:CD2	2.48	0.45
1:A:169:PHE:O	1:A:209:LYS:HE2	2.17	0.45
1:C:252:VAL:HA	1:D:271:PHE:HZ	1.82	0.45
1:B:248:ARG:O	1:B:252:VAL:HG23	2.16	0.45
1:B:91:ILE:HG22	1:B:95:LYS:HE3	1.99	0.45
1:C:112:ILE:HD11	1:C:154:LEU:CD2	2.46	0.45
1:C:291:ILE:HG22	1:C:302:TYR:CD1	2.52	0.45
1:D:427:LYS:HB2	1:D:427:LYS:HE3	1.76	0.45
1:B:510:ASP:HB3	1:B:513:LYS:HB2	1.97	0.45
1:A:199:SER:N	1:A:202:GLY:HA2	2.32	0.45
1:A:399:PRO:HG2	1:A:466:PHE:CB	2.46	0.45
1:C:128:LEU:O	1:C:195:PHE:HB2	2.17	0.45
1:A:272:GLU:HB2	1:A:323:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:THR:HG22	1:B:232:ILE:H	1.81	0.45
1:B:330:ARG:HG3	1:B:342:PHE:HE1	1.82	0.45
1:C:222:PRO:HG2	1:C:243:ILE:HD11	1.98	0.45
1:A:408:GLU:HG2	1:A:415:LEU:H	1.82	0.45
1:C:145:SER:OG	1:C:150:ARG:NH1	2.49	0.45
1:B:440:PRO:C	1:B:441:ASN:ND2	2.63	0.45
1:C:84:PHE:CD1	1:C:218:LEU:HB3	2.52	0.45
1:C:501:VAL:O	2:C:601:KRS:H20	2.17	0.45
1:D:143:SER:HB2	1:D:151:PHE:H	1.81	0.45
1:A:504:ALA:HB2	1:A:553:LEU:HG	1.99	0.44
1:B:257:ILE:CD1	1:B:564:LEU:HD12	2.46	0.44
1:C:455:HIS:ND1	1:C:456:PHE:HD2	2.14	0.44
1:C:149:LEU:HD23	1:C:166:ASN:HA	1.99	0.44
1:C:234:TYR:OH	1:C:572:ASP:OD1	2.17	0.44
1:A:329:PHE:O	1:A:330:ARG:HG2	2.16	0.44
1:B:425:ILE:O	1:B:429:ILE:HG13	2.17	0.44
1:B:455:HIS:C	1:B:455:HIS:CD2	2.91	0.44
1:B:79:ASP:HA	1:B:80:PRO:HD3	1.86	0.44
1:B:419:PHE:C	1:B:421:SER:H	2.20	0.44
1:C:482:HIS:HB3	1:C:485:LYS:O	2.18	0.44
1:D:334:ILE:HG22	1:D:340:PRO:HD3	2.00	0.44
1:D:501:VAL:O	2:D:601:KRS:H20	2.17	0.44
1:B:283:GLY:N	1:B:289:PRO:HB3	2.33	0.44
1:C:138:ARG:NH2	1:C:189:ILE:HD11	2.32	0.44
1:C:418:PRO:HG2	1:C:421:SER:HB2	2.00	0.44
1:C:471:HIS:CE1	1:C:491:ARG:HE	2.36	0.44
1:D:570:ILE:O	1:D:573:VAL:HG22	2.18	0.44
1:B:308:GLU:HG3	1:B:309:LEU:HG	2.00	0.44
1:B:473:GLN:H	1:B:473:GLN:HG2	1.56	0.44
1:C:260:PHE:O	1:C:264:PHE:HB2	2.18	0.44
1:D:112:ILE:O	1:D:116:ILE:HG13	2.18	0.44
1:A:547:LEU:HD12	1:A:548:PRO:HD2	2.00	0.43
1:B:147:GLN:HB2	1:B:148:LYS:H	1.43	0.43
1:B:252:VAL:O	1:B:256:LYS:HG3	2.18	0.43
1:B:500:GLU:HB3	1:B:559:ARG:HH12	1.83	0.43
1:C:288:ARG:H	1:C:288:ARG:HG2	1.58	0.43
1:A:291:ILE:HG12	1:A:302:TYR:CE2	2.53	0.43
1:A:264:PHE:CZ	1:A:364:PHE:HA	2.53	0.43
1:A:398:TYR:HB2	1:A:467:PHE:CE2	2.53	0.43
1:B:453:ALA:HA	1:B:457:ILE:HD12	2.00	0.43
1:C:84:PHE:CE1	1:C:218:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:PHE:HE2	1:D:181:TYR:HD1	1.66	0.43
1:D:260:PHE:O	1:D:264:PHE:HB2	2.19	0.43
1:D:429:ILE:HG13	1:D:448:LEU:HD11	1.99	0.43
1:A:199:SER:C	1:A:202:GLY:H	2.22	0.43
1:D:92:GLN:NE2	1:D:96:ASP:OD1	2.52	0.43
1:B:116:ILE:O	1:B:120:LYS:HG3	2.18	0.43
1:B:260:PHE:O	1:B:264:PHE:HB2	2.18	0.43
1:C:290:PHE:CD1	1:C:329:PHE:HB3	2.51	0.43
1:C:432:ILE:HG13	1:C:448:LEU:HD22	2.00	0.43
1:A:292:THR:HG1	1:B:290:PHE:HD1	1.67	0.43
1:A:442:PRO:HA	1:A:443:PRO:HD3	1.83	0.43
1:B:164:LEU:O	1:B:208:PRO:HD2	2.18	0.43
1:B:473:GLN:HB3	1:B:489:THR:HG23	2.01	0.43
1:D:404:VAL:HG23	1:D:415:LEU:HD11	2.00	0.43
1:A:164:LEU:HD13	1:A:207:PHE:HE1	1.83	0.43
1:B:354:TYR:O	1:B:358:ILE:HD12	2.19	0.43
1:C:164:LEU:HD22	1:C:207:PHE:CE1	2.54	0.43
1:C:567:LYS:HA	1:C:567:LYS:HD3	1.74	0.43
1:A:425:ILE:HG22	1:A:426:GLU:N	2.33	0.43
1:B:559:ARG:O	1:B:562:MET:HB2	2.18	0.43
1:C:303:LEU:HB3	1:C:329:PHE:CD1	2.54	0.43
1:D:143:SER:OG	1:D:151:PHE:HB2	2.18	0.43
1:D:342:PHE:CE1	2:D:601:KRS:H5	2.54	0.43
1:D:425:ILE:HA	1:D:428:MET:HE2	1.99	0.43
1:D:559:ARG:O	1:D:562:MET:HB2	2.19	0.43
1:A:399:PRO:HG2	1:A:466:PHE:HB3	2.01	0.43
1:B:240:ASP:OD1	1:B:244:ASN:ND2	2.52	0.43
1:C:279:ASN:HB2	1:C:281:ILE:HG22	2.01	0.43
1:B:387:ASN:H	1:B:387:ASN:HD22	1.65	0.42
1:C:111:SER:HB3	1:C:114:GLU:HG3	2.01	0.42
1:C:134:ASN:HA	1:C:192:ILE:O	2.18	0.42
1:D:108:ARG:CZ	1:D:111:SER:HB2	2.49	0.42
1:A:420:ASP:O	1:A:425:ILE:HG12	2.19	0.42
1:C:291:ILE:O	1:C:291:ILE:HG13	2.19	0.42
1:D:432:ILE:C	1:D:432:ILE:HD12	2.38	0.42
1:D:94:GLN:HG3	1:D:99:ILE:CG2	2.49	0.42
2:D:601:KRS:H11	2:D:601:KRS:H8	1.81	0.42
1:B:293:HIS:HD2	1:B:294:HIS:N	2.17	0.42
1:C:369:VAL:HG21	1:C:394:PHE:CD2	2.55	0.42
1:A:199:SER:HB3	1:A:203:GLU:H	1.84	0.42
1:C:199:SER:OG	1:C:200:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ILE:H	1:C:305:ILE:HD12	1.85	0.42
1:C:369:VAL:HG21	1:C:394:PHE:CG	2.54	0.42
1:B:112:ILE:O	1:B:116:ILE:HG12	2.20	0.42
1:C:504:ALA:HB2	1:C:553:LEU:HG	2.01	0.42
1:D:90:PHE:O	1:D:94:GLN:HB2	2.19	0.42
1:A:422:ASN:HB3	1:A:423:GLU:H	1.50	0.42
1:A:128:LEU:O	1:A:195:PHE:HB2	2.20	0.41
1:B:429:ILE:O	1:B:432:ILE:HG22	2.20	0.41
1:C:559:ARG:O	1:C:562:MET:HB2	2.21	0.41
1:D:228:LYS:HA	1:D:229:ASP:HA	1.48	0.41
1:B:339:ASN:ND2	1:B:574:ILE:HD12	2.33	0.41
1:C:338:HIS:HD2	1:C:559:ARG:HH21	1.67	0.41
1:C:347:PHE:CE2	1:C:553:LEU:HB3	2.55	0.41
1:A:275:THR:HG22	1:A:304:ARG:HH11	1.85	0.41
1:D:162:GLN:HB3	1:D:205:SER:HB3	2.03	0.41
1:A:403:ILE:HG23	1:A:404:VAL:H	1.85	0.41
1:A:411:THR:HG23	1:A:413:THR:H	1.85	0.41
1:C:112:ILE:O	1:C:116:ILE:HG13	2.21	0.41
1:C:477:PRO:O	1:C:478:LEU:HB2	2.20	0.41
1:D:448:LEU:O	1:D:452:LEU:HD12	2.21	0.41
1:A:154:LEU:HD22	1:A:192:ILE:HD12	2.03	0.41
1:B:154:LEU:HB2	1:B:163:VAL:HG23	2.03	0.41
1:B:244:ASN:C	1:B:246:SER:H	2.24	0.41
1:B:357:LEU:HD13	1:B:504:ALA:HB1	2.03	0.41
1:C:506:THR:HA	1:C:551:GLY:HA2	2.01	0.41
1:D:142:VAL:HB	1:D:152:PHE:CE1	2.56	0.41
1:A:127:HIS:HB3	1:A:195:PHE:CE1	2.56	0.41
1:B:463:ASP:OD2	1:B:464:LYS:HG3	2.21	0.41
1:B:511:PRO:HG3	1:B:543:LEU:HB3	2.01	0.41
1:C:398:TYR:HB3	1:C:465:PRO:O	2.19	0.41
1:D:112:ILE:HD12	1:D:156:GLY:N	2.35	0.41
1:D:353:ASP:O	1:D:357:LEU:HD12	2.21	0.41
1:B:240:ASP:O	1:B:244:ASN:HB2	2.20	0.41
1:D:112:ILE:HG12	1:D:135:ILE:HD11	2.01	0.41
1:A:198:LYS:HB3	1:A:198:LYS:HE2	1.83	0.41
1:A:509:ASN:N	1:A:509:ASN:OD1	2.50	0.41
1:C:393:ASP:HB3	1:C:463:ASP:O	2.21	0.41
1:A:116:ILE:O	1:A:120:LYS:N	2.54	0.41
1:A:413:THR:HG21	1:A:431:ILE:HD11	2.03	0.41
1:A:462:ASN:O	1:A:464:LYS:N	2.54	0.41
1:C:308:GLU:O	1:C:312:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ILE:HG21	1:C:400:LYS:HE3	2.02	0.41
1:A:228:LYS:H	1:A:233:ARG:NH1	2.18	0.40
1:B:275:THR:OG1	1:B:324:GLU:OE1	2.22	0.40
1:B:411:THR:HG23	1:B:413:THR:N	2.34	0.40
1:C:417:GLN:HA	1:C:418:PRO:C	2.41	0.40
1:D:353:ASP:OD1	1:D:356:ASP:N	2.54	0.40
1:A:115:PHE:CE2	1:A:196:PRO:HB3	2.56	0.40
1:A:164:LEU:HD13	1:A:207:PHE:CE1	2.55	0.40
1:A:193:VAL:HB	1:A:210:GLU:HG2	2.03	0.40
1:A:222:PRO:HD2	1:A:243:ILE:HD11	2.04	0.40
1:B:442:PRO:HA	1:B:443:PRO:HD3	1.74	0.40
1:A:150:ARG:HG3	1:A:150:ARG:NH1	2.31	0.40
1:A:155:VAL:HG12	1:A:160:LYS:HD3	2.03	0.40
1:A:270:PHE:HB3	1:A:323:TYR:CD1	2.57	0.40
1:A:432:ILE:HG21	1:A:439:LEU:HA	2.03	0.40
1:C:162:GLN:HB3	1:C:205:SER:HG	1.86	0.40
1:C:164:LEU:O	1:C:208:PRO:HD2	2.22	0.40
1:A:425:ILE:HD13	1:A:448:LEU:HD12	2.03	0.40
1:A:501:VAL:O	2:A:601:KRS:H20	2.21	0.40
1:A:138:ARG:NH2	1:B:316:VAL:O	2.55	0.40
1:B:447:LYS:HA	1:B:447:LYS:HD2	1.78	0.40
1:C:164:LEU:O	1:C:207:PHE:HA	2.20	0.40
1:C:428:MET:HA	1:C:431:ILE:HD12	2.03	0.40
1:D:192:ILE:HG12	1:D:211:THR:HG23	2.03	0.40
1:D:362:GLU:O	1:D:366:SER:OG	2.22	0.40
1:A:502:LEU:HD12	1:A:555:LEU:HD21	2.02	0.40
1:C:84:PHE:HD1	1:C:218:LEU:HB3	1.86	0.40
1:C:265:LEU:HD21	1:C:360:TRP:CZ2	2.56	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	477/516 (92%)	457 (96%)	20 (4%)	0	100	100
1	B	480/516 (93%)	460 (96%)	20 (4%)	0	100	100
1	C	477/516 (92%)	455 (95%)	22 (5%)	0	100	100
1	D	469/516 (91%)	450 (96%)	19 (4%)	0	100	100
All	All	1903/2064 (92%)	1822 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	407/464 (88%)	400 (98%)	7 (2%)	66	86
1	B	403/464 (87%)	394 (98%)	9 (2%)	57	83
1	C	384/464 (83%)	375 (98%)	9 (2%)	56	82
1	D	388/464 (84%)	380 (98%)	8 (2%)	59	83
All	All	1582/1856 (85%)	1549 (98%)	33 (2%)	59	83

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	127	HIS
1	A	129	GLU
1	A	231	GLU
1	A	332	GLU
1	A	425	ILE
1	A	454	SER
1	B	82	LEU
1	B	147	GLN
1	B	227	LEU
1	B	232	ILE
1	B	294	HIS
1	B	339	ASN

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Mol	Chain	Res	Type
1	B	421	SER
1	B	441	ASN
1	B	482	HIS
1	C	227	LEU
1	C	268	ARG
1	C	328	VAL
1	C	339	ASN
1	C	355	ASN
1	C	449	LEU
1	C	464	LYS
1	C	501	VAL
1	C	572	ASP
1	D	108	ARG
1	D	176	ASN
1	D	227	LEU
1	D	235	ARG
1	D	383	ASP
1	D	415	LEU
1	D	425	ILE
1	D	459	ASN

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

Mol	Chain	Res	Type
1	A	104	HIS
1	A	381	ASN
1	A	462	ASN
1	B	387	ASN
1	B	441	ASN
1	B	455	HIS
1	B	471	HIS
1	C	134	ASN
1	C	339	ASN
1	C	417	GLN
1	C	459	ASN
1	C	566	ASN
1	D	170	HIS
1	D	171	ASN
1	D	430	ASN
1	D	514	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

4 ligands 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	KRS	A	601	-	23,23,23	1.99	3 (13%)	32,33,33	1.84	6 (18%)
2	KRS	B	601	-	23,23,23	2.03	3 (13%)	32,33,33	1.43	5 (15%)
2	KRS	C	601	-	23,23,23	2.00	3 (13%)	32,33,33	1.71	6 (18%)
2	KRS	D	601	-	23,23,23	1.91	3 (13%)	32,33,33	2.21	7 (21%)

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	KRS	A	601	-	-	0/4/26/26	0/3/3/3
2	KRS	B	601	-	-	0/4/26/26	0/3/3/3
2	KRS	C	601	-	-	0/4/26/26	0/3/3/3
2	KRS	D	601	-	-	0/4/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	KRS	C9-C5	3.00	1.47	1.41
2	C	601	KRS	C9-C5	3.11	1.47	1.41
2	D	601	KRS	C9-C5	3.16	1.48	1.41
2	A	601	KRS	C9-C5	3.21	1.48	1.41
2	D	601	KRS	C9-C1	4.02	1.48	1.41
2	C	601	KRS	C9-C1	4.19	1.48	1.41
2	B	601	KRS	C9-C1	4.23	1.48	1.41
2	A	601	KRS	C9-C1	4.41	1.48	1.41
2	D	601	KRS	O3-C8	7.22	1.45	1.35
2	A	601	KRS	O3-C8	7.34	1.45	1.35
2	C	601	KRS	O3-C8	7.64	1.46	1.35
2	B	601	KRS	O3-C8	7.86	1.46	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	KRS	C14-C13-C12	-5.63	107.12	110.99
2	D	601	KRS	C11-C10-C7	-5.41	107.51	114.44
2	D	601	KRS	C7-O3-C8	-5.25	109.88	118.83
2	A	601	KRS	C7-O3-C8	-4.91	110.46	118.83
2	A	601	KRS	C11-C10-C7	-4.87	108.20	114.44
2	C	601	KRS	C11-C10-C7	-4.83	108.25	114.44
2	D	601	KRS	O5-C12-C13	-4.75	107.02	109.97
2	A	601	KRS	C14-C13-C12	-3.56	108.54	110.99
2	B	601	KRS	C7-O3-C8	-3.43	112.98	118.83
2	C	601	KRS	C7-O3-C8	-3.39	113.05	118.83
2	A	601	KRS	O5-C12-C13	-3.20	107.99	109.97
2	B	601	KRS	C10-C7-C6	-3.01	107.51	113.25
2	C	601	KRS	C14-C13-C12	-2.90	109.00	110.99
2	C	601	KRS	O5-C12-C13	-2.67	108.31	109.97
2	C	601	KRS	C10-C7-C6	-2.61	108.27	113.25
2	B	601	KRS	C14-C13-C12	-2.12	109.53	110.99
2	D	601	KRS	C10-C7-C6	-2.09	109.26	113.25
2	B	601	KRS	C11-C10-C7	-2.06	111.80	114.44
2	A	601	KRS	O3-C8-O4	2.00	120.00	117.62
2	D	601	KRS	O3-C8-O4	2.45	120.53	117.62
2	D	601	KRS	C1-C9-C8	2.92	122.99	119.61
2	B	601	KRS	C1-C9-C8	3.26	123.39	119.61
2	A	601	KRS	C1-C9-C8	3.60	123.79	119.61
2	C	601	KRS	C1-C9-C8	3.70	123.91	119.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	KRS	1	0
2	C	601	KRS	3	0
2	D	601	KRS	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	485/516 (93%)	-0.01	3 (0%)	89	86	29, 51, 73, 94	0
1	B	486/516 (94%)	0.05	10 (2%)	64	60	31, 50, 78, 101	0
1	C	485/516 (93%)	0.24	28 (5%)	24	23	41, 64, 92, 120	0
1	D	479/516 (92%)	0.20	17 (3%)	44	40	40, 65, 87, 109	0
All	All	1935/2064 (93%)	0.12	58 (2%)	51	47	29, 57, 87, 120	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	202	GLY	4.5
1	C	123	GLY	3.8
1	D	197	GLY	3.7
1	A	462	ASN	3.4
1	C	199	SER	3.3
1	C	429	ILE	3.3
1	C	443	PRO	3.2
1	B	440	PRO	3.2
1	C	204	LEU	3.0
1	D	435	HIS	3.0
1	C	411	THR	2.9
1	C	415	LEU	2.9
1	D	443	PRO	2.9
1	D	421	SER	2.9
1	C	122	LEU	2.8
1	C	198	LYS	2.8
1	C	196	PRO	2.7
1	C	169	PHE	2.7
1	C	130	ASP	2.7
1	B	434	GLU	2.7
1	C	124	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	432	ILE	2.6
1	D	295	ASN	2.6
1	B	581	PRO	2.6
1	A	82	LEU	2.5
1	C	197	GLY	2.5
1	D	121	ASP	2.5
1	C	419	PHE	2.5
1	B	439	LEU	2.4
1	B	415	LEU	2.4
1	D	411	THR	2.4
1	B	432	ILE	2.4
1	B	441	ASN	2.4
1	D	286	ASN	2.3
1	B	431	ILE	2.3
1	C	517	CYS	2.3
1	C	440	PRO	2.3
1	C	229	ASP	2.3
1	C	295	ASN	2.3
1	D	166	ASN	2.3
1	C	456	PHE	2.3
1	D	431	ILE	2.2
1	C	126	GLU	2.2
1	A	197	GLY	2.2
1	B	443	PRO	2.2
1	D	79	ASP	2.2
1	D	581	PRO	2.2
1	C	125	GLY	2.2
1	B	430	ASN	2.2
1	D	445	ALA	2.2
1	D	517	CYS	2.1
1	C	127	HIS	2.1
1	C	448	LEU	2.1
1	C	207	PHE	2.1
1	D	96	ASP	2.1
1	D	440	PRO	2.1
1	C	430	ASN	2.0
1	C	413	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	KRS	A	601	21/21	0.94	0.23	0.67	35,36,38,39	0
2	KRS	B	601	21/21	0.94	0.24	0.53	40,41,43,44	0
2	KRS	C	601	21/21	0.94	0.21	-0.62	50,54,55,56	0
2	KRS	D	601	21/21	0.94	0.20	-0.91	49,51,53,54	0

6.5 Other polymers (i)

There are no such residues in this entry.