



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:56 AM GMT

PDB ID : 3KAK
Title : Structure of homoglutathione synthetase from Glycine max in open conformation with gamma-glutamyl-cysteine bound.
Authors : Galant, A.; Arkus, K.A.J.; Zubieta, C.; Cahoon, R.E.; Jez, J.M.
Deposited on : 2009-10-19
Resolution : 2.11 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

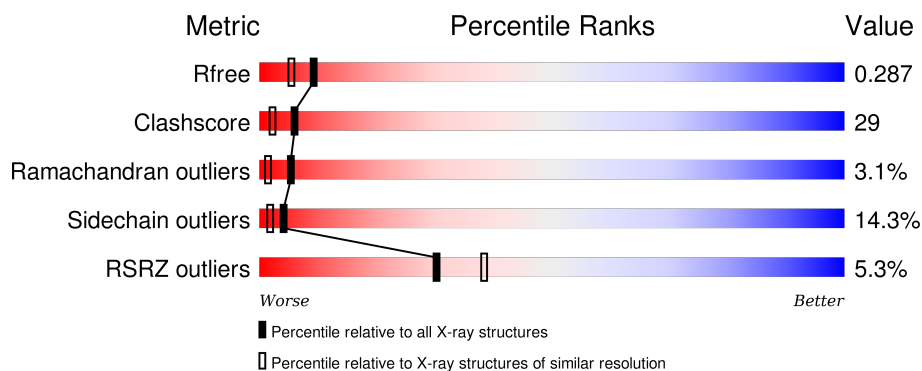
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	91344	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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 $\leq 5\%$. 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	499	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>28%</div> <div>8%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	499	<div> <div>6%</div> <div> <div></div> <div>50%</div> <div>26%</div> <div>8%</div> <div>•</div> <div>12%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3GC	A	501	X	-	X	X
2	3GC	B	501	X	-	-	X
2	3GC	B	502	X	-	X	-

2 Entry composition [i](#)

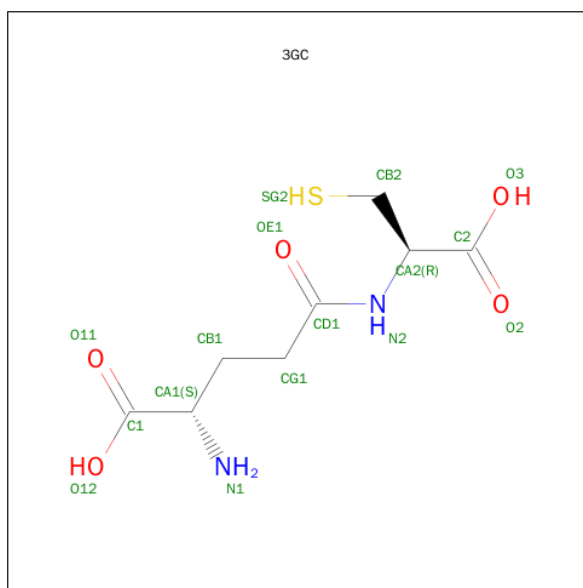
There are 3 unique types of molecules in this entry. The entry contains 7414 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Homoglutathione synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	6	0
			3574	2275	619	665	15			
1	B	437	Total	C	N	O	S	0	6	0
			3511	2230	608	658	15			

- Molecule 2 is GAMMA-GLUTAMYLCYSTEINE (three-letter code: 3GC) (formula: $C_8H_{14}N_2O_5S$).

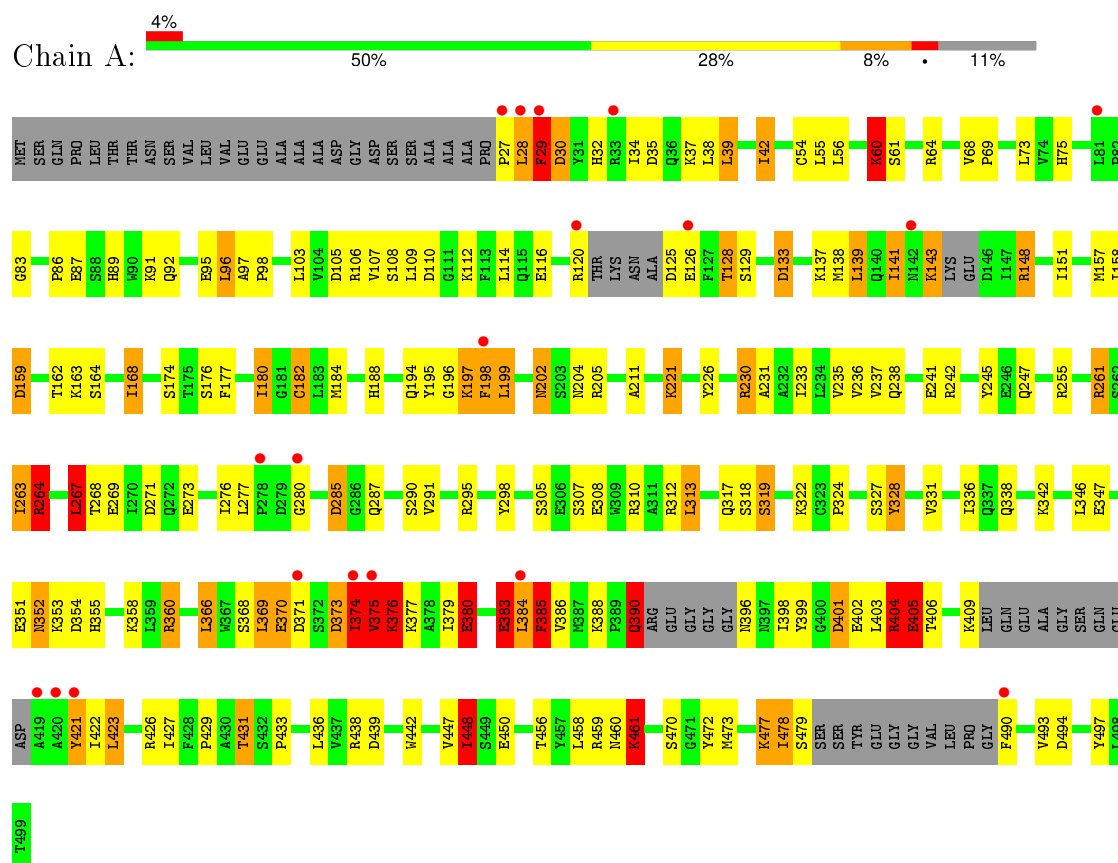


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total 130	O 130	0	0
3	B	151	Total 151	O 151	0	0

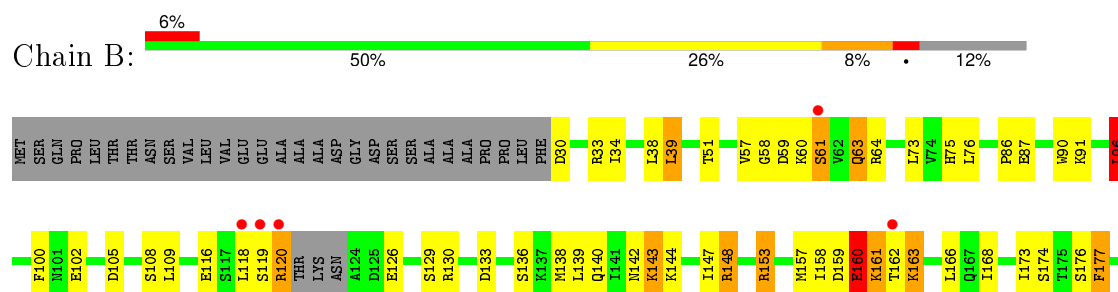
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Homogluthathione synthetase



• Molecule 1: Homogluthathione synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.88Å 80.95Å 89.12Å 90.00° 95.96° 90.00°	Depositor
Resolution (Å)	19.80 – 2.11 19.80 – 2.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.80-2.11) 99.7 (19.80-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.288 0.210 , 0.287	Depositor DCC
R_{free} test set	2635 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 52692 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7414	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.16 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2346e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 3GC

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	1.30	20/3639 (0.5%)	1.25	37/4913 (0.8%)
1	B	1.30	10/3578 (0.3%)	1.27	26/4835 (0.5%)
All	All	1.30	30/7217 (0.4%)	1.26	63/9748 (0.6%)

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	7
1	B	0	10
All	All	0	17

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	GLU	CB-CG	10.16	1.71	1.52
1	B	328	TYR	CD1-CE1	8.04	1.51	1.39
1	A	54	CYS	CB-SG	7.89	1.95	1.82
1	A	383	GLU	CG-CD	7.45	1.63	1.51
1	A	402	GLU	CB-CG	7.02	1.65	1.52
1	B	469	GLU	CD-OE1	6.86	1.33	1.25
1	A	404	ARG	N-CA	6.49	1.59	1.46
1	B	210	ASN	CB-CG	6.48	1.66	1.51
1	B	245	TYR	CD1-CE1	-6.31	1.29	1.39
1	A	375	VAL	CB-CG1	6.03	1.65	1.52
1	A	116	GLU	CG-CD	6.01	1.60	1.51
1	A	328	TYR	CD1-CE1	5.85	1.48	1.39
1	A	380	GLU	CB-CG	5.80	1.63	1.52
1	A	402	GLU	CG-CD	5.75	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	ARG	CA-C	5.74	1.67	1.52
1	B	298	TYR	CE2-CZ	5.70	1.46	1.38
1	B	351	GLU	CB-CG	5.58	1.62	1.52
1	A	405	GLU	CB-CG	-5.56	1.41	1.52
1	B	197	LYS	CD-CE	5.48	1.65	1.51
1	A	472	TYR	CE1-CZ	5.45	1.45	1.38
1	A	384	LEU	CG-CD2	5.43	1.72	1.51
1	B	226	TYR	CD1-CE1	-5.42	1.31	1.39
1	A	385	PHE	N-CA	-5.35	1.35	1.46
1	B	351	GLU	CG-CD	5.34	1.59	1.51
1	A	261	ARG	CG-CD	5.29	1.65	1.51
1	A	390	GLN	CG-CD	5.26	1.63	1.51
1	B	102	GLU	CB-CG	5.24	1.62	1.52
1	A	60	LYS	CD-CE	5.19	1.64	1.51
1	A	404	ARG	C-O	5.12	1.33	1.23
1	A	375	VAL	CA-CB	5.09	1.65	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ARG	NE-CZ-NH2	-13.07	113.77	120.30
1	B	148	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	264	ARG	NE-CZ-NH1	-8.97	115.82	120.30
1	A	255	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	148	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	148	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	B	264	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	439	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	375	VAL	N-CA-C	-7.20	91.56	111.00
1	B	197	LYS	CD-CE-NZ	7.18	128.22	111.70
1	A	295	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	459	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	384	LEU	CB-CA-C	-6.74	97.39	110.20
1	B	490	PHE	CA-CB-CG	6.64	129.83	113.90
1	B	205	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	139	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	376	LYS	N-CA-C	6.49	128.53	111.00
1	A	346	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	267	LEU	CB-CG-CD1	6.48	122.01	111.00
1	A	401	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	182	CYS	CB-CA-C	6.17	122.75	110.40
1	B	489	GLY	CA-C-N	-6.12	103.73	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LEU	CA-C-N	-6.09	103.80	117.20
1	B	489	GLY	O-C-N	6.07	132.42	122.70
1	A	380	GLU	O-C-N	-6.05	113.02	122.70
1	B	478	ILE	CA-C-N	-6.05	103.89	117.20
1	A	267	LEU	CB-CG-CD2	-6.02	100.76	111.00
1	A	255	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	383	GLU	OE1-CD-OE2	-5.98	116.12	123.30
1	B	487	LEU	N-CA-C	-5.98	94.85	111.00
1	A	295	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	422	ILE	N-CA-C	5.88	126.89	111.00
1	B	310	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	423	LEU	CA-CB-CG	5.83	128.70	115.30
1	B	205	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	199	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	153	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	489	GLY	C-N-CA	5.77	136.12	121.70
1	B	314	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	A	28	LEU	O-C-N	5.61	131.68	122.70
1	B	219	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	A	29	PHE	CA-C-N	-5.58	104.94	117.20
1	A	384	LEU	CA-CB-CG	5.58	128.12	115.30
1	B	96	LEU	CA-CB-CG	5.50	127.94	115.30
1	B	130	ARG	CG-CD-NE	5.49	123.32	111.80
1	A	404	ARG	CB-CA-C	-5.48	99.45	110.40
1	B	204	ASN	CB-CA-C	-5.39	99.63	110.40
1	B	38	LEU	CB-CG-CD1	5.34	120.08	111.00
1	B	143	LYS	CD-CE-NZ	-5.32	99.47	111.70
1	B	478	ILE	C-N-CA	5.31	134.99	121.70
1	A	405	GLU	CB-CA-C	-5.24	99.92	110.40
1	A	448	ILE	CG1-CB-CG2	-5.24	99.88	111.40
1	A	383	GLU	N-CA-C	5.22	125.09	111.00
1	B	148	ARG	CG-CD-NE	-5.22	100.84	111.80
1	A	366	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	A	385	PHE	CB-CA-C	5.20	120.79	110.40
1	A	346	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	B	489	GLY	N-CA-C	-5.19	100.13	113.10
1	B	166	LEU	CB-CG-CD2	5.09	119.65	111.00
1	A	438	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	404	ARG	N-CA-C	5.08	124.71	111.00
1	A	312	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	375	VAL	CB-CA-C	5.04	120.97	111.40

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	LEU	Peptide
1	A	373	ASP	Peptide
1	A	374	ILE	Peptide
1	A	375	VAL	Peptide
1	A	380	GLU	Mainchain
1	A	403	LEU	Peptide
1	A	404	ARG	Peptide
1	B	160	GLU	Peptide
1	B	368	SER	Peptide
1	B	384	LEU	Mainchain
1	B	388	LYS	Peptide
1	B	389	PRO	Peptide
1	B	422	ILE	Peptide
1	B	478	ILE	Mainchain
1	B	479	SER	Peptide
1	B	486	VAL	Peptide
1	B	487	LEU	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	3574	0	3616	173	0
1	B	3511	0	3541	236	0
2	A	16	0	11	7	0
2	B	32	0	22	17	0
3	A	130	0	0	15	0
3	B	151	0	0	29	0
All	All	7414	0	7190	409	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 29.

All (409) 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:B:384:LEU:O	1:B:426:ARG:HB2	1.26	1.29
1:A:398:ILE:HG21	1:A:405:GLU:OE1	1.28	1.28
1:A:39:LEU:HD12	1:A:442:TRP:CZ3	1.69	1.25
1:B:374:ILE:O	1:B:376:LYS:N	1.72	1.19
1:B:479:SER:HB3	3:B:640:HOH:O	1.51	1.11
1:A:404:ARG:HG2	1:A:404:ARG:O	1.11	1.10
1:B:487:LEU:HB2	1:B:489:GLY:H	1.18	1.08
1:B:375:VAL:HG22	1:B:379:ILE:HG13	1.29	1.06
1:A:384:LEU:O	1:A:426:ARG:HB2	1.57	1.04
1:B:344:GLY:HA2	3:B:649:HOH:O	1.57	1.03
1:B:375:VAL:HG23	1:B:388:LYS:HG3	1.38	1.03
1:B:378:ALA:HB1	1:B:388:LYS:NZ	1.72	1.03
1:B:479:SER:CB	3:B:640:HOH:O	2.01	1.02
1:A:404:ARG:CG	1:A:404:ARG:O	2.06	1.02
1:A:373:ASP:HB2	1:A:374:ILE:HG22	1.39	1.01
1:A:374:ILE:HD12	1:A:374:ILE:O	1.61	1.01
1:B:207:PRO:HA	2:B:502:3GC:H22	1.25	0.99
1:A:383:GLU:OE1	1:A:384:LEU:HB2	1.60	0.99
1:B:360:ARG:HH11	1:B:360:ARG:HG3	1.26	0.98
1:B:384:LEU:O	1:B:426:ARG:CB	2.12	0.97
1:A:60:LYS:HD3	1:A:242[A]:ARG:NH1	1.81	0.96
1:B:138:MET:CE	1:B:143:LYS:HD2	1.94	0.96
1:A:39:LEU:HD12	1:A:442:TRP:HZ3	1.17	0.96
1:A:277:LEU:HD11	3:A:605:HOH:O	1.67	0.94
1:B:337:GLN:HG3	3:B:613:HOH:O	1.65	0.94
1:B:238:GLN:NE2	2:B:501:3GC:H22	1.66	0.93
1:B:160:GLU:C	1:B:163:LYS:HZ1	1.72	0.93
1:B:346:LEU:HA	3:B:623:HOH:O	1.69	0.91
1:B:384:LEU:C	1:B:426:ARG:HB2	1.91	0.90
1:B:378:ALA:HB1	1:B:388:LYS:HZ3	1.33	0.90
1:B:160:GLU:C	1:B:163:LYS:NZ	2.25	0.90
1:A:384:LEU:HG	1:A:426:ARG:H	1.37	0.90
1:B:208:ALA:HB3	2:B:502:3GC:HA1	1.52	0.89
1:B:430:ALA:HA	3:B:617:HOH:O	1.72	0.89
1:B:349:PHE:HD1	3:B:623:HOH:O	1.56	0.88
1:B:423:LEU:HD12	1:B:424:MET:N	1.87	0.88
1:B:160:GLU:O	1:B:163:LYS:NZ	2.06	0.88
1:B:487:LEU:HB2	1:B:489:GLY:N	1.88	0.88
1:A:202:ASN:HD22	1:A:204:ASN:H	1.18	0.87
1:B:159:ASP:HB3	3:B:603:HOH:O	1.75	0.87
1:B:161:LYS:O	1:B:162:THR:HG22	1.76	0.86
1:A:384:LEU:O	1:A:385:PHE:O	1.93	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD21	1:B:336:ILE:HG12	1.56	0.86
1:A:379:ILE:HD11	1:A:406:THR:HG22	1.59	0.85
1:A:373:ASP:HB2	1:A:374:ILE:CG2	2.07	0.85
1:B:377:LYS:HE2	3:B:643:HOH:O	1.77	0.84
1:B:207:PRO:HA	2:B:502:3GC:N1	1.93	0.84
1:A:261:ARG:HH11	1:A:287:GLN:NE2	1.75	0.83
1:A:277:LEU:CD1	3:A:605:HOH:O	2.21	0.83
1:B:423:LEU:HB2	3:B:580:HOH:O	1.79	0.83
1:A:379:ILE:CG1	1:A:406:THR:HG22	2.07	0.82
1:B:138:MET:HE3	1:B:143:LYS:HD2	1.62	0.82
1:A:39:LEU:CD1	1:A:442:TRP:CZ3	2.61	0.82
1:B:390:GLN:HG2	3:B:615:HOH:O	1.79	0.82
1:A:247:GLN:OE1	1:A:264:ARG:NH1	2.11	0.81
1:B:375:VAL:HG13	1:B:379:ILE:HB	1.62	0.81
1:B:375:VAL:HG23	1:B:388:LYS:CG	2.11	0.81
1:A:285:ASP:OD1	1:A:285:ASP:O	1.99	0.81
1:B:374:ILE:C	1:B:376:LYS:H	1.84	0.80
1:B:422:ILE:HG23	1:B:423:LEU:H	1.47	0.79
1:B:422:ILE:HG23	1:B:423:LEU:N	1.97	0.79
1:A:398:ILE:CG2	1:A:405:GLU:OE1	2.23	0.78
1:A:371:ASP:HA	1:A:375:VAL:HG23	1.64	0.78
1:A:125:ASP:OD2	1:A:128:THR:HB	1.85	0.77
1:A:39:LEU:CD1	1:A:442:TRP:HZ3	1.97	0.77
1:A:176:SER:OG	2:A:501:3GC:HG11	1.84	0.77
1:B:384:LEU:O	1:B:385:PHE:O	2.02	0.77
1:A:261:ARG:HH11	1:A:287:GLN:HE22	1.32	0.77
1:A:379:ILE:CD1	1:A:406:THR:HG22	2.15	0.76
1:B:161:LYS:HA	1:B:163:LYS:HZ1	1.51	0.76
1:B:421:TYR:CD1	1:B:421:TYR:O	2.39	0.76
1:B:423:LEU:HD12	1:B:424:MET:H	1.50	0.75
1:A:230:ARG:HD3	3:A:558:HOH:O	1.85	0.75
1:B:344:GLY:CA	3:B:649:HOH:O	2.22	0.74
1:B:90:TRP:CD1	2:B:502:3GC:HA2	2.22	0.74
1:B:160:GLU:N	1:B:428:PHE:O	2.16	0.74
1:B:484:GLY:HA3	3:B:525:HOH:O	1.86	0.74
1:A:379:ILE:CG1	1:A:406:THR:CG2	2.65	0.74
1:B:390:GLN:CG	3:B:615:HOH:O	2.36	0.73
1:A:384:LEU:O	1:A:385:PHE:C	2.22	0.73
1:A:383:GLU:OE1	1:A:384:LEU:N	2.21	0.73
1:A:268:THR:HG22	3:A:554:HOH:O	1.87	0.73
1:B:378:ALA:HB1	1:B:388:LYS:HZ1	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ILE:HG13	1:A:406:THR:HG21	1.68	0.73
1:A:268:THR:HB	1:A:308:GLU:OE2	1.89	0.73
1:B:374:ILE:HG22	1:B:375:VAL:HB	1.71	0.72
1:B:207:PRO:CA	2:B:502:3GC:H22	2.02	0.72
1:A:370:GLU:O	1:A:374:ILE:HG13	1.88	0.72
1:B:142:ASN:O	1:B:142:ASN:ND2	2.23	0.72
1:A:374:ILE:CD1	1:A:374:ILE:O	2.36	0.72
1:B:375:VAL:CG2	1:B:379:ILE:HG13	2.15	0.72
1:B:379:ILE:CD1	3:B:532:HOH:O	2.38	0.71
2:B:502:3GC:SG2	2:B:502:3GC:OE1	2.49	0.71
1:B:386:VAL:O	1:B:423:LEU:HD13	1.90	0.70
1:A:368:SER:OG	1:A:369:LEU:N	2.23	0.70
1:B:208:ALA:CB	2:B:502:3GC:HA1	2.21	0.70
1:B:105:ASP:OD1	1:B:148:ARG:HD2	1.91	0.70
1:B:366:LEU:HA	1:B:423:LEU:O	1.92	0.70
2:B:502:3GC:HB11	2:B:502:3GC:O2	1.93	0.69
1:A:379:ILE:HG13	1:A:406:THR:CG2	2.22	0.69
1:B:279:ASP:OD1	1:B:281:THR:CG2	2.40	0.69
1:B:360:ARG:NH1	1:B:360:ARG:HG3	2.03	0.69
1:B:194[A]:GLN:O	1:B:197:LYS:HD2	1.93	0.69
1:B:241:GLU:OE1	2:B:501:3GC:N1	2.26	0.69
1:B:376:LYS:C	1:B:378:ALA:H	1.95	0.69
1:B:374:ILE:HG22	1:B:375:VAL:N	2.07	0.68
1:B:238:GLN:HE21	2:B:501:3GC:H22	1.37	0.68
1:A:241:GLU:OE1	2:A:501:3GC:N1	2.26	0.68
1:B:138:MET:CE	1:B:143:LYS:CD	2.71	0.67
1:B:161:LYS:HA	1:B:163:LYS:NZ	2.09	0.67
1:B:120:ARG:HD2	1:B:335:LYS:CE	2.24	0.67
1:B:161:LYS:O	1:B:162:THR:CG2	2.43	0.67
1:B:120:ARG:HD2	1:B:335:LYS:HD3	1.77	0.67
1:A:384:LEU:HG	1:A:426:ARG:N	2.08	0.66
1:B:90:TRP:HD1	2:B:502:3GC:HA2	1.61	0.65
1:B:202:ASN:ND2	1:B:204:ASN:HB2	2.10	0.65
1:A:86:PRO:HD2	1:A:158:ILE:HD11	1.76	0.65
1:B:379:ILE:HD11	3:B:532:HOH:O	1.95	0.65
1:A:390:GLN:CG	1:A:422:ILE:HG23	2.26	0.65
1:A:138:MET:SD	1:A:143:LYS:HD2	2.37	0.64
1:B:269:GLU:O	1:B:273:GLU:HB2	1.97	0.64
1:B:334:LYS:HZ3	1:B:421:TYR:HB2	1.62	0.64
1:B:374:ILE:CG2	1:B:375:VAL:N	2.60	0.64
1:A:384:LEU:C	1:A:426:ARG:HB2	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LYS:C	3:A:546:HOH:O	2.36	0.64
1:A:34:ILE:HB	1:A:39:LEU:CD2	2.28	0.64
1:B:346:LEU:HD12	1:B:356:ILE:HG23	1.80	0.64
1:A:383:GLU:OE1	1:A:384:LEU:CB	2.40	0.64
1:A:269:GLU:O	1:A:273:GLU:HB2	1.97	0.64
1:B:120:ARG:NE	1:B:335:LYS:HD3	2.12	0.63
1:B:475:ARG:NH2	1:B:490:PHE:O	2.32	0.63
1:A:261:ARG:NH1	1:A:287:GLN:NE2	2.47	0.63
1:B:194[A]:GLN:HA	1:B:194[A]:GLN:HE21	1.63	0.63
1:B:334:LYS:NZ	1:B:421:TYR:HB2	2.13	0.63
1:B:384:LEU:O	1:B:426:ARG:HD2	1.99	0.63
1:A:69:PRO:HA	1:A:245:TYR:OH	1.98	0.63
1:B:358:LYS:HE2	3:B:576:HOH:O	1.99	0.62
1:B:138:MET:HE1	1:B:143:LYS:HG3	1.81	0.62
1:B:159:ASP:OD1	1:B:428:PHE:N	2.25	0.62
1:B:138:MET:HE3	1:B:143:LYS:CD	2.29	0.62
1:A:396:ASN:N	3:A:611:HOH:O	2.31	0.62
1:B:338:GLN:OE1	1:B:422:ILE:HG22	1.99	0.62
1:B:479:SER:HB2	3:B:640:HOH:O	1.78	0.62
1:B:475:ARG:CZ	1:B:490:PHE:O	2.48	0.61
1:B:118:LEU:HD21	1:B:336:ILE:CG1	2.30	0.61
1:B:87:GLU:OE2	1:B:91:LYS:NZ	2.33	0.61
1:B:108:SER:HB2	1:B:327:SER:HB2	1.81	0.61
1:A:174:SER:O	2:A:501:3GC:HB22	2.01	0.61
1:B:384:LEU:HB2	3:B:504:HOH:O	2.00	0.60
1:B:388:LYS:O	1:B:390:GLN:HB3	2.01	0.60
1:B:279:ASP:OD1	1:B:281:THR:HG23	2.00	0.60
1:A:86:PRO:HD2	1:A:158:ILE:CD1	2.31	0.60
1:B:63:GLN:CD	1:B:63:GLN:N	2.55	0.60
1:A:108:SER:HB2	1:A:327:SER:HB2	1.82	0.60
1:B:364:ALA:HB3	1:B:424:MET:CE	2.31	0.60
1:B:375:VAL:HG13	1:B:379:ILE:CB	2.30	0.60
1:B:120:ARG:CD	1:B:335:LYS:HD3	2.32	0.60
1:B:334:LYS:HG2	1:B:338:GLN:HE21	1.65	0.60
1:A:442:TRP:CD1	1:A:442:TRP:N	2.68	0.60
1:B:129:SER:O	1:B:133[A]:ASP:OD1	2.20	0.60
1:A:405:GLU:OE2	1:A:405:GLU:CA	2.49	0.59
1:B:375:VAL:O	1:B:379:ILE:HB	2.03	0.59
1:B:118:LEU:HD22	1:B:335:LYS:HB3	1.85	0.59
1:B:168:ILE:HG21	1:B:450:GLU:OE2	2.02	0.59
1:A:34:ILE:HB	1:A:39:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PHE:HD2	1:B:199:LEU:HG	1.68	0.58
1:A:157:MET:HG3	1:A:168[B]:ILE:HD13	1.84	0.58
1:B:174:SER:OG	1:B:174:SER:O	2.14	0.58
1:A:379:ILE:HD11	1:A:406:THR:CG2	2.33	0.58
1:B:279:ASP:OD1	1:B:281:THR:HG22	2.03	0.58
1:B:365:GLY:O	1:B:424:MET:HA	2.04	0.58
1:B:120:ARG:HD2	1:B:335:LYS:CD	2.33	0.58
1:B:360:ARG:NH1	1:B:360:ARG:CG	2.65	0.58
1:A:133:ASP:O	1:A:137:LYS:HG3	2.04	0.57
1:B:430:ALA:CA	3:B:617:HOH:O	2.43	0.57
1:B:389:PRO:HB2	3:B:557:HOH:O	2.04	0.57
1:A:450:GLU:OE2	1:A:477:LYS:HE2	2.03	0.57
1:B:478:ILE:HG22	1:B:479:SER:N	2.19	0.57
1:A:233:ILE:HG12	1:A:291:VAL:HB	1.85	0.57
1:B:383:GLU:O	1:B:428:PHE:HZ	1.88	0.57
1:A:379:ILE:HG12	1:A:406:THR:HG22	1.84	0.57
1:B:369:LEU:O	1:B:370:GLU:HG3	2.04	0.57
1:B:376:LYS:C	1:B:378:ALA:N	2.58	0.57
1:B:488:PRO:HG2	1:B:490:PHE:HA	1.87	0.56
1:B:160:GLU:O	1:B:161:LYS:HG3	2.06	0.56
1:B:377:LYS:O	1:B:385:PHE:CE1	2.58	0.56
1:B:210:ASN:OD1	1:B:214:GLN:HG3	2.06	0.56
1:B:147:ILE:HB	1:B:321:ILE:CD1	2.35	0.56
1:B:322:LYS:HD3	1:B:322:LYS:N	2.21	0.56
1:B:160:GLU:C	1:B:163:LYS:HZ3	2.05	0.56
1:B:202:ASN:HD22	1:B:204:ASN:H	1.52	0.56
1:A:129:SER:O	1:A:133:ASP:OD1	2.24	0.55
1:B:208:ALA:H	2:B:502:3GC:CA1	2.19	0.55
1:A:236:VAL:HG11	1:A:267:LEU:HD13	1.89	0.55
1:B:313:LEU:O	1:B:317:GLN:HG3	2.07	0.55
1:A:352:ASN:HD22	1:A:352:ASN:C	2.10	0.55
1:B:376:LYS:O	1:B:378:ALA:N	2.38	0.55
1:A:353:LYS:HE3	3:A:555:HOH:O	2.07	0.55
1:B:161:LYS:CA	1:B:163:LYS:HZ1	2.18	0.55
1:A:409:LYS:HE3	3:A:586:HOH:O	2.06	0.55
1:A:197:LYS:HE3	1:A:198:PHE:H	1.71	0.55
1:B:298:TYR:CE1	2:B:501:3GC:HG12	2.42	0.55
1:A:176:SER:HG	2:A:501:3GC:HG11	1.68	0.55
1:A:388:LYS:NZ	3:A:596:HOH:O	2.29	0.54
1:B:120:ARG:HD2	1:B:335:LYS:NZ	2.23	0.54
1:B:59:ASP:OD1	1:B:61:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ILE:CG2	1:B:423:LEU:N	2.70	0.54
1:A:376:LYS:HZ3	1:A:380:GLU:CG	2.21	0.54
1:B:147:ILE:HB	1:B:321:ILE:HD11	1.90	0.54
1:B:153:ARG:HD2	1:B:452:GLY:HA3	1.89	0.54
1:A:386:VAL:HG22	1:A:399:TYR:CD2	2.42	0.54
1:B:378:ALA:CB	1:B:388:LYS:NZ	2.59	0.54
1:A:298:TYR:CZ	2:A:501:3GC:OE1	2.61	0.54
1:A:157:MET:CE	1:A:429:PRO:HB3	2.38	0.53
1:B:324:PRO:HB2	1:B:328:TYR:HB2	1.90	0.53
1:B:423:LEU:C	1:B:423:LEU:HD12	2.28	0.53
1:A:377:LYS:O	1:A:380:GLU:O	2.26	0.53
1:A:157:MET:HE2	1:A:429:PRO:HB3	1.90	0.53
1:A:276:ILE:CG2	1:A:280:GLY:HA2	2.39	0.53
1:B:364:ALA:HB3	1:B:424:MET:HE2	1.89	0.53
1:A:352:ASN:ND2	1:A:354:ASP:H	2.06	0.53
1:A:202:ASN:ND2	1:A:204:ASN:CG	2.62	0.53
1:A:109:LEU:HD11	1:A:148:ARG:NH1	2.23	0.53
1:A:56:LEU:HD23	1:A:75:HIS:HA	1.90	0.53
1:B:379:ILE:HD13	3:B:532:HOH:O	2.07	0.53
1:A:370:GLU:HB2	1:A:374:ILE:HG23	1.91	0.53
1:A:352:ASN:ND2	1:A:354:ASP:N	2.57	0.53
1:B:163:LYS:HA	1:B:163:LYS:HE3	1.91	0.52
1:B:266:THR:OG1	1:B:269:GLU:HG3	2.09	0.52
1:B:138:MET:CE	1:B:143:LYS:CG	2.87	0.52
1:B:378:ALA:CB	1:B:388:LYS:HZ1	2.20	0.52
1:A:322:LYS:N	1:A:322:LYS:HD3	2.24	0.52
1:B:138:MET:HE3	1:B:143:LYS:CG	2.39	0.52
1:B:34:ILE:CG2	1:B:39:LEU:HD13	2.40	0.52
1:B:120:ARG:HE	1:B:335:LYS:HD3	1.73	0.52
1:B:375:VAL:HA	1:B:379:ILE:N	2.24	0.52
1:A:384:LEU:CG	1:A:426:ARG:H	2.17	0.52
1:B:138:MET:CE	1:B:143:LYS:HG3	2.39	0.52
1:A:401:ASP:O	1:A:404:ARG:HB3	2.10	0.52
1:B:63:GLN:OE1	1:B:64:ARG:N	2.38	0.52
1:B:339:GLU:O	1:B:345:VAL:HG21	2.10	0.51
1:B:118:LEU:HD12	1:B:330:LEU:HD22	1.91	0.51
1:B:375:VAL:HA	1:B:379:ILE:H	1.76	0.51
1:B:30:ASP:HA	1:B:433:PRO:HG2	1.93	0.50
1:A:374:ILE:CG1	1:A:374:ILE:O	2.59	0.50
1:B:194[A]:GLN:HE21	1:B:194[A]:GLN:CA	2.24	0.50
1:B:460:ASN:O	1:B:463:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASN:HD21	1:A:354:ASP:HB3	1.76	0.50
1:B:388:LYS:HG2	1:B:389:PRO:HD2	1.94	0.50
1:A:267:LEU:HD22	3:A:513:HOH:O	2.12	0.50
1:A:55:LEU:HD21	1:A:184:MET:SD	2.52	0.50
1:B:204:ASN:HB3	1:B:205:ARG:HG2	1.93	0.50
1:B:198:PHE:HZ	3:B:524:HOH:O	1.95	0.50
1:B:173:ILE:HD12	1:B:324:PRO:HD2	1.92	0.50
1:B:221:LYS:HD2	1:B:466:ILE:HD11	1.94	0.50
1:B:210:ASN:HB3	3:B:631:HOH:O	2.12	0.50
1:A:338:GLN:HG2	1:A:366:LEU:HD11	1.94	0.49
1:B:328:TYR:O	1:B:329:HIS:C	2.50	0.49
1:B:196:GLY:O	1:B:200:GLY:N	2.45	0.49
1:B:375:VAL:C	1:B:379:ILE:H	2.16	0.49
1:A:390:GLN:HG2	1:A:422:ILE:HG23	1.93	0.49
1:B:324:PRO:HB2	1:B:328:TYR:CB	2.43	0.49
1:B:489:GLY:C	1:B:491:GLY:H	2.16	0.49
1:B:63:GLN:NE2	1:B:63:GLN:H	2.10	0.48
1:A:159:ASP:HB2	1:A:427:ILE:HG23	1.94	0.48
1:B:368:SER:HB3	1:B:422:ILE:HG12	1.95	0.48
1:B:426:ARG:HD3	1:B:428:PHE:CZ	2.49	0.48
1:A:376:LYS:NZ	1:A:380:GLU:HB2	2.29	0.48
1:B:426:ARG:NH1	1:B:428:PHE:CE2	2.82	0.48
1:A:245:TYR:CE2	1:B:51:THR:HG21	2.48	0.48
1:A:32:HIS:CD2	1:A:433:PRO:HB3	2.48	0.48
1:A:174:SER:OG	2:A:501:3GC:HG12	2.14	0.48
1:B:193:SER:O	1:B:197:LYS:HE3	2.12	0.48
1:B:341:ALA:HB1	1:B:366:LEU:HD13	1.96	0.47
1:B:488:PRO:HD2	1:B:490:PHE:HA	1.95	0.47
1:A:231:ALA:CB	1:A:290:SER:HB3	2.45	0.47
1:B:360:ARG:HA	1:B:363:PHE:HB2	1.96	0.47
1:B:438:ARG:HD3	3:B:552:HOH:O	2.13	0.47
1:A:226:TYR:CG	1:A:290:SER:HB2	2.50	0.47
1:A:271:ASP:HB2	1:A:307:SER:O	2.14	0.47
1:A:313:LEU:HD22	1:A:317:GLN:HG3	1.95	0.47
1:B:375:VAL:H	1:B:388:LYS:HE2	1.80	0.47
1:A:370:GLU:O	1:A:374:ILE:CG1	2.59	0.47
1:B:63:GLN:CD	1:B:63:GLN:H	2.17	0.47
1:A:73:LEU:HB2	1:B:73:LEU:HB2	1.96	0.47
1:A:405:GLU:HA	1:A:405:GLU:OE2	2.13	0.47
1:B:138:MET:HE2	1:B:143:LYS:HD2	1.88	0.47
1:A:92:GLN:NE2	3:A:634:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:NE2	2:A:501:3GC:H22	2.13	0.47
1:A:180:ILE:HG21	1:A:493:VAL:HG11	1.96	0.46
1:B:161:LYS:N	1:B:163:LYS:HZ1	2.12	0.46
1:B:34:ILE:HG22	1:B:39:LEU:HD13	1.98	0.46
1:A:87:GLU:OE2	1:A:91:LYS:NZ	2.46	0.46
1:A:151:ILE:HG12	1:A:456:THR:HG22	1.98	0.46
1:B:176:SER:O	1:B:177:PHE:HB2	2.15	0.46
1:B:479:SER:HA	3:B:525:HOH:O	2.15	0.46
1:B:205:ARG:HB2	1:B:497:TYR:CE2	2.51	0.46
1:A:318[B]:SER:O	1:A:322:LYS:NZ	2.48	0.46
1:A:347:GLU:OE1	1:A:360:ARG:NH1	2.49	0.46
1:A:404:ARG:NH2	3:A:609:HOH:O	2.47	0.46
1:A:237:VAL:HG11	1:A:264:ARG:NH1	2.31	0.46
1:B:388:LYS:CG	1:B:389:PRO:HD2	2.45	0.46
1:B:75:HIS:ND1	1:B:76:LEU:O	2.42	0.46
1:A:83:GLY:O	1:A:497:TYR:N	2.47	0.46
1:B:341:ALA:CB	1:B:366:LEU:HD13	2.45	0.46
1:A:120:ARG:HD2	1:A:120:ARG:HA	1.80	0.46
1:A:383:GLU:OE1	1:A:384:LEU:CA	2.64	0.45
1:A:431:THR:HG23	3:A:529:HOH:O	2.16	0.45
1:A:221:LYS:HB3	1:A:458:LEU:CD2	2.46	0.45
1:A:352:ASN:HD22	1:A:354:ASP:N	2.15	0.45
1:A:38:LEU:O	1:A:42:ILE:HG13	2.17	0.45
1:B:375:VAL:HG13	1:B:379:ILE:CG1	2.46	0.45
1:A:376:LYS:HZ2	1:A:380:GLU:HB2	1.81	0.45
1:B:118:LEU:HD21	1:B:336:ILE:CD1	2.46	0.45
1:B:488:PRO:CG	1:B:490:PHE:HA	2.46	0.45
1:A:197:LYS:NZ	1:A:198:PHE:HB2	2.31	0.45
1:A:105:ASP:OD1	1:A:148:ARG:HD2	2.16	0.45
1:A:460:ASN:O	1:A:461:LYS:C	2.55	0.45
1:B:426:ARG:NH1	1:B:428:PHE:HE2	2.15	0.45
1:A:271:ASP:OD1	1:A:310:ARG:HD2	2.17	0.45
1:A:226:TYR:HE2	1:A:319[B]:SER:O	2.00	0.45
1:B:487:LEU:N	1:B:487:LEU:HD22	2.32	0.45
1:B:39:LEU:HA	1:B:39:LEU:HD12	1.61	0.45
1:A:177:PHE:CD1	1:A:180:ILE:HG12	2.52	0.45
1:A:404:ARG:C	1:A:406:THR:N	2.70	0.44
1:A:95:GLU:OE2	1:A:358:LYS:HE2	2.17	0.44
1:A:369:LEU:HA	1:A:374:ILE:HD11	1.99	0.44
1:A:376:LYS:O	1:A:376:LYS:CD	2.65	0.44
1:B:488:PRO:HB2	1:B:491:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:SER:HB2	1:A:327:SER:CB	2.48	0.44
1:B:379:ILE:HG12	3:B:615:HOH:O	2.18	0.44
1:A:376:LYS:HD3	1:A:379:ILE:HB	1.98	0.44
1:A:64:ARG:HB3	1:A:68:VAL:HG23	1.99	0.44
1:A:188:HIS:HE1	1:A:494:ASP:OD1	2.01	0.44
1:B:384:LEU:O	1:B:426:ARG:CG	2.66	0.44
1:A:352:ASN:HD22	1:A:355:HIS:H	1.66	0.44
1:A:386:VAL:CG2	1:A:399:TYR:CE2	3.01	0.44
1:A:105:ASP:OD2	1:A:148:ARG:NH1	2.51	0.43
1:B:136:SER:O	1:B:140:GLN:HB2	2.18	0.43
1:B:194[B]:GLN:O	1:B:197:LYS:HD2	2.18	0.43
1:B:364:ALA:HB3	1:B:424:MET:HE3	1.99	0.43
1:A:379:ILE:CD1	1:A:406:THR:CG2	2.91	0.43
1:A:376:LYS:NZ	1:A:380:GLU:CG	2.81	0.43
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.66	0.43
1:A:195:TYR:O	1:A:199:LEU:HD12	2.17	0.43
1:B:364:ALA:CB	1:B:424:MET:HE2	2.48	0.43
1:A:386:VAL:HG22	1:A:399:TYR:CE2	2.54	0.43
1:B:274:GLY:HA2	1:B:283:SER:O	2.19	0.43
1:B:86:PRO:HA	1:B:499:THR:HA	2.00	0.43
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.85	0.43
1:B:247:GLN:OE1	1:B:264:ARG:NH2	2.51	0.43
1:A:383:GLU:CG	1:A:384:LEU:N	2.81	0.43
1:B:118:LEU:CD1	1:B:330:LEU:HD22	2.48	0.43
1:B:233:ILE:O	1:B:262:SER:HA	2.19	0.42
1:A:342:LYS:O	1:A:360:ARG:NH2	2.52	0.42
1:A:331:VAL:HA	1:A:336:ILE:HG21	2.01	0.42
1:B:256:GLU:HB3	3:B:635:HOH:O	2.19	0.42
1:A:450:GLU:CD	1:A:477:LYS:HE2	2.40	0.42
1:A:27:PRO:CB	1:A:30:ASP:HB3	2.49	0.42
1:B:87:GLU:HB2	1:B:498:LEU:HB3	2.00	0.42
1:B:157:MET:HB2	1:B:168:ILE:HD11	2.01	0.42
1:A:352:ASN:ND2	1:A:352:ASN:C	2.72	0.42
1:A:110:ASP:O	1:A:114:LEU:HG	2.20	0.42
1:A:448:ILE:HD12	1:A:448:ILE:HG21	1.73	0.42
1:A:236:VAL:CG1	1:A:267:LEU:HD13	2.50	0.42
1:A:107:VAL:HG23	1:A:107:VAL:H	1.63	0.42
1:B:58:GLY:HA3	1:B:242[B]:ARG:HG2	2.02	0.42
1:A:97:ALA:HB3	1:A:98:PRO:HD3	2.02	0.42
1:B:422:ILE:CG2	1:B:423:LEU:H	2.23	0.42
1:B:265:LYS:HA	1:B:269:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ALA:O	1:B:365:GLY:C	2.58	0.41
1:A:376:LYS:O	1:A:377:LYS:C	2.56	0.41
1:A:384:LEU:HA	1:A:426:ARG:HB3	2.01	0.41
1:A:263:ILE:HG21	1:A:263:ILE:HD12	1.83	0.41
1:B:287:GLN:HB2	1:B:287:GLN:HE21	1.70	0.41
1:B:208:ALA:N	2:B:502:3GC:HA1	2.35	0.41
1:A:162:THR:OG1	1:A:164:SER:HB2	2.20	0.41
1:B:238:GLN:NE2	2:B:501:3GC:N1	2.49	0.41
1:B:147:ILE:HA	1:B:459:ARG:O	2.20	0.41
1:A:352:ASN:ND2	1:A:355:HIS:H	2.18	0.41
1:B:247:GLN:HG3	1:B:247:GLN:H	1.63	0.41
1:B:118:LEU:CD2	1:B:335:LYS:HG2	2.50	0.41
1:B:331:VAL:HA	1:B:336:ILE:HG21	2.03	0.41
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.46	0.41
1:A:103:LEU:O	1:A:107:VAL:HG23	2.20	0.41
1:B:384:LEU:HG	1:B:426:ARG:H	1.85	0.41
1:B:247:GLN:OE1	1:B:264:ARG:NH1	2.52	0.41
1:B:299:THR:OG1	1:B:301:LYS:HG3	2.20	0.41
1:A:436:LEU:HD21	1:A:447:VAL:HG11	2.02	0.41
1:A:261:ARG:NH1	1:A:287:GLN:HE21	2.17	0.41
1:B:208:ALA:N	2:B:502:3GC:N1	2.63	0.41
1:B:120:ARG:HD2	1:B:335:LYS:HZ3	1.86	0.41
1:B:331:VAL:O	1:B:337:GLN:OE1	2.38	0.41
1:B:147:ILE:HB	1:B:321:ILE:HD12	2.02	0.41
1:A:211:ALA:HA	1:A:470:SER:O	2.20	0.41
1:B:226:TYR:CD1	1:B:290:SER:HB2	2.56	0.41
1:B:96:LEU:HG	1:B:100:PHE:CE2	2.56	0.41
1:A:143:LYS:HE2	1:A:143:LYS:HB2	1.22	0.41
1:A:421:TYR:HA	1:A:421:TYR:HD2	1.46	0.41
1:A:478:ILE:O	1:A:479:SER:HB2	2.21	0.41
1:B:385:PHE:HB3	1:B:423:LEU:HD11	2.01	0.40
1:B:374:ILE:HG22	1:B:375:VAL:CB	2.47	0.40
1:B:148:ARG:NH2	3:B:629:HOH:O	2.51	0.40
1:B:118:LEU:HG	1:B:336:ILE:HD11	2.04	0.40
1:A:197:LYS:N	3:A:628:HOH:O	2.39	0.40
1:B:385:PHE:N	1:B:385:PHE:CD1	2.78	0.40
1:B:197:LYS:CG	1:B:198:PHE:H	2.34	0.40
1:A:409:LYS:HE2	3:A:563:HOH:O	2.21	0.40
1:A:324:PRO:HB2	1:A:328:TYR:HB2	2.03	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	437/499 (88%)	406 (93%)	23 (5%)	8 (2%)	11	4
1	B	437/499 (88%)	387 (89%)	31 (7%)	19 (4%)	3	1
All	All	874/998 (88%)	793 (91%)	54 (6%)	27 (3%)	5	1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	ARG
1	A	461	LYS
1	B	197	LYS
1	B	370	GLU
1	B	375	VAL
1	B	385	PHE
1	B	387	MET
1	B	389	PRO
1	B	483	GLU
1	B	487	LEU
1	B	490	PHE
1	A	383	GLU
1	A	385	PHE
1	B	204	ASN
1	B	478	ILE
1	B	479	SER
1	B	480	SER
1	A	29	PHE
1	B	422	ILE
1	A	196	GLY
1	B	198	PHE
1	B	376	LYS
1	B	386	VAL
1	A	141	ILE
1	B	177	PHE

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Mol	Chain	Res	Type
1	A	375	VAL
1	B	484	GLY

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	397/431 (92%)	337 (85%)	60 (15%)	3	1
1	B	390/431 (90%)	336 (86%)	54 (14%)	4	2
All	All	787/862 (91%)	673 (86%)	114 (14%)	4	2

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	30	ASP
1	A	35	ASP
1	A	37	LYS
1	A	39	LEU
1	A	42	ILE
1	A	60	LYS
1	A	61	SER
1	A	89	HIS
1	A	96	LEU
1	A	106	ARG
1	A	112	LYS
1	A	126	GLU
1	A	128	THR
1	A	133	ASP
1	A	139	LEU
1	A	141	ILE
1	A	143	LYS
1	A	159	ASP
1	A	163	LYS
1	A	168[A]	ILE

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Mol	Chain	Res	Type
1	A	168[B]	ILE
1	A	180	ILE
1	A	182	CYS
1	A	194	GLN
1	A	197	LYS
1	A	198	PHE
1	A	202	ASN
1	A	205	ARG
1	A	221	LYS
1	A	230	ARG
1	A	235	VAL
1	A	263	ILE
1	A	264	ARG
1	A	267	LEU
1	A	285	ASP
1	A	305	SER
1	A	313	LEU
1	A	319[A]	SER
1	A	319[B]	SER
1	A	351	GLU
1	A	352	ASN
1	A	360	ARG
1	A	369	LEU
1	A	370	GLU
1	A	374	ILE
1	A	376	LYS
1	A	383	GLU
1	A	390	GLN
1	A	404	ARG
1	A	405	GLU
1	A	421	TYR
1	A	423	LEU
1	A	431	THR
1	A	448	ILE
1	A	461	LYS
1	A	473	MET
1	A	477	LYS
1	A	478	ILE
1	A	490	PHE
1	B	33	ARG
1	B	39	LEU
1	B	57	VAL

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Mol	Chain	Res	Type
1	B	60	LYS
1	B	61	SER
1	B	63	GLN
1	B	96	LEU
1	B	116	GLU
1	B	119	SER
1	B	120	ARG
1	B	126	GLU
1	B	139	LEU
1	B	144	LYS
1	B	158	ILE
1	B	160	GLU
1	B	161	LYS
1	B	163	LYS
1	B	194[A]	GLN
1	B	194[B]	GLN
1	B	197	LYS
1	B	202	ASN
1	B	206	VAL
1	B	229	PRO
1	B	230	ARG
1	B	235	VAL
1	B	237	VAL
1	B	240	GLU
1	B	247	GLN
1	B	281	THR
1	B	287	GLN
1	B	322	LYS
1	B	324	PRO
1	B	327	SER
1	B	346	LEU
1	B	352	ASN
1	B	363	PHE
1	B	366	LEU
1	B	369	LEU
1	B	371	ASP
1	B	373	ASP
1	B	376	LYS
1	B	379	ILE
1	B	386	VAL
1	B	388	LYS
1	B	421	TYR

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Mol	Chain	Res	Type
1	B	422	ILE
1	B	438	ARG
1	B	473	MET
1	B	475	ARG
1	B	477	LYS
1	B	479	SER
1	B	480	SER
1	B	487	LEU
1	B	490	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	202	ASN
1	A	238	GLN
1	A	287	GLN
1	A	352	ASN
1	A	397	ASN
1	A	468	ASN
1	B	40	GLN
1	B	142	ASN
1	B	171	ASN
1	B	202	ASN
1	B	238	GLN
1	B	272	GLN
1	B	287	GLN
1	B	337	GLN
1	B	338	GLN
1	B	352	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	3GC	A	501	-	9,15,15	2.13	2 (22%)	7,19,19	3.80	1 (14%)
2	3GC	B	501	-	9,15,15	2.05	2 (22%)	7,19,19	2.71	5 (71%)
2	3GC	B	502	-	9,15,15	2.95	2 (22%)	7,19,19	5.76	6 (85%)

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	3GC	A	501	-	1/1/5/6	0/11/19/19	0/0/0/0
2	3GC	B	501	-	1/1/5/6	0/11/19/19	0/0/0/0
2	3GC	B	502	-	1/1/5/6	0/11/19/19	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	3GC	CD1-N2	-4.31	1.25	1.34
2	A	501	3GC	CD1-N2	-3.75	1.26	1.34
2	B	501	3GC	CD1-N2	-3.57	1.26	1.34
2	B	501	3GC	OE1-CD1	4.65	1.33	1.23
2	A	501	3GC	OE1-CD1	4.79	1.33	1.23
2	B	502	3GC	OE1-CD1	7.42	1.38	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	3GC	CB2-CA2-N2	-9.86	97.55	111.40
2	B	502	3GC	CG1-CD1-N2	-8.91	101.31	115.83
2	B	502	3GC	CA2-CB2-SG2	-7.70	104.69	114.16
2	B	502	3GC	CB1-CG1-CD1	-5.83	99.41	113.27
2	B	502	3GC	CB2-CA2-N2	-5.15	104.17	111.40
2	B	501	3GC	CB1-CG1-CD1	-3.35	105.31	113.27
2	B	501	3GC	OE1-CD1-CG1	-2.42	117.80	121.98
2	B	501	3GC	OE1-CD1-N2	-2.26	119.17	123.01
2	B	501	3GC	CB2-CA2-N2	-2.14	108.40	111.40
2	B	502	3GC	OE1-CD1-N2	3.50	128.94	123.01
2	B	501	3GC	CG1-CD1-N2	4.41	123.03	115.83
2	B	502	3GC	OE1-CD1-CG1	4.50	129.74	121.98

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	501	3GC	CA1
2	A	501	3GC	CA1
2	B	502	3GC	CA1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	3GC	7	0
2	B	501	3GC	5	0
2	B	502	3GC	12	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 ⓘ

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	443/499 (88%)	0.14	19 (4%) 39 47	14, 27, 46, 71	0
1	B	437/499 (87%)	0.20	28 (6%) 23 30	12, 25, 59, 78	0
All	All	880/998 (88%)	0.17	47 (5%) 30 38	12, 26, 52, 78	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	484	GLY	9.6
1	B	487	LEU	7.5
1	B	369	LEU	7.0
1	B	375	VAL	6.7
1	A	374	ILE	6.0
1	B	486	VAL	6.0
1	A	490	PHE	5.8
1	B	379	ILE	5.7
1	A	375	VAL	5.1
1	B	485	GLY	4.7
1	B	488	PRO	4.6
1	B	479	SER	4.5
1	A	27	PRO	4.4
1	A	120	ARG	4.3
1	B	421	TYR	4.2
1	A	421	TYR	4.0
1	A	419	ALA	3.6
1	B	490	PHE	3.6
1	B	499	THR	3.5
1	B	162	THR	3.3
1	A	142	ASN	3.1
1	B	370	GLU	3.1
1	A	33	ARG	3.1
1	B	489	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	120	ARG	2.9
1	B	388	LYS	2.9
1	B	389	PRO	2.9
1	A	280	GLY	2.8
1	A	198	PHE	2.8
1	B	374	ILE	2.6
1	B	480	SER	2.5
1	A	371	ASP	2.5
1	A	126	GLU	2.5
1	A	81	LEU	2.4
1	B	385	PHE	2.4
1	B	384	LEU	2.4
1	B	387	MET	2.3
1	B	118	LEU	2.3
1	A	28	LEU	2.3
1	B	119	SER	2.2
1	B	422	ILE	2.2
1	B	61	SER	2.2
1	A	384	LEU	2.1
1	A	420	ALA	2.1
1	A	29	PHE	2.1
1	B	423	LEU	2.1
1	A	278	PRO	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(\AA^2)	Q<0.9
2	3GC	B	501	16/16	0.89	0.18	2.71	35,43,47,50	0
2	3GC	A	501	16/16	0.89	0.18	2.02	46,51,57,61	0
2	3GC	B	502	16/16	0.88	0.22	1.72	13,20,24,24	16

6.5 Other polymers [i](#)

There are no such residues in this entry.