



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:56 AM UTC

PDB ID : 4KZT / pdb_00004kzt
Title : Structure mmNAGS bound with L-arginine
Authors : Zhao, G.; Jin, Z.; Allewell, N.M.; Tuchman, M.; Shi, D.
Deposited on : 2013-05-30
Resolution : 2.80 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
Mogul : 2022.3.0, CSD as543be (2022)
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

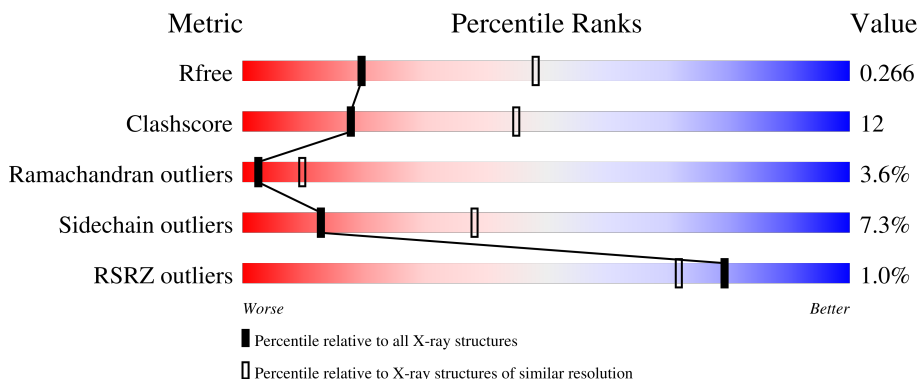
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	461	% 62% 26% 5% 7%
1	B	461	% 64% 25% • 7%
1	X	461	% 69% 21% • 7%
1	Y	461	% 62% 27% • • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13338 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 N-acetylglutamate kinase / N-acetylglutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3311	2079	597	626	9			
1	B	431	Total	C	N	O	S	0	0	0
			3311	2079	597	626	9			
1	X	431	Total	C	N	O	S	0	0	0
			3311	2079	597	626	9			
1	Y	431	Total	C	N	O	S	0	0	0
			3311	2079	597	626	9			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q0ASS9
A	-18	GLY	-	expression tag	UNP Q0ASS9
A	-17	SER	-	expression tag	UNP Q0ASS9
A	-16	SER	-	expression tag	UNP Q0ASS9
A	-15	HIS	-	expression tag	UNP Q0ASS9
A	-14	HIS	-	expression tag	UNP Q0ASS9
A	-13	HIS	-	expression tag	UNP Q0ASS9
A	-12	HIS	-	expression tag	UNP Q0ASS9
A	-11	HIS	-	expression tag	UNP Q0ASS9
A	-10	HIS	-	expression tag	UNP Q0ASS9
A	-9	SER	-	expression tag	UNP Q0ASS9
A	-8	SER	-	expression tag	UNP Q0ASS9
A	-7	GLY	-	expression tag	UNP Q0ASS9
A	-6	LEU	-	expression tag	UNP Q0ASS9
A	-5	VAL	-	expression tag	UNP Q0ASS9
A	-4	PRO	-	expression tag	UNP Q0ASS9
A	-3	ARG	-	expression tag	UNP Q0ASS9
A	-2	GLY	-	expression tag	UNP Q0ASS9
A	-1	SER	-	expression tag	UNP Q0ASS9
A	0	HIS	-	expression tag	UNP Q0ASS9
A	106	MET	ILE	engineered mutation	UNP Q0ASS9

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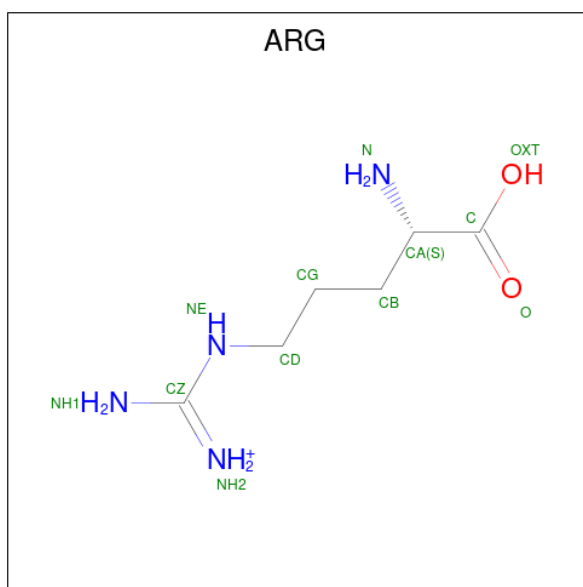
Chain	Residue	Modelled	Actual	Comment	Reference
A	294	MET	ILE	engineered mutation	UNP Q0ASS9
A	376	MET	LEU	engineered mutation	UNP Q0ASS9
B	-19	MET	-	expression tag	UNP Q0ASS9
B	-18	GLY	-	expression tag	UNP Q0ASS9
B	-17	SER	-	expression tag	UNP Q0ASS9
B	-16	SER	-	expression tag	UNP Q0ASS9
B	-15	HIS	-	expression tag	UNP Q0ASS9
B	-14	HIS	-	expression tag	UNP Q0ASS9
B	-13	HIS	-	expression tag	UNP Q0ASS9
B	-12	HIS	-	expression tag	UNP Q0ASS9
B	-11	HIS	-	expression tag	UNP Q0ASS9
B	-10	HIS	-	expression tag	UNP Q0ASS9
B	-9	SER	-	expression tag	UNP Q0ASS9
B	-8	SER	-	expression tag	UNP Q0ASS9
B	-7	GLY	-	expression tag	UNP Q0ASS9
B	-6	LEU	-	expression tag	UNP Q0ASS9
B	-5	VAL	-	expression tag	UNP Q0ASS9
B	-4	PRO	-	expression tag	UNP Q0ASS9
B	-3	ARG	-	expression tag	UNP Q0ASS9
B	-2	GLY	-	expression tag	UNP Q0ASS9
B	-1	SER	-	expression tag	UNP Q0ASS9
B	0	HIS	-	expression tag	UNP Q0ASS9
B	106	MET	ILE	engineered mutation	UNP Q0ASS9
B	294	MET	ILE	engineered mutation	UNP Q0ASS9
B	376	MET	LEU	engineered mutation	UNP Q0ASS9
X	-19	MET	-	expression tag	UNP Q0ASS9
X	-18	GLY	-	expression tag	UNP Q0ASS9
X	-17	SER	-	expression tag	UNP Q0ASS9
X	-16	SER	-	expression tag	UNP Q0ASS9
X	-15	HIS	-	expression tag	UNP Q0ASS9
X	-14	HIS	-	expression tag	UNP Q0ASS9
X	-13	HIS	-	expression tag	UNP Q0ASS9
X	-12	HIS	-	expression tag	UNP Q0ASS9
X	-11	HIS	-	expression tag	UNP Q0ASS9
X	-10	HIS	-	expression tag	UNP Q0ASS9
X	-9	SER	-	expression tag	UNP Q0ASS9
X	-8	SER	-	expression tag	UNP Q0ASS9
X	-7	GLY	-	expression tag	UNP Q0ASS9
X	-6	LEU	-	expression tag	UNP Q0ASS9
X	-5	VAL	-	expression tag	UNP Q0ASS9
X	-4	PRO	-	expression tag	UNP Q0ASS9
X	-3	ARG	-	expression tag	UNP Q0ASS9

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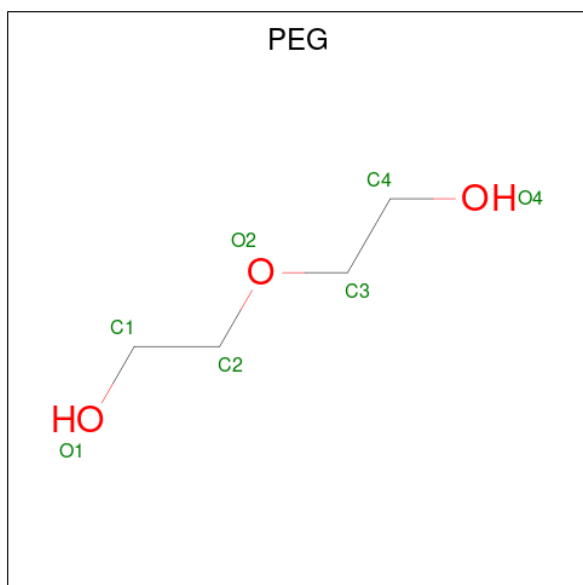
Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	GLY	-	expression tag	UNP Q0ASS9
X	-1	SER	-	expression tag	UNP Q0ASS9
X	0	HIS	-	expression tag	UNP Q0ASS9
X	106	MET	ILE	engineered mutation	UNP Q0ASS9
X	294	MET	ILE	engineered mutation	UNP Q0ASS9
X	376	MET	LEU	engineered mutation	UNP Q0ASS9
Y	-19	MET	-	expression tag	UNP Q0ASS9
Y	-18	GLY	-	expression tag	UNP Q0ASS9
Y	-17	SER	-	expression tag	UNP Q0ASS9
Y	-16	SER	-	expression tag	UNP Q0ASS9
Y	-15	HIS	-	expression tag	UNP Q0ASS9
Y	-14	HIS	-	expression tag	UNP Q0ASS9
Y	-13	HIS	-	expression tag	UNP Q0ASS9
Y	-12	HIS	-	expression tag	UNP Q0ASS9
Y	-11	HIS	-	expression tag	UNP Q0ASS9
Y	-10	HIS	-	expression tag	UNP Q0ASS9
Y	-9	SER	-	expression tag	UNP Q0ASS9
Y	-8	SER	-	expression tag	UNP Q0ASS9
Y	-7	GLY	-	expression tag	UNP Q0ASS9
Y	-6	LEU	-	expression tag	UNP Q0ASS9
Y	-5	VAL	-	expression tag	UNP Q0ASS9
Y	-4	PRO	-	expression tag	UNP Q0ASS9
Y	-3	ARG	-	expression tag	UNP Q0ASS9
Y	-2	GLY	-	expression tag	UNP Q0ASS9
Y	-1	SER	-	expression tag	UNP Q0ASS9
Y	0	HIS	-	expression tag	UNP Q0ASS9
Y	106	MET	ILE	engineered mutation	UNP Q0ASS9
Y	294	MET	ILE	engineered mutation	UNP Q0ASS9
Y	376	MET	LEU	engineered mutation	UNP Q0ASS9

- Molecule 2 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		
2	B	1	Total	C	N	O	0	0
			12	6	4	2		
2	X	1	Total	C	N	O	0	0
			12	6	4	2		
2	Y	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

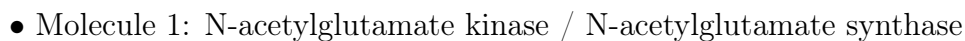


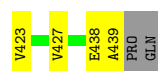
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	X	1	Total C O 7 4 3	0	0
3	Y	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

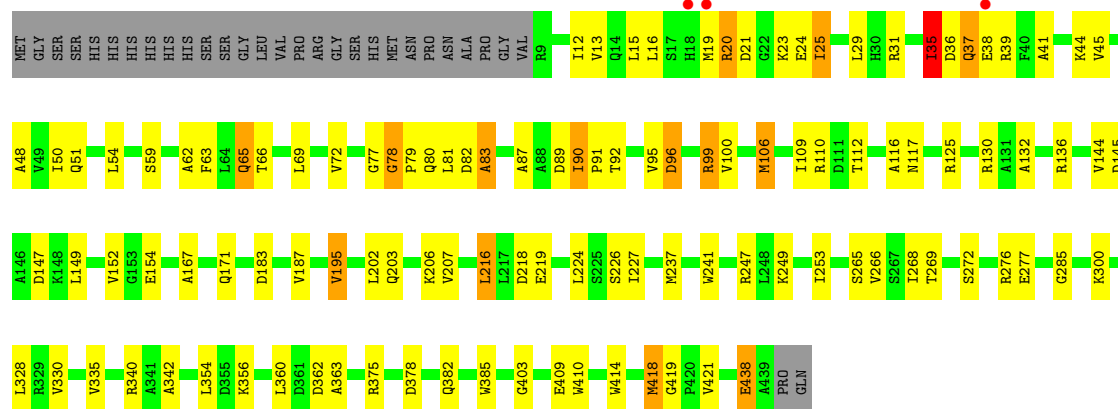
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	5	Total O 5 5	0	0
4	X	2	Total O 2 2	0	0
4	Y	7	Total O 7 7	0	0

- Molecule 1: N-acetylglutamate kinase / N-acetylglutamate synthase

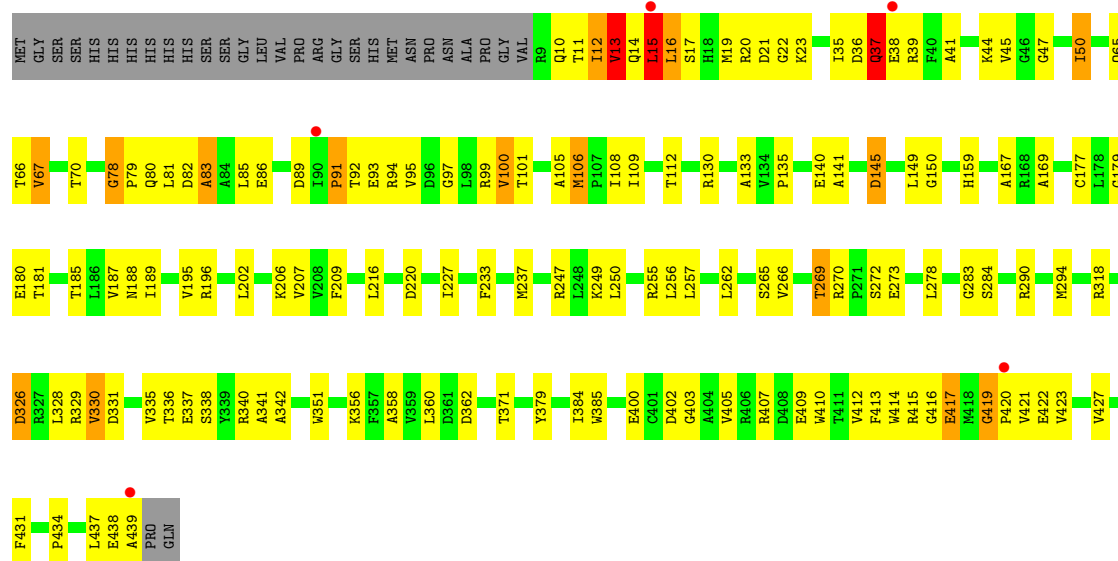




• Molecule 1: N-acetylglutamate kinase / N-acetylglutamate synthase



• Molecule 1: N-acetylglutamate kinase / N-acetylglutamate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.83Å 110.82Å 117.20Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	39.30 – 2.80 39.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.8 (39.30-2.80) 85.3 (39.30-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.196 , 0.265 0.198 , 0.266	Depositor DCC
R_{free} test set	2004 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13338	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.61	1/3369 (0.0%)	1.01	8/4576 (0.2%)
1	B	0.65	0/3369	1.00	6/4576 (0.1%)
1	X	0.58	0/3369	0.98	9/4576 (0.2%)
1	Y	0.60	0/3369	1.02	5/4576 (0.1%)
All	All	0.61	1/13476 (0.0%)	1.00	28/18304 (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
1	A	0	1
1	Y	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	ALA	CA-CB	-5.31	1.45	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ALA	N-CA-C	-9.31	101.17	114.12
1	A	35	ILE	N-CA-C	8.45	118.50	110.30
1	A	419	GLY	CA-C-N	8.39	130.33	119.84
1	A	419	GLY	C-N-CA	8.39	130.33	119.84
1	X	87	ALA	N-CA-C	-8.06	102.92	114.12
1	X	154	GLU	CA-C-N	6.93	127.34	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	154	GLU	C-N-CA	6.93	127.34	119.93
1	Y	108	ILE	N-CA-C	-6.15	104.75	110.53
1	Y	422	GLU	N-CA-C	-6.08	105.90	113.38
1	X	419	GLY	CA-C-N	5.96	127.29	119.84
1	X	419	GLY	C-N-CA	5.96	127.29	119.84
1	A	34	GLY	N-CA-C	-5.88	99.25	113.18
1	Y	179	GLY	N-CA-C	5.78	119.54	111.10
1	B	419	GLY	CA-C-N	5.63	126.88	119.84
1	B	419	GLY	C-N-CA	5.63	126.88	119.84
1	B	331	ASP	N-CA-C	-5.62	106.55	113.41
1	Y	434	PRO	O-C-N	5.55	123.87	121.31
1	X	24	GLU	N-CA-C	-5.46	106.62	113.28
1	A	35	ILE	CB-CA-C	-5.37	105.10	111.81
1	A	154	GLU	CA-C-N	5.34	126.51	119.84
1	A	154	GLU	C-N-CA	5.34	126.51	119.84
1	Y	402	ASP	N-CA-C	-5.26	106.88	113.72
1	X	25	ILE	CB-CA-C	-5.25	105.25	111.97
1	A	434	PRO	O-C-N	5.21	123.71	121.31
1	X	35	ILE	CB-CA-C	-5.11	105.34	112.04
1	X	195	VAL	CB-CA-C	-5.10	105.36	111.88
1	B	95	VAL	CB-CA-C	-5.06	106.12	111.23
1	B	402	ASP	N-CA-C	-5.04	107.11	114.12

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	LEU	Peptide
1	Y	15	LEU	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	3311	0	3302	101	0
1	B	3311	0	3302	87	0
1	X	3311	0	3302	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	3311	0	3302	94	0
2	A	12	0	12	2	0
2	B	12	0	12	1	0
2	X	12	0	12	1	0
2	Y	12	0	12	2	0
3	A	7	0	10	3	0
3	B	7	0	10	1	0
3	X	7	0	10	0	0
3	Y	7	0	10	0	0
4	A	4	0	0	3	0
4	B	5	0	0	4	0
4	X	2	0	0	0	0
4	Y	7	0	0	3	0
All	All	13338	0	13296	327	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 12.

All (327) 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:329:ARG:NH2	4:B:605:HOH:O	1.85	1.07
1:Y:249:LYS:NZ	4:Y:606:HOH:O	1.93	0.98
1:Y:65:GLN:HG2	1:Y:130:ARG:H	1.40	0.87
1:Y:12:ILE:HG21	1:Y:67:VAL:HA	1.57	0.86
1:A:65:GLN:HG2	1:A:130:ARG:H	1.39	0.84
1:A:38:GLU:HG2	1:A:167:ALA:HB2	1.64	0.80
1:A:37:GLN:HB3	4:A:604:HOH:O	1.83	0.78
1:X:300:LYS:NZ	1:X:328:LEU:O	2.18	0.76
1:A:207:VAL:HB	1:A:266:VAL:HG22	1.67	0.76
1:B:300:LYS:NZ	1:B:328:LEU:O	2.18	0.75
1:Y:409:GLU:HG2	1:Y:410:TRP:CD1	2.22	0.75
1:B:38:GLU:HG2	1:B:167:ALA:HB2	1.69	0.74
1:B:145:ASP:HB2	1:B:149:LEU:HB2	1.71	0.72
1:A:142:ASP:OD1	1:A:156:ARG:NH2	2.23	0.71
1:B:70:THR:HG21	1:B:167:ALA:HA	1.73	0.71
1:X:136:ARG:NH2	1:Y:180:GLU:OE2	2.23	0.70
1:B:59:SER:HB3	1:Y:14:GLN:HG2	1.72	0.69
1:A:14:GLN:HG2	1:X:59:SER:HB3	1.73	0.69
1:A:228:ASN:ND2	1:A:291:GLY:HA3	2.06	0.69
1:X:39:ARG:NH1	1:X:203:GLN:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLU:HG2	1:A:410:TRP:CD1	2.29	0.68
1:B:218:ASP:HB3	1:B:224:LEU:HD13	1.75	0.68
1:A:37:GLN:OE1	1:A:168:ARG:NH1	2.27	0.68
1:A:21:ASP:O	1:A:23:LYS:N	2.27	0.66
1:A:437:LEU:HD22	3:A:502:PEG:H12	1.77	0.66
1:Y:318:ARG:HD2	1:Y:439:ALA:HB3	1.77	0.66
1:B:148:LYS:HG2	1:B:149:LEU:HD23	1.77	0.66
1:Y:257:LEU:HD21	1:Y:266:VAL:HG23	1.78	0.65
1:Y:206:LYS:NZ	1:Y:265:SER:OG	2.27	0.65
1:Y:38:GLU:HG2	1:Y:167:ALA:HB2	1.77	0.65
1:X:38:GLU:HG2	1:X:167:ALA:HB2	1.80	0.64
1:A:50:ILE:HG22	1:A:54:LEU:HD13	1.81	0.63
1:X:19:MET:O	1:X:21:ASP:N	2.32	0.63
1:A:44:LYS:HB2	1:A:195:VAL:HG21	1.81	0.63
1:Y:21:ASP:O	1:Y:23:LYS:N	2.32	0.63
1:Y:15:LEU:HB3	1:Y:16:LEU:HD23	1.81	0.62
1:A:35:ILE:C	1:A:37:GLN:H	2.08	0.62
1:Y:262:LEU:HG	1:Y:290:ARG:HH21	1.64	0.62
1:B:39:ARG:NH1	1:B:203:GLN:O	2.32	0.62
1:Y:421:VAL:HG13	4:Y:604:HOH:O	1.99	0.61
1:X:382:GLN:HB3	1:X:418:MET:HE1	1.82	0.61
1:A:151:ARG:HG3	1:A:187:VAL:HG23	1.83	0.60
1:B:340:ARG:HG2	1:B:360:LEU:HD12	1.84	0.60
1:A:20:ARG:HE	1:X:276:ARG:HE	1.50	0.60
1:A:265:SER:HB2	1:A:287:LEU:HD11	1.84	0.60
1:Y:409:GLU:HG2	1:Y:410:TRP:HD1	1.64	0.60
1:X:110:ARG:NH1	1:Y:180:GLU:OE1	2.35	0.60
1:X:409:GLU:HG2	1:X:410:TRP:HD1	1.67	0.60
1:Y:419:GLY:O	1:Y:421:VAL:N	2.32	0.60
1:A:242:VAL:HG12	1:A:247:ARG:HG3	1.84	0.59
1:B:106:MET:HA	1:B:106:MET:HE2	1.84	0.59
1:B:375:ARG:HH11	1:B:375:ARG:HB2	1.67	0.59
1:X:409:GLU:HG2	1:X:410:TRP:CD1	2.37	0.59
1:B:19:MET:O	1:B:21:ASP:N	2.34	0.58
1:X:39:ARG:HD2	1:X:202:LEU:O	2.04	0.58
1:A:16:LEU:HA	1:A:19:MET:HG3	1.84	0.58
1:A:294:MET:HE2	1:A:371:THR:HG22	1.85	0.58
1:B:39:ARG:HD2	1:B:202:LEU:O	2.03	0.57
1:Y:278:LEU:O	2:Y:501:ARG:N	2.38	0.57
1:B:323:GLY:C	1:B:327:ARG:HH21	2.13	0.57
1:A:318:ARG:HD2	1:A:439:ALA:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:CZ	4:B:605:HOH:O	2.42	0.56
1:Y:35:ILE:HG22	1:Y:37:GLN:H	1.70	0.56
1:Y:400:GLU:O	1:Y:415:ARG:NH1	2.38	0.56
1:Y:145:ASP:HB2	1:Y:149:LEU:HB2	1.86	0.56
1:A:38:GLU:HB3	1:A:72:VAL:HG23	1.88	0.56
1:A:419:GLY:O	1:A:421:VAL:N	2.33	0.56
1:B:276:ARG:NH2	1:Y:20:ARG:O	2.37	0.55
1:A:38:GLU:OE2	1:A:70:THR:OG1	2.20	0.55
1:X:106:MET:HA	1:X:106:MET:HE2	1.89	0.55
1:X:340:ARG:HB3	1:X:363:ALA:HB2	1.89	0.55
1:Y:140:GLU:OE1	1:Y:159:HIS:NE2	2.40	0.55
1:B:99:ARG:O	1:B:152:VAL:HG21	2.07	0.55
1:Y:85:LEU:HD12	1:Y:112:THR:HG23	1.89	0.55
1:Y:177:CYS:HB3	1:Y:189:ILE:O	2.06	0.55
1:A:106:MET:HE3	1:A:188:ASN:HB2	1.89	0.54
1:B:19:MET:HE3	1:Y:19:MET:HA	1.88	0.54
1:A:14:GLN:HG3	1:A:18:HIS:NE2	2.22	0.54
1:A:38:GLU:CG	1:A:167:ALA:HB2	2.36	0.54
1:B:62:ALA:O	1:B:66:THR:HG23	2.07	0.54
1:B:65:GLN:HA	1:B:69:LEU:O	2.08	0.54
1:A:19:MET:HG2	1:X:19:MET:HG3	1.89	0.53
1:A:257:LEU:HD21	1:A:266:VAL:HG23	1.90	0.53
1:A:31:ARG:HD3	1:A:205:TYR:OH	2.08	0.53
1:B:406:ARG:HD2	1:B:411:THR:OG1	2.08	0.53
1:A:351:TRP:HB3	1:A:384:ILE:HD13	1.91	0.53
1:X:237:MET:SD	1:X:247:ARG:HG2	2.49	0.53
1:B:25:ILE:HG23	1:B:279:PHE:HB3	1.91	0.53
1:Y:207:VAL:HB	1:Y:266:VAL:HG22	1.90	0.53
1:A:133:ALA:C	1:A:135:PRO:HD3	2.34	0.53
1:Y:145:ASP:OD1	1:Y:150:GLY:N	2.41	0.53
1:A:340:ARG:HG2	1:A:360:LEU:HD12	1.90	0.53
1:B:269:THR:HG21	1:B:277:GLU:HB2	1.91	0.53
1:Y:269:THR:CG2	1:Y:273:GLU:HB2	2.39	0.53
1:B:113:LEU:HD12	1:B:178:LEU:HD21	1.90	0.52
1:B:196:ARG:HH11	1:B:255:ARG:HD2	1.75	0.52
1:Y:106:MET:HE3	1:Y:188:ASN:HB2	1.91	0.52
1:B:19:MET:C	1:B:21:ASP:H	2.17	0.52
1:Y:196:ARG:HH11	1:Y:255:ARG:HD2	1.74	0.52
1:Y:412:VAL:HG23	1:Y:431:PHE:CE1	2.44	0.52
1:A:362:ASP:O	1:A:366:GLU:HG3	2.10	0.52
1:A:81:LEU:HB3	1:A:112:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:249:LYS:O	1:X:253:ILE:HG13	2.10	0.52
1:Y:405:VAL:HG21	1:Y:427:VAL:HG11	1.91	0.52
1:A:145:ASP:CG	1:A:149:LEU:HB2	2.35	0.52
1:B:106:MET:HE1	1:B:188:ASN:HB2	1.92	0.52
1:Y:81:LEU:HB3	1:Y:112:THR:HG21	1.92	0.51
1:X:96:ASP:HB2	1:X:100:VAL:HG13	1.93	0.51
1:A:16:LEU:HD12	1:A:17:SER:H	1.76	0.51
1:B:65:GLN:OE1	1:B:130:ARG:HB2	2.10	0.51
1:X:35:ILE:O	1:X:37:GLN:N	2.39	0.51
1:X:44:LYS:HD2	1:X:195:VAL:HG21	1.91	0.51
1:B:331:ASP:OD2	1:B:379:TYR:OH	2.21	0.51
1:X:340:ARG:HG2	1:X:360:LEU:HD12	1.93	0.51
1:Y:328:LEU:HG	1:Y:330:VAL:HG23	1.93	0.51
1:B:190:ASN:HB3	1:B:193:VAL:HG22	1.93	0.50
1:X:403:GLY:HA3	1:X:414:TRP:CZ2	2.46	0.50
1:B:17:SER:HB2	1:B:18:HIS:CD2	2.45	0.50
1:X:41:ALA:HA	1:X:206:LYS:O	2.11	0.50
1:A:120:LEU:O	1:A:124:ILE:HG13	2.11	0.50
1:B:38:GLU:CG	1:B:167:ALA:HB2	2.40	0.50
1:A:244:GLY:HA2	1:A:247:ARG:HD3	1.93	0.50
1:X:269:THR:HG21	1:X:277:GLU:HB2	1.93	0.50
1:A:328:LEU:HG	1:A:330:VAL:HG23	1.93	0.50
1:Y:81:LEU:O	1:Y:86:GLU:HB2	2.12	0.50
1:Y:331:ASP:OD2	1:Y:379:TYR:OH	2.18	0.50
1:A:20:ARG:HB2	1:X:20:ARG:CG	2.42	0.49
1:B:81:LEU:C	1:B:83:ALA:H	2.20	0.49
1:X:81:LEU:C	1:X:83:ALA:H	2.20	0.49
1:B:269:THR:HG22	1:B:285:GLY:HA3	1.94	0.49
1:X:65:GLN:HA	1:X:69:LEU:O	2.11	0.49
1:X:81:LEU:HD12	1:X:82:ASP:N	2.27	0.49
1:A:35:ILE:O	1:A:37:GLN:N	2.32	0.49
1:A:136:ARG:HH21	1:B:137:GLY:HA2	1.76	0.49
1:X:354:LEU:HB3	1:X:385:TRP:HB3	1.95	0.49
1:X:99:ARG:O	1:X:152:VAL:HG21	2.13	0.49
1:Y:233:PHE:CE1	1:Y:237:MET:HE2	2.48	0.49
1:B:38:GLU:HG3	1:B:163:VAL:HG12	1.94	0.49
1:Y:340:ARG:HG2	1:Y:360:LEU:HD12	1.95	0.49
1:B:362:ASP:OD2	1:B:362:ASP:N	2.41	0.48
1:A:22:GLY:HA2	1:A:25:ILE:HD12	1.95	0.48
1:B:13:VAL:O	1:B:16:LEU:HD11	2.13	0.48
1:B:354:LEU:HB3	1:B:385:TRP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:78:GLY:O	1:X:82:ASP:HB3	2.14	0.48
1:A:269:THR:HG22	1:A:270:ARG:H	1.77	0.48
1:B:270:ARG:HG2	1:B:273:GLU:HG2	1.95	0.48
1:X:81:LEU:HD22	1:X:109:ILE:HG12	1.96	0.48
1:B:147:ASP:OD1	1:B:147:ASP:N	2.46	0.48
1:X:125:ARG:HD3	1:Y:169:ALA:HB2	1.96	0.48
1:A:86:GLU:HG2	1:A:91:PRO:HG2	1.95	0.47
1:A:99:ARG:O	1:A:152:VAL:HG21	2.14	0.47
1:A:228:ASN:HD21	1:A:291:GLY:HA3	1.79	0.47
1:Y:269:THR:HG22	1:Y:270:ARG:H	1.78	0.47
1:A:196:ARG:NH1	1:A:252:GLU:OE1	2.46	0.47
1:A:347:ARG:NH1	1:A:350:GLY:O	2.47	0.47
1:A:331:ASP:OD2	1:A:379:TYR:OH	2.26	0.47
1:B:357:PHE:H	3:B:502:PEG:H21	1.78	0.47
1:X:269:THR:HG22	1:X:285:GLY:HA3	1.96	0.47
1:Y:421:VAL:N	4:Y:604:HOH:O	2.48	0.47
1:Y:14:GLN:NE2	1:Y:17:SER:HB2	2.30	0.47
1:Y:294:MET:HE2	1:Y:371:THR:HG22	1.96	0.47
1:A:81:LEU:HD12	1:A:82:ASP:N	2.30	0.47
1:B:134:VAL:HG13	1:B:162:LEU:HD13	1.97	0.47
1:Y:362:ASP:OD2	1:Y:362:ASP:N	2.47	0.47
1:A:186:LEU:HB3	1:B:184:GLY:HA3	1.95	0.47
1:B:257:LEU:HD21	1:B:266:VAL:HG23	1.97	0.47
1:Y:97:GLY:H	1:Y:149:LEU:HD21	1.80	0.47
1:A:37:GLN:HB3	1:A:38:GLU:H	1.47	0.46
1:B:81:LEU:HD22	1:B:109:ILE:HG12	1.97	0.46
1:B:86:GLU:HG2	1:B:91:PRO:HG2	1.97	0.46
1:A:412:VAL:HG23	1:A:431:PHE:CE1	2.51	0.46
1:Y:141:ALA:O	1:Y:181:THR:HA	2.15	0.46
1:Y:89:ASP:C	1:Y:91:PRO:HD3	2.41	0.46
1:A:200:HIS:ND1	1:A:259:ASP:OD2	2.47	0.46
1:Y:16:LEU:HA	1:Y:19:MET:HG3	1.97	0.46
1:A:196:ARG:NH1	1:A:255:ARG:HD2	2.30	0.46
1:B:96:ASP:HB2	1:B:100:VAL:HG13	1.98	0.46
1:X:65:GLN:CD	1:X:130:ARG:H	2.24	0.46
1:Y:36:ASP:O	1:Y:37:GLN:HB2	2.16	0.46
1:Y:39:ARG:HD2	1:Y:202:LEU:O	2.16	0.46
1:Y:105:ALA:O	1:Y:109:ILE:HG13	2.16	0.46
1:B:354:LEU:HB3	1:B:385:TRP:CB	2.47	0.45
1:X:90:ILE:N	1:X:91:PRO:HD3	2.31	0.45
1:Y:237:MET:O	1:Y:247:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:403:GLY:HA3	1:Y:414:TRP:CZ2	2.51	0.45
1:A:94:ARG:O	1:A:100:VAL:HG13	2.16	0.45
1:A:346:THR:HG23	1:A:355:ASP:HB2	1.97	0.45
1:Y:38:GLU:OE2	1:Y:70:THR:OG1	2.30	0.45
1:Y:89:ASP:HB3	1:Y:91:PRO:HD3	1.98	0.45
1:Y:336:THR:HG22	1:Y:341:ALA:O	2.16	0.45
1:B:308:LEU:HA	1:B:308:LEU:HD23	1.76	0.45
1:X:19:MET:C	1:X:21:ASP:H	2.23	0.45
1:X:207:VAL:HB	1:X:266:VAL:HG22	1.99	0.45
1:Y:38:GLU:CG	1:Y:167:ALA:HB2	2.44	0.45
1:A:50:ILE:O	1:A:54:LEU:HB2	2.15	0.45
1:B:38:GLU:OE2	1:B:38:GLU:HA	2.15	0.45
1:Y:227:ILE:HD13	1:Y:250:LEU:HD21	1.98	0.45
1:A:130:ARG:HH11	1:A:130:ARG:CG	2.30	0.45
1:A:113:LEU:HD12	1:A:178:LEU:HD21	1.99	0.45
1:Y:196:ARG:HA	1:Y:256:LEU:HD21	1.99	0.45
1:A:125:ARG:HA	1:A:129:GLY:O	2.17	0.45
1:A:136:ARG:NH2	1:B:137:GLY:HA2	2.31	0.45
1:B:294:MET:HE2	1:B:371:THR:HG22	1.99	0.45
1:A:206:LYS:HZ3	2:A:501:ARG:C	2.25	0.44
1:X:132:ALA:HB2	1:X:171:GLN:OE1	2.17	0.44
1:B:106:MET:CE	1:B:188:ASN:HB2	2.47	0.44
1:B:351:TRP:HB3	1:B:384:ILE:HD13	1.99	0.44
1:B:422:GLU:HB2	4:B:603:HOH:O	2.17	0.44
1:X:12:ILE:HG23	1:X:15:LEU:HB3	1.99	0.44
1:X:51:GLN:HB2	1:X:80:GLN:NE2	2.32	0.44
1:Y:326:ASP:OD1	1:Y:326:ASP:N	2.50	0.44
1:A:38:GLU:HB2	4:A:604:HOH:O	2.17	0.44
1:A:199:VAL:HG13	1:A:260:LEU:HD21	1.99	0.44
1:X:216:LEU:HD22	1:X:268:ILE:HD12	1.99	0.44
1:Y:44:LYS:HD3	1:Y:209:PHE:CE1	2.52	0.44
1:A:409:GLU:HG2	1:A:410:TRP:HD1	1.79	0.44
1:X:12:ILE:HG23	1:X:15:LEU:HD23	2.00	0.44
1:Y:269:THR:HG21	1:Y:273:GLU:HB2	1.99	0.44
1:Y:233:PHE:CZ	1:Y:237:MET:HE2	2.52	0.44
1:A:20:ARG:O	1:X:276:ARG:NH2	2.49	0.44
1:B:276:ARG:HE	1:Y:20:ARG:HA	1.83	0.44
1:B:318:ARG:HD2	1:B:439:ALA:HB3	1.99	0.44
1:A:44:LYS:HD3	1:A:209:PHE:CE1	2.53	0.44
1:A:89:ASP:C	1:A:91:PRO:HD3	2.43	0.43
1:A:81:LEU:C	1:A:83:ALA:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:VAL:HG13	1:A:342:ALA:HB2	2.00	0.43
1:B:207:VAL:HB	1:B:266:VAL:HG22	1.99	0.43
1:B:354:LEU:HD21	1:B:357:PHE:HB2	2.00	0.43
1:X:438:GLU:H	1:X:438:GLU:HG2	1.57	0.43
1:Y:41:ALA:HA	1:Y:206:LYS:O	2.18	0.43
1:A:180:GLU:OE1	1:B:110:ARG:NH1	2.51	0.43
1:A:287:LEU:HB2	2:A:501:ARG:NE	2.33	0.43
1:X:356:LYS:HA	1:X:356:LYS:HD3	1.76	0.43
1:A:196:ARG:HA	1:A:256:LEU:HD21	1.99	0.43
1:B:412:VAL:HG11	1:B:427:VAL:HG22	1.98	0.43
1:B:418:MET:HG3	1:B:423:VAL:CG1	2.49	0.43
1:A:269:THR:CG2	1:A:273:GLU:HB2	2.48	0.43
1:X:206:LYS:HE2	2:X:501:ARG:OXT	2.19	0.43
1:A:35:ILE:C	1:A:37:GLN:N	2.71	0.43
1:A:177:CYS:HB3	1:A:189:ILE:O	2.18	0.43
1:Y:133:ALA:C	1:Y:135:PRO:HD3	2.43	0.43
1:A:316:PHE:HE1	3:A:502:PEG:H21	1.83	0.43
1:Y:12:ILE:O	1:Y:16:LEU:HD21	2.18	0.43
1:Y:416:GLY:O	1:Y:417:GLU:C	2.62	0.43
1:B:389:THR:HG21	1:B:407:ARG:O	2.19	0.43
1:A:11:THR:C	1:A:12:ILE:HD12	2.44	0.42
1:Y:97:GLY:HA3	1:Y:149:LEU:HD21	2.01	0.42
1:Y:181:THR:HG23	1:Y:185:THR:O	2.19	0.42
1:B:287:LEU:HG	1:B:288:ILE:N	2.34	0.42
1:A:35:ILE:HG22	1:A:37:GLN:N	2.34	0.42
1:A:39:ARG:HD2	1:A:202:LEU:O	2.19	0.42
1:B:143:ILE:O	1:B:145:ASP:N	2.52	0.42
1:Y:81:LEU:C	1:Y:83:ALA:H	2.27	0.42
1:A:233:PHE:CZ	1:A:237:MET:HE2	2.55	0.42
1:A:410:TRP:HH2	3:A:502:PEG:H11	1.83	0.42
1:B:354:LEU:HD13	1:B:376:MET:HE2	2.01	0.42
1:A:12:ILE:HG21	1:A:67:VAL:HA	2.01	0.42
1:X:65:GLN:HE22	1:X:130:ARG:HD3	1.85	0.42
1:Y:412:VAL:HG23	1:Y:431:PHE:CZ	2.55	0.42
1:A:290:ARG:HD3	4:A:602:HOH:O	2.20	0.42
1:B:91:PRO:O	1:B:92:THR:OG1	2.33	0.42
1:B:285:GLY:O	2:B:501:ARG:NH2	2.53	0.42
1:Y:351:TRP:HB3	1:Y:384:ILE:HD13	2.02	0.42
1:A:14:GLN:NE2	1:A:17:SER:HB2	2.35	0.42
1:X:35:ILE:C	1:X:37:GLN:N	2.78	0.42
1:Y:47:GLY:O	1:Y:50:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.91	0.42
1:B:86:GLU:O	1:B:91:PRO:HG2	2.20	0.42
1:A:326:ASP:OD1	1:A:326:ASP:N	2.52	0.42
1:B:19:MET:SD	1:Y:19:MET:HG2	2.58	0.42
1:X:38:GLU:CG	1:X:167:ALA:HB2	2.46	0.42
1:A:15:LEU:HB3	1:A:16:LEU:HD23	2.02	0.41
1:B:403:GLY:HA3	1:B:414:TRP:CZ2	2.55	0.41
1:Y:78:GLY:C	1:Y:80:GLN:H	2.28	0.41
1:Y:336:THR:O	1:Y:338:SER:N	2.53	0.41
1:B:90:ILE:N	1:B:91:PRO:HD3	2.35	0.41
1:Y:101:THR:O	1:Y:101:THR:OG1	2.34	0.41
1:A:216:LEU:HB2	1:A:286:THR:HG21	2.02	0.41
1:B:38:GLU:OE1	1:B:70:THR:HG22	2.20	0.41
1:B:81:LEU:HD12	1:B:82:ASP:N	2.36	0.41
1:X:25:ILE:H	1:X:25:ILE:HG12	1.75	0.41
1:X:38:GLU:HB3	1:X:72:VAL:CG2	2.51	0.41
1:X:48:ALA:HA	1:X:79:PRO:HG2	2.02	0.41
1:Y:196:ARG:NH1	1:Y:255:ARG:HD2	2.35	0.41
1:Y:341:ALA:HA	1:Y:358:ALA:O	2.21	0.41
1:A:15:LEU:HD22	1:X:63:PHE:HE1	1.85	0.41
1:B:78:GLY:O	1:B:82:ASP:HB3	2.20	0.41
1:X:218:ASP:HB3	1:X:224:LEU:HD13	2.02	0.41
1:A:78:GLY:HA3	1:A:79:PRO:HD3	1.89	0.41
1:X:219:GLU:HB2	1:X:241:TRP:CE2	2.56	0.41
1:B:104:GLU:H	1:B:104:GLU:HG2	1.64	0.41
1:B:294:MET:SD	1:B:375:ARG:HD2	2.60	0.41
1:X:50:ILE:HD12	1:X:116:ALA:HB1	2.02	0.41
1:Y:269:THR:HG22	1:Y:273:GLU:HB2	2.02	0.41
1:A:294:MET:HB3	1:A:294:MET:HE3	1.77	0.41
1:A:407:ARG:NH2	1:A:428:GLU:OE1	2.53	0.41
1:B:253:ILE:HD11	1:B:268:ILE:HD11	2.03	0.41
1:Y:10:GLN:O	1:Y:13:VAL:HG23	2.20	0.41
1:A:356:LYS:HD3	1:A:356:LYS:HA	1.81	0.41
1:B:23:LYS:N	4:B:601:HOH:O	2.53	0.41
1:B:38:GLU:OE2	1:B:70:THR:HB	2.21	0.41
1:B:48:ALA:HA	1:B:79:PRO:HG2	2.03	0.41
1:X:224:LEU:HD23	1:X:227:ILE:HD11	2.03	0.41
1:Y:38:GLU:OE2	1:Y:38:GLU:HA	2.21	0.41
1:Y:81:LEU:HD12	1:Y:82:ASP:N	2.36	0.41
1:Y:385:TRP:CE2	1:Y:413:PHE:HB2	2.56	0.41
1:Y:403:GLY:HA3	1:Y:414:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:HG23	1:B:49:VAL:HB	2.03	0.41
1:B:336:THR:HG22	1:B:341:ALA:O	2.20	0.41
1:X:50:ILE:O	1:X:54:LEU:HB2	2.21	0.41
1:Y:140:GLU:HB2	1:Y:159:HIS:CD2	2.55	0.41
1:A:19:MET:HA	1:X:19:MET:HE3	2.02	0.40
1:A:20:ARG:HA	1:X:276:ARG:HE	1.86	0.40
1:A:139:PHE:CZ	1:A:194:ALA:HB1	2.56	0.40
1:B:39:ARG:O	1:B:204:PRO:HA	2.21	0.40
1:Y:356:LYS:HE3	1:Y:437:LEU:HD13	2.03	0.40
1:X:77:GLY:O	1:X:81:LEU:HG	2.21	0.40
1:Y:283:GLY:HA3	2:Y:501:ARG:NH1	2.36	0.40
1:A:251:GLU:HG2	1:A:255:ARG:NH2	2.36	0.40
1:B:253:ILE:HG21	1:B:288:ILE:HD12	2.04	0.40
1:Y:335:VAL:HG13	1:Y:342:ALA:HB2	2.02	0.40
1:X:62:ALA:O	1:X:66:THR:HG23	2.21	0.40
1:X:219:GLU:HB2	1:X:241:TRP:CD2	2.56	0.40
1:X:335:VAL:HG22	1:X:342:ALA:HB1	2.03	0.40
1:Y:11:THR:C	1:Y:12:ILE:HD12	2.46	0.40
1:Y:44:LYS:HB2	1:Y:195:VAL:HG21	2.03	0.40
1:Y:94:ARG:O	1:Y:100:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/461 (93%)	376 (88%)	36 (8%)	17 (4%)	2	8
1	B	429/461 (93%)	382 (89%)	33 (8%)	14 (3%)	3	11
1	X	429/461 (93%)	383 (89%)	34 (8%)	12 (3%)	4	14
1	Y	429/461 (93%)	381 (89%)	30 (7%)	18 (4%)	2	7
All	All	1716/1844 (93%)	1522 (89%)	133 (8%)	61 (4%)	2	10

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	22	GLY
1	A	37	GLN
1	A	145	ASP
1	A	417	GLU
1	A	420	PRO
1	B	20	ARG
1	B	96	ASP
1	B	144	VAL
1	B	145	ASP
1	X	20	ARG
1	X	37	GLN
1	X	144	VAL
1	X	145	ASP
1	Y	15	LEU
1	Y	22	GLY
1	Y	37	GLN
1	Y	417	GLU
1	Y	420	PRO
1	A	36	ASP
1	A	78	GLY
1	A	83	ALA
1	A	92	THR
1	A	93	GLU
1	A	419	GLY
1	B	23	LYS
1	B	78	GLY
1	B	84	ALA
1	X	23	LYS
1	X	78	GLY
1	X	96	ASP
1	Y	83	ALA
1	Y	93	GLU
1	Y	145	ASP
1	B	31	ARG
1	B	37	GLN
1	B	83	ALA
1	X	83	ALA
1	Y	92	THR
1	Y	330	VAL
1	Y	337	GLU
1	A	330	VAL

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Mol	Chain	Res	Type
1	B	146	ALA
1	X	31	ARG
1	X	92	THR
1	X	330	VAL
1	Y	13	VAL
1	Y	78	GLY
1	Y	419	GLY
1	A	91	PRO
1	A	329	ARG
1	B	92	THR
1	B	330	VAL
1	Y	91	PRO
1	Y	284	SER
1	X	36	ASP
1	Y	329	ARG
1	B	420	PRO
1	Y	79	PRO
1	A	13	VAL
1	A	79	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	342/367 (93%)	319 (93%)	23 (7%)	15	42
1	B	342/367 (93%)	313 (92%)	29 (8%)	10	31
1	X	342/367 (93%)	315 (92%)	27 (8%)	11	35
1	Y	342/367 (93%)	321 (94%)	21 (6%)	17	46
All	All	1368/1468 (93%)	1268 (93%)	100 (7%)	13	38

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	13	VAL

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Mol	Chain	Res	Type
1	A	16	LEU
1	A	37	GLN
1	A	45	VAL
1	A	50	ILE
1	A	66	THR
1	A	67	VAL
1	A	95	VAL
1	A	100	VAL
1	A	106	MET
1	A	130	ARG
1	A	148	LYS
1	A	157	HIS
1	A	199	VAL
1	A	216	LEU
1	A	220	ASP
1	A	269	THR
1	A	272	SER
1	A	295	VAL
1	A	326	ASP
1	A	407	ARG
1	A	423	VAL
1	B	13	VAL
1	B	16	LEU
1	B	29	LEU
1	B	35	ILE
1	B	45	VAL
1	B	65	GLN
1	B	89	ASP
1	B	90	ILE
1	B	95	VAL
1	B	99	ARG
1	B	112	THR
1	B	138	VAL
1	B	145	ASP
1	B	183	ASP
1	B	187	VAL
1	B	216	LEU
1	B	226	SER
1	B	253	ILE
1	B	265	SER
1	B	272	SER
1	B	287	LEU

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Mol	Chain	Res	Type
1	B	327	ARG
1	B	362	ASP
1	B	372	VAL
1	B	375	ARG
1	B	378	ASP
1	B	418	MET
1	B	421	VAL
1	B	438	GLU
1	X	13	VAL
1	X	16	LEU
1	X	29	LEU
1	X	35	ILE
1	X	45	VAL
1	X	65	GLN
1	X	89	ASP
1	X	90	ILE
1	X	95	VAL
1	X	99	ARG
1	X	106	MET
1	X	112	THR
1	X	117	ASN
1	X	147	ASP
1	X	149	LEU
1	X	183	ASP
1	X	187	VAL
1	X	216	LEU
1	X	226	SER
1	X	265	SER
1	X	272	SER
1	X	362	ASP
1	X	375	ARG
1	X	378	ASP
1	X	418	MET
1	X	421	VAL
1	X	438	GLU
1	Y	12	ILE
1	Y	13	VAL
1	Y	16	LEU
1	Y	37	GLN
1	Y	45	VAL
1	Y	50	ILE
1	Y	66	THR

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Mol	Chain	Res	Type
1	Y	67	VAL
1	Y	95	VAL
1	Y	99	ARG
1	Y	100	VAL
1	Y	106	MET
1	Y	187	VAL
1	Y	216	LEU
1	Y	220	ASP
1	Y	269	THR
1	Y	272	SER
1	Y	326	ASP
1	Y	407	ARG
1	Y	423	VAL
1	Y	438	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	228	ASN
1	B	30	HIS
1	B	115	GLN
1	B	117	ASN
1	B	159	HIS
1	X	159	HIS
1	Y	14	GLN
1	Y	310	ASN
1	Y	382	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 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	ARG	A	501	-	10,11,11	0.81	0	9,13,13	1.01	1 (11%)
2	ARG	B	501	-	10,11,11	0.62	0	9,13,13	1.01	1 (11%)
2	ARG	X	501	-	10,11,11	0.70	1 (10%)	9,13,13	0.92	1 (11%)
3	PEG	X	502	-	6,6,6	0.67	0	5,5,5	1.31	0
3	PEG	B	502	-	6,6,6	0.48	0	5,5,5	1.61	1 (20%)
3	PEG	Y	502	-	6,6,6	0.53	0	5,5,5	1.38	0
2	ARG	Y	501	-	10,11,11	0.77	1 (10%)	9,13,13	0.95	1 (11%)
3	PEG	A	502	-	6,6,6	0.49	0	5,5,5	1.62	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	A	501	-	-	0/11/11/11	-
2	ARG	B	501	-	-	0/11/11/11	-
2	ARG	X	501	-	-	0/11/11/11	-
3	PEG	X	502	-	-	4/4/4/4	-
3	PEG	B	502	-	-	2/4/4/4	-
3	PEG	Y	502	-	-	3/4/4/4	-
2	ARG	Y	501	-	-	0/11/11/11	-
3	PEG	A	502	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	501	ARG	OXT-C	-2.10	1.24	1.30
2	Y	501	ARG	OXT-C	-2.07	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ARG	OXT-C-O	-2.86	117.58	124.08
2	B	501	ARG	OXT-C-O	-2.76	117.82	124.08
2	X	501	ARG	OXT-C-O	-2.62	118.14	124.08
2	Y	501	ARG	OXT-C-O	-2.53	118.34	124.08
3	A	502	PEG	O2-C3-C4	2.12	119.45	110.11
3	B	502	PEG	O2-C3-C4	2.04	119.08	110.11

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	PEG	C1-C2-O2-C3
3	X	502	PEG	O1-C1-C2-O2
3	X	502	PEG	O2-C3-C4-O4
3	B	502	PEG	O2-C3-C4-O4
3	Y	502	PEG	O2-C3-C4-O4
3	X	502	PEG	C4-C3-O2-C2
3	Y	502	PEG	C4-C3-O2-C2
3	X	502	PEG	C1-C2-O2-C3
3	Y	502	PEG	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ARG	2	0
2	B	501	ARG	1	0
2	X	501	ARG	1	0
3	B	502	PEG	1	0
2	Y	501	ARG	2	0
3	A	502	PEG	3	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	431/461 (93%)	-0.50	4 (0%) 81 74	59, 96, 163, 205	0
1	B	431/461 (93%)	-0.49	6 (1%) 73 64	43, 84, 154, 193	0
1	X	431/461 (93%)	-0.49	3 (0%) 84 77	68, 102, 167, 199	0
1	Y	431/461 (93%)	-0.41	5 (1%) 76 68	57, 98, 174, 214	0
All	All	1724/1844 (93%)	-0.47	18 (1%) 79 72	43, 96, 166, 214	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	38	GLU	4.6
1	Y	90	ILE	3.9
1	B	15	LEU	3.0
1	B	85	LEU	2.7
1	X	38	GLU	2.7
1	B	35	ILE	2.7
1	B	11	THR	2.7
1	A	36	ASP	2.7
1	A	38	GLU	2.4
1	Y	420	PRO	2.3
1	B	22	GLY	2.3
1	B	19	MET	2.3
1	X	19	MET	2.2
1	Y	439	ALA	2.2
1	X	18	HIS	2.2
1	A	15	LEU	2.2
1	Y	15	LEU	2.2
1	A	82	ASP	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	PEG	X	502	7/7	0.79	0.13	55,81,109,119	0
3	PEG	A	502	7/7	0.82	0.12	53,70,86,92	0
3	PEG	B	502	7/7	0.91	0.09	55,95,101,111	0
2	ARG	Y	501	12/12	0.92	0.06	50,62,79,88	0
3	PEG	Y	502	7/7	0.92	0.10	66,85,107,113	0
2	ARG	B	501	12/12	0.93	0.07	53,67,86,103	0
2	ARG	A	501	12/12	0.93	0.06	47,62,84,85	0
2	ARG	X	501	12/12	0.95	0.07	61,70,87,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.