



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:16 PM UTC

PDB ID : 2WIU / pdb_00002wiu
Title : Mercury-modified bacterial persistence regulator hipBA
Authors : Evdokimov, A.; Voznesensky, I.; Fennell, K.; Anderson, M.; Smith, J.F.;
Fisher, D.A.
Deposited on : 2009-05-17
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

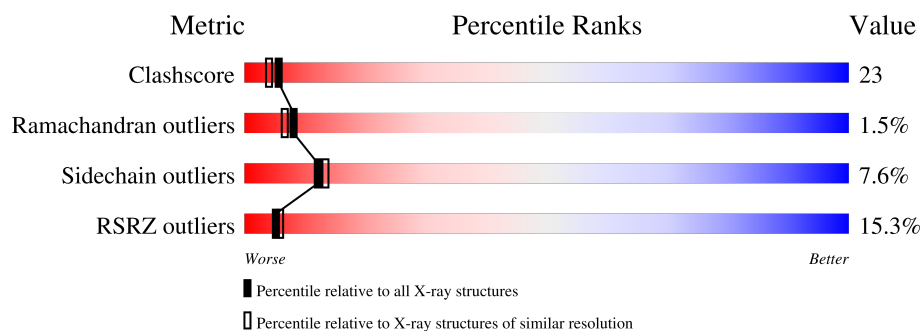
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	446	17% 61% 28% 6% • •
1	C	446	13% 54% 31% • 10%
2	B	88	8% 47% 32% • 19%
2	D	88	10% 48% 24% 9% 19%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8029 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 PROTEIN HIPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3397	2171	593	620	13			
1	C	401	Total	C	N	O	S	0	3	0
			3190	2043	557	576	14			

- Molecule 2 is a protein called HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	S	0	1	0
			576	366	96	111	3			
2	D	71	Total	C	N	O	S	0	0	0
			571	362	95	111	3			

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Hg	0	0
			2	2		
3	B	1	Total	Hg	0	0
			1	1		
3	C	3	Total	Hg	0	0
			3	3		
3	D	1	Total	Hg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	2	Total	Cl	0	0
			2	2		

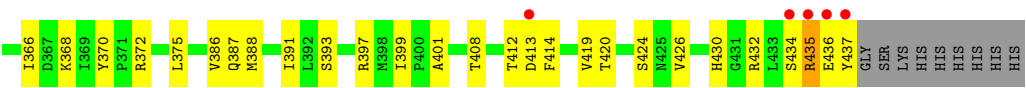
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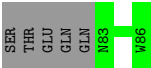
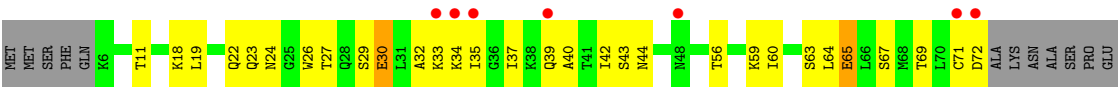
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	Cl 3	0	0
4	D	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total 108	O 108	0	0
5	B	18	Total 18	O 18	0	0
5	C	135	Total 135	O 135	0	0
5	D	17	Total 17	O 17	0	0



● Molecule 2: HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB



● Molecule 2: HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	166.93Å 166.93Å 124.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	166.67 – 2.35 166.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (166.67-2.35) 88.8 (166.67-2.35)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.264 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8029	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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 27.39 % 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 2.2189e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, HG

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	1.17	5/3470 (0.1%)	1.39	39/4701 (0.8%)
1	C	1.12	4/3264 (0.1%)	1.30	20/4418 (0.5%)
2	B	1.28	2/587 (0.3%)	1.19	3/790 (0.4%)
2	D	1.37	1/579 (0.2%)	1.30	3/780 (0.4%)
All	All	1.18	12/7900 (0.2%)	1.33	65/10689 (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	4
1	C	0	4
2	B	0	1
2	D	0	2
All	All	0	11

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	LEU	C-N	-30.53	0.91	1.33
2	B	33	LYS	CG-CD	6.47	1.71	1.52
2	D	9	SER	C-O	-5.78	1.18	1.24
1	A	357	ASN	CG-OD1	5.78	1.34	1.23
1	C	344	GLY	C-O	-5.71	1.17	1.24
1	A	399	ILE	C-O	-5.51	1.20	1.24
1	C	22	GLY	C-O	-5.43	1.16	1.24
1	C	57	VAL	CA-CB	5.37	1.60	1.54
1	A	158	THR	C-O	-5.33	1.18	1.23
2	B	18	LYS	C-O	-5.31	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	LEU	C-O	-5.25	1.18	1.24
1	C	257	GLN	C-O	-5.23	1.18	1.24

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LEU	O-C-N	-14.89	103.83	123.19
1	A	161	LEU	CA-C-N	12.25	144.93	121.54
1	A	161	LEU	C-N-CA	12.25	144.93	121.54
1	A	162	ARG	CA-C-N	10.91	138.11	123.06
1	A	162	ARG	C-N-CA	10.91	138.11	123.06
1	A	265	VAL	N-CA-C	-10.90	102.46	113.47
1	A	162	ARG	O-C-N	-10.89	108.11	122.59
1	C	339	VAL	N-CA-C	-7.71	105.49	112.90
1	C	397	ARG	N-CA-C	7.70	119.67	111.28
1	C	426	VAL	N-CA-C	7.67	117.78	110.42
1	A	119	LYS	N-CA-C	7.32	119.75	110.24
1	A	74	ARG	N-CA-C	7.18	119.73	111.11
1	A	75	ILE	N-CA-C	-7.18	103.30	110.62
1	C	391	ILE	N-CA-C	-7.16	103.87	110.82
1	A	436	GLU	N-CA-C	7.11	121.78	113.18
1	C	275	ILE	N-CA-C	6.98	117.12	110.42
1	A	271	GLY	N-CA-C	6.96	123.06	110.95
1	C	304	LEU	N-CA-C	6.66	118.20	111.07
1	A	275	ILE	N-CA-C	6.55	117.30	110.62
1	A	38	ALA	N-CA-C	6.45	119.34	110.24
1	C	37	TYR	N-CA-C	6.44	120.24	112.38
1	A	200	VAL	N-CA-C	6.36	116.50	110.53
1	C	368	LYS	N-CA-C	6.27	120.61	113.15
1	A	70	ILE	N-CA-C	6.19	116.31	110.30
2	B	22	GLN	N-CA-C	6.17	117.81	111.14
2	D	59	LYS	N-CA-C	6.06	118.41	111.02
1	C	419	VAL	CB-CA-C	-6.04	104.15	111.88
1	C	311	HIS	N-CA-C	6.03	118.49	110.53
2	D	64	LEU	N-CA-C	-5.99	105.62	113.17
1	A	379	LYS	N-CA-C	-5.94	104.78	112.68
1	C	408	THR	N-CA-C	5.92	118.50	111.33
1	A	210	ALA	N-CA-C	-5.86	104.97	111.36
1	A	123	ALA	N-CA-C	-5.78	105.12	111.82
1	A	423	GLU	CB-CA-C	-5.74	101.21	110.74
1	C	414	PHE	N-CA-C	5.72	117.72	109.48
1	A	62	ASP	N-CA-C	-5.66	105.19	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	SER	CA-C-N	5.64	125.49	119.28
1	A	68	SER	C-N-CA	5.64	125.49	119.28
1	C	305	ILE	N-CA-C	5.58	119.22	112.80
2	B	11	THR	N-CA-C	5.48	117.26	111.28
1	A	168	CYS	N-CA-C	5.47	118.15	109.50
1	A	197	SER	N-CA-C	-5.41	106.38	112.87
1	C	276	ALA	N-CA-C	5.41	117.61	111.02
1	C	54	SER	N-CA-C	5.38	117.23	110.24
1	A	57	VAL	CB-CA-C	-5.38	104.84	111.94
1	A	95	ARG	N-CA-C	5.36	118.03	111.82
1	A	304	LEU	N-CA-C	5.31	117.48	111.11
1	A	116	ALA	N-CA-C	5.31	116.02	108.54
1	A	397	ARG	N-CA-C	5.30	117.97	111.82
1	A	195	ASP	N-CA-C	5.29	117.76	108.56
1	C	75	ILE	CB-CA-C	-5.28	105.11	112.02
1	A	423	GLU	N-CA-C	5.28	120.08	111.37
1	C	375	LEU	N-CA-C	5.26	117.02	111.28
1	A	432	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	A	39	ARG	CA-C-N	5.22	125.14	119.76
1	A	39	ARG	C-N-CA	5.22	125.14	119.76
1	C	208	LEU	N-CA-C	5.21	116.64	111.07
1	A	201	ASP	N-CA-C	5.17	116.92	111.28
1	A	112	HIS	CA-C-N	5.15	125.07	119.76
1	A	112	HIS	C-N-CA	5.15	125.07	119.76
1	C	174	THR	CA-C-N	5.11	125.09	120.03
1	C	174	THR	C-N-CA	5.11	125.09	120.03
1	A	388	MET	N-CA-C	5.02	116.76	111.28
2	D	9	SER	N-CA-C	5.02	113.92	108.14
2	B	42	ILE	CB-CA-C	-5.01	105.45	112.02

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ASP	Peptide
1	A	164	GLY	Peptide
1	A	270	ASP	Peptide
1	A	358	ALA	Peptide
2	B	71	CYS	Peptide
1	C	120	LEU	Peptide
1	C	165	ASN	Peptide
1	C	170	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	C	99	GLY	Peptide
2	D	24	ASN	Peptide
2	D	71	CYS	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	3397	0	3426	147	2
1	C	3190	0	3237	168	0
2	B	576	0	586	28	0
2	D	571	0	575	26	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	1	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	1	0
5	A	108	0	0	3	0
5	B	18	0	0	1	0
5	C	135	0	0	5	0
5	D	17	0	0	0	0
All	All	8029	0	7824	364	2

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 23.

All (364) 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:121:THR:HG22	1:C:124:ARG:NH1	1.21	1.48
1:A:263:SER:O	1:A:266:LYS:HG2	1.16	1.28
1:C:63:ASN:ND2	1:C:256[B]:CYS:SG	2.08	1.27
1:C:121:THR:CG2	1:C:124:ARG:NH1	1.99	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:THR:CG2	1:C:124:ARG:HH12	1.53	1.19
1:C:142:ARG:NH1	1:C:146:ASP:OD2	1.76	1.18
1:A:79:TYR:HE2	1:A:140:MET:CE	1.56	1.16
1:A:79:TYR:CE2	1:A:140:MET:HE3	1.80	1.16
1:C:241:ASN:HD22	1:C:245:THR:HG23	1.10	1.15
1:C:124:ARG:CB	1:C:124:ARG:HH11	1.59	1.14
1:A:79:TYR:CE2	1:A:140:MET:CE	2.31	1.13
1:C:279:MET:HE3	1:C:295:PHE:CD2	1.84	1.11
1:A:79:TYR:CZ	1:A:140:MET:HE3	1.84	1.10
1:C:279:MET:HE3	1:C:295:PHE:HD2	0.94	1.10
1:C:279:MET:CE	1:C:295:PHE:HD2	1.65	1.10
1:A:263:SER:O	1:A:266:LYS:CG	2.00	1.08
1:C:279:MET:CE	1:C:295:PHE:CD2	2.37	1.07
1:A:79:TYR:OH	1:A:140:MET:HE3	1.54	1.07
1:C:78:ARG:HG3	1:C:78:ARG:HH11	0.93	1.06
1:C:124:ARG:O	1:C:128:VAL:HG23	1.54	1.04
1:A:11:GLN:HG2	1:A:32:TRP:HZ3	1.21	1.04
2:D:35:ILE:CD1	2:D:37:ILE:HG12	1.88	1.03
1:C:125:LEU:C	1:C:127:GLU:H	1.67	1.02
2:D:35:ILE:HD12	2:D:37:ILE:HG12	1.42	1.01
1:C:124:ARG:NH1	1:C:124:ARG:HB3	1.77	1.00
1:C:279:MET:HE1	1:C:295:PHE:HB3	1.44	0.99
1:C:78:ARG:HH11	1:C:78:ARG:CG	1.75	0.98
1:A:79:TYR:HE2	1:A:140:MET:HE1	1.26	0.98
1:A:128:VAL:HG22	1:A:141:ILE:HD11	1.45	0.97
1:A:119:LYS:HZ2	1:A:166:ASP:CG	1.73	0.96
1:C:124:ARG:HH11	1:C:124:ARG:HB2	1.31	0.94
1:C:129:LEU:HB3	1:C:182:LEU:HD11	1.50	0.94
1:C:124:ARG:NH1	1:C:124:ARG:CB	2.30	0.93
1:C:120:LEU:HG	1:C:124:ARG:NH2	1.85	0.92
2:B:27:THR:HG23	2:B:29:SER:H	1.33	0.91
1:A:185:GLY:HA2	1:A:197:SER:HA	1.52	0.91
2:D:24:ASN:O	2:D:26:TRP:N	2.04	0.90
2:B:35:ILE:CG2	2:B:63:SER:HB3	2.02	0.89
2:D:24:ASN:ND2	2:D:26:TRP:CZ3	2.40	0.88
1:A:288:ALA:O	1:A:292:ARG:HG3	1.73	0.88
1:C:78:ARG:HG3	1:C:78:ARG:NH1	1.74	0.88
1:C:187:ILE:HD12	1:C:196:LEU:HD12	1.56	0.88
1:C:63:ASN:CG	1:C:256[B]:CYS:SG	2.58	0.87
1:A:11:GLN:HG2	1:A:32:TRP:CZ3	2.10	0.87
1:A:141:ILE:HG22	1:A:143:GLU:H	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:HG22	1:C:170:PRO:O	1.74	0.86
2:B:69:THR:HG22	2:D:69:THR:HG22	1.56	0.85
1:A:243:GLU:O	1:A:245:THR:HG23	1.75	0.85
1:A:268:GLU:OE2	1:A:362:LYS:NZ	2.09	0.85
1:C:105:PRO:O	1:C:107:ASP:N	2.11	0.84
1:C:121:THR:HG22	1:C:124:ARG:HH11	1.39	0.84
1:C:121:THR:HG23	1:C:124:ARG:H	1.42	0.84
1:C:279:MET:CE	1:C:295:PHE:HB3	2.08	0.83
1:C:241:ASN:ND2	1:C:245:THR:HG23	1.92	0.83
1:A:128:VAL:CG2	1:A:141:ILE:HD11	2.08	0.83
1:C:229:ARG:HH11	1:C:229:ARG:HG3	1.44	0.82
2:B:27:THR:CG2	2:B:30:GLU:H	1.92	0.82
1:C:125:LEU:C	1:C:127:GLU:N	2.36	0.81
2:D:24:ASN:O	2:D:25:GLY:C	2.22	0.81
1:C:167:TRP:C	1:C:168[A]:CYS:SG	2.64	0.81
2:D:24:ASN:ND2	2:D:26:TRP:CH2	2.49	0.81
1:A:119:LYS:NZ	1:A:166:ASP:CG	2.39	0.80
1:C:120:LEU:HG	1:C:124:ARG:CZ	2.12	0.80
1:C:288:ALA:O	1:C:292:ARG:HG3	1.82	0.80
2:B:35:ILE:HG21	2:B:63:SER:HB3	1.62	0.79
1:A:363:LYS:HD3	1:A:373:HIS:CD2	2.16	0.79
1:A:243:GLU:HB2	1:A:245:THR:HG23	1.62	0.79
1:A:82:LYS:O	1:A:83:SER:CB	2.30	0.78
1:C:434:SER:C	1:C:436:GLU:H	1.92	0.78
1:C:121:THR:CG2	1:C:124:ARG:HH11	1.94	0.78
1:A:191:ASN:O	1:A:192:ALA:HB2	1.83	0.78
1:A:128:VAL:HG22	1:A:141:ILE:CD1	2.13	0.78
1:C:279:MET:HE2	1:C:295:PHE:CD2	2.17	0.77
1:C:124:ARG:O	1:C:128:VAL:CG2	2.30	0.77
1:A:79:TYR:CE2	1:A:140:MET:HE1	2.09	0.77
1:C:105:PRO:C	1:C:107:ASP:H	1.91	0.76
2:D:35:ILE:HD11	2:D:37:ILE:HG12	1.67	0.76
1:C:256[A]:CYS:SG	3:C:1440:HG:HG	2.04	0.76
1:C:121:THR:HG22	1:C:124:ARG:HB3	1.68	0.76
1:C:124:ARG:O	1:C:127:GLU:HB3	1.84	0.76
2:D:31:LEU:HD22	2:D:63:SER:HB3	1.66	0.76
1:A:121:THR:O	1:A:122:GLU:CB	2.30	0.75
1:C:122:GLU:C	1:C:122:GLU:OE1	2.30	0.75
2:D:35:ILE:HD11	2:D:37:ILE:CG1	2.16	0.74
1:C:106:GLU:C	1:C:107:ASP:OD1	2.29	0.74
2:B:27:THR:HG22	2:B:30:GLU:H	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HZ2	1:A:166:ASP:CB	2.00	0.73
1:C:125:LEU:HA	1:C:128:VAL:HG23	1.68	0.73
1:C:120:LEU:CG	1:C:124:ARG:NH2	2.52	0.73
2:D:35:ILE:CD1	2:D:37:ILE:CG1	2.67	0.73
1:A:357:ASN:HD22	1:A:380:VAL:HG21	1.53	0.73
2:B:27:THR:HG23	2:B:29:SER:N	2.04	0.72
1:A:130:THR:O	1:A:130:THR:CG2	2.37	0.72
1:A:78:ARG:NH2	1:A:141:ILE:O	2.19	0.72
1:C:121:THR:O	1:C:123:ALA:N	2.23	0.72
2:B:35:ILE:HG23	2:B:63:SER:HB3	1.72	0.71
1:C:292:ARG:NH1	5:C:2086:HOH:O	2.21	0.71
2:B:69:THR:CG2	2:D:69:THR:HG22	2.19	0.71
1:A:263:SER:C	1:A:266:LYS:HG2	2.13	0.71
1:C:241:ASN:HD22	1:C:245:THR:CG2	1.98	0.70
1:A:145:ASN:O	1:A:146:ASP:HB2	1.92	0.69
1:A:83:SER:OG	1:A:84:ARG:N	2.23	0.69
2:B:69:THR:HG22	2:D:69:THR:CG2	2.21	0.69
1:C:124:ARG:C	1:C:127:GLU:HB3	2.17	0.69
2:D:21:ARG:HG2	2:D:21:ARG:HH11	1.56	0.69
1:C:129:LEU:CB	1:C:182:LEU:HD11	2.23	0.68
1:A:264:SER:HA	1:A:266:LYS:HZ2	1.56	0.68
2:B:35:ILE:HG23	2:B:63:SER:CB	2.23	0.68
1:A:119:LYS:NZ	1:A:166:ASP:CB	2.56	0.68
1:C:241:ASN:O	1:C:244:ARG:N	2.26	0.68
1:C:121:THR:HG22	1:C:124:ARG:HH12	0.82	0.68
2:D:23:GLN:HE21	2:D:23:GLN:HA	1.59	0.68
1:A:83:SER:HB3	1:A:88:ASP:OD2	1.95	0.67
2:B:27:THR:HG22	2:B:30:GLU:HB2	1.76	0.66
1:A:185:GLY:HA2	1:A:197:SER:CA	2.23	0.66
1:A:78:ARG:HD2	1:A:78:ARG:C	2.21	0.65
1:C:125:LEU:O	1:C:127:GLU:N	2.29	0.65
1:A:78:ARG:HD2	1:A:78:ARG:O	1.96	0.65
1:A:107:ASP:O	1:A:108:GLU:HB2	1.96	0.65
1:A:121:THR:O	1:A:122:GLU:HB2	1.96	0.65
1:A:264:SER:HA	1:A:266:LYS:NZ	2.11	0.65
1:C:107:ASP:N	1:C:107:ASP:OD1	2.30	0.65
1:C:121:THR:O	1:C:124:ARG:N	2.30	0.65
1:A:268:GLU:CD	1:A:362:LYS:NZ	2.55	0.65
1:A:75:ILE:HA	1:A:137:PRO:HG3	1.79	0.65
1:A:78:ARG:O	1:A:78:ARG:CD	2.45	0.65
1:A:265:VAL:O	1:A:267:TYR:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ALA:HB1	2:D:37:ILE:O	1.96	0.64
1:C:121:THR:HG21	1:C:124:ARG:NH1	2.11	0.64
1:C:242:ALA:C	1:C:244:ARG:H	2.05	0.64
1:C:434:SER:O	1:C:436:GLU:N	2.30	0.64
1:A:78:ARG:C	1:A:78:ARG:CD	2.72	0.63
1:C:121:THR:CG2	1:C:124:ARG:HB3	2.28	0.63
1:C:167:TRP:O	1:C:168[A]:CYS:SG	2.57	0.63
1:C:121:THR:O	1:C:122:GLU:C	2.42	0.63
1:C:173:ILE:O	1:C:173:ILE:HG22	1.98	0.62
1:A:115:MET:CE	1:A:247:LEU:H	2.12	0.62
1:A:187:ILE:HG22	1:A:189:GLN:HG3	1.79	0.62
1:A:357:ASN:ND2	1:A:380:VAL:HG11	2.15	0.62
1:C:155:GLN:O	1:C:155:GLN:HG2	1.98	0.62
1:C:63:ASN:CG	1:C:256[B]:CYS:HG	2.07	0.62
1:A:141:ILE:HG22	1:A:143:GLU:N	2.14	0.62
1:C:162:ARG:HD2	1:C:167:TRP:CZ3	2.34	0.62
1:C:241:ASN:HB2	1:C:246:VAL:H	1.63	0.62
1:A:292:ARG:NH1	5:A:2067:HOH:O	2.32	0.61
1:C:420:THR:O	1:C:424:SER:OG	2.16	0.61
1:A:115:MET:HE1	1:A:247:LEU:H	1.65	0.61
1:A:243:GLU:O	1:A:245:THR:CG2	2.47	0.61
2:D:27:THR:OG1	2:D:30:GLU:HG3	2.00	0.61
1:A:82:LYS:O	1:A:83:SER:HB3	1.99	0.61
1:C:121:THR:CG2	1:C:124:ARG:CB	2.79	0.61
1:A:267:TYR:HB2	1:A:270:ASP:OD2	2.00	0.60
1:A:275:ILE:HG22	1:A:381:LEU:HD11	1.83	0.60
1:A:92:GLU:O	1:A:148:ARG:HD2	2.02	0.60
1:A:357:ASN:ND2	1:A:380:VAL:HG21	2.17	0.60
1:A:216:ASN:OD1	1:A:329:PRO:HG3	2.01	0.60
1:A:191:ASN:O	1:A:192:ALA:CB	2.50	0.60
1:C:78:ARG:CG	1:C:78:ARG:NH1	2.45	0.60
1:A:130:THR:O	1:A:130:THR:HG22	2.01	0.59
1:A:363:LYS:HD3	1:A:373:HIS:NE2	2.17	0.59
1:C:241:ASN:HB3	1:C:245:THR:H	1.67	0.58
1:A:146:ASP:O	1:A:171:LYS:HA	2.03	0.58
1:A:79:TYR:OH	1:A:140:MET:CE	2.41	0.58
1:C:370:TYR:CE1	1:C:432:ARG:HD3	2.39	0.58
1:A:189:GLN:N	1:A:192:ALA:O	2.34	0.57
2:B:29:SER:OG	2:B:39:GLN:OE1	2.23	0.57
2:D:21:ARG:HG2	2:D:21:ARG:NH1	2.18	0.57
1:C:399:ILE:HB	1:C:430:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:NH2	1:A:148:ARG:HG3	2.20	0.56
1:C:160:LEU:O	1:C:176:THR:HB	2.05	0.56
2:D:71:CYS:HB3	4:D:1088:CL:CL	2.42	0.56
1:C:171:LYS:HD3	5:C:2050:HOH:O	2.04	0.56
1:C:434:SER:C	1:C:436:GLU:N	2.50	0.56
1:C:296:MET:HE3	1:C:388:MET:HE1	1.88	0.56
2:B:35:ILE:HD12	2:B:59:LYS:HB3	1.86	0.56
1:C:149:ILE:HD12	5:C:2045:HOH:O	2.05	0.56
1:C:241:ASN:O	1:C:244:ARG:HA	2.07	0.55
1:A:113:PRO:HB2	1:A:116:ALA:HB2	1.89	0.55
1:A:189:GLN:O	1:A:190:PRO:C	2.49	0.55
1:A:243:GLU:O	1:A:244:ARG:C	2.48	0.55
1:C:229:ARG:HG3	1:C:229:ARG:NH1	2.09	0.55
1:A:243:GLU:HB2	1:A:245:THR:CG2	2.36	0.55
1:C:162:ARG:HD2	1:C:167:TRP:CH2	2.42	0.55
1:C:159:ALA:HB1	1:C:176:THR:OG1	2.05	0.55
1:C:8:MET:HE2	1:C:100:ALA:HB3	1.89	0.55
1:A:376:ALA:O	1:A:380:VAL:HG23	2.06	0.55
1:A:141:ILE:CG2	1:A:143:GLU:H	2.18	0.55
2:B:72:ASP:O	5:B:2018:HOH:O	2.18	0.55
2:D:35:ILE:HD11	2:D:37:ILE:CD1	2.37	0.55
1:A:81:ALA:O	1:A:83:SER:N	2.40	0.54
1:C:162:ARG:O	1:C:162:ARG:HG2	1.91	0.54
1:C:120:LEU:CD1	1:C:124:ARG:NH2	2.70	0.54
1:A:67:ASP:N	1:A:67:ASP:OD1	2.41	0.54
1:C:142:ARG:NH2	1:C:148:ARG:H	2.06	0.54
1:A:119:LYS:NZ	1:A:166:ASP:HB2	2.23	0.53
1:A:237:ASP:HB3	1:A:252:GLN:OE1	2.07	0.53
1:A:185:GLY:CA	1:A:197:SER:HA	2.33	0.53
1:A:120:LEU:HB2	1:A:167:TRP:O	2.09	0.53
1:C:161:LEU:HD12	1:C:177:THR:HG23	1.91	0.53
1:A:31:GLU:HB3	5:A:2008:HOH:O	2.08	0.53
1:C:237:ASP:HB3	1:C:252:GLN:OE1	2.10	0.53
2:B:30:GLU:O	2:B:34[A]:LYS:HG3	2.10	0.52
1:C:155:GLN:O	1:C:155:GLN:CG	2.57	0.52
1:A:81:ALA:C	1:A:83:SER:H	2.16	0.52
1:C:8:MET:HG2	1:C:100:ALA:HB1	1.91	0.52
2:D:35:ILE:HD11	2:D:37:ILE:HD11	1.91	0.52
1:C:121:THR:HG23	1:C:124:ARG:N	2.18	0.52
1:C:279:MET:CE	1:C:295:PHE:CG	2.92	0.52
1:A:296:MET:HE3	1:A:388:MET:HE1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ALA:O	1:C:127:GLU:HB2	2.10	0.52
1:A:79:TYR:O	1:A:80:HIS:C	2.50	0.52
1:A:115:MET:HE1	1:A:247:LEU:N	2.24	0.52
1:C:120:LEU:HD23	1:C:121:THR:H	1.75	0.52
1:C:279:MET:CE	1:C:295:PHE:CB	2.85	0.52
1:A:402:ALA:O	1:A:406:VAL:HG23	2.10	0.52
1:C:242:ALA:C	1:C:244:ARG:N	2.68	0.52
1:A:357:ASN:HD21	1:A:380:VAL:HG11	1.75	0.51
2:B:26:TRP:CD1	2:B:34[A]:LYS:NZ	2.79	0.51
2:B:64:LEU:O	2:B:65:GLU:HB2	2.09	0.51
1:C:11:GLN:HG2	1:C:32:TRP:HZ3	1.74	0.51
1:C:173:ILE:O	1:C:173:ILE:CG2	2.59	0.51
1:C:7:TRP:CD1	1:C:104:ILE:HD12	2.46	0.50
1:C:356:LEU:O	1:C:357:ASN:HB2	2.11	0.50
1:C:121:THR:HG22	1:C:124:ARG:CB	2.39	0.50
1:C:121:THR:HG23	1:C:121:THR:O	2.10	0.50
1:C:176:THR:O	1:C:238:ARG:HG3	2.11	0.50
1:A:78:ARG:O	1:A:78:ARG:HD3	2.10	0.50
1:A:267:TYR:O	1:A:271:GLY:HA2	2.12	0.50
1:A:263:SER:O	1:A:266:LYS:N	2.39	0.50
1:A:119:LYS:HZ3	1:A:166:ASP:HB2	1.76	0.50
1:A:95:ARG:CZ	1:A:148:ARG:HG3	2.42	0.50
1:C:105:PRO:C	1:C:107:ASP:N	2.56	0.50
1:A:11:GLN:CG	1:A:32:TRP:HZ3	2.09	0.49
1:C:122:GLU:OE1	1:C:122:GLU:O	2.30	0.49
1:C:179:ILE:HD12	1:C:235:ARG:HG2	1.93	0.49
1:C:145:ASN:OD1	1:C:190:PRO:HD2	2.12	0.49
1:C:259:PHE:HD2	1:C:273:PRO:HG2	1.76	0.49
1:A:187:ILE:O	1:A:194:LEU:N	2.38	0.49
1:A:115:MET:HA	1:A:174:THR:HG23	1.94	0.49
1:A:270:ASP:N	1:A:271:GLY:HA2	2.27	0.49
2:B:35:ILE:HG23	2:B:63:SER:HB2	1.94	0.49
1:C:121:THR:C	1:C:123:ALA:N	2.69	0.49
1:C:370:TYR:CD1	1:C:432:ARG:HD3	2.48	0.48
1:C:241:ASN:CB	1:C:245:THR:H	2.26	0.48
1:C:259:PHE:CD1	1:C:277:ARG:NH2	2.80	0.48
1:A:126:GLU:OE1	1:A:226:GLY:HA3	2.13	0.48
1:C:42:SER:HB2	1:C:60:PHE:CD1	2.48	0.48
1:C:125:LEU:HA	1:C:128:VAL:CG2	2.40	0.48
1:A:215:LEU:HD21	1:A:297:LYS:HG2	1.95	0.48
1:C:170:PRO:HG3	1:C:176:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ALA:O	1:C:339:VAL:HG22	2.14	0.48
1:A:263:SER:O	1:A:266:LYS:CB	2.61	0.48
1:C:189:GLN:HB2	1:C:190:PRO:CD	2.43	0.48
1:A:224:LYS:HA	1:A:228:VAL:O	2.13	0.48
1:A:9:ASN:O	1:A:10:ASN:HB2	2.14	0.48
1:A:161:LEU:HG	1:A:162:ARG:N	2.27	0.48
2:B:27:THR:HG23	2:B:30:GLU:H	1.74	0.47
1:C:129:LEU:O	1:C:130:THR:OG1	2.30	0.47
1:A:302:GLN:OE1	1:A:310:GLY:HA3	2.14	0.47
2:D:64:LEU:O	2:D:65:GLU:HB2	2.14	0.47
1:A:96:ASP:HB3	1:A:149:ILE:HG22	1.97	0.47
1:C:32:TRP:C	1:C:34:ALA:H	2.22	0.47
1:C:76:VAL:HG23	1:C:89:LEU:HD21	1.96	0.47
2:D:29:SER:O	2:D:30:GLU:C	2.53	0.47
2:B:56:THR:O	2:B:60:ILE:HG13	2.14	0.47
1:A:121:THR:OG1	1:A:124:ARG:HB2	2.14	0.47
1:A:371:PRO:HB3	1:A:392:LEU:HD13	1.97	0.47
1:C:120:LEU:HD12	1:C:124:ARG:HH21	1.79	0.47
1:A:142:ARG:O	1:A:142:ARG:HG3	2.15	0.47
1:A:58:PHE:CE1	1:A:86:PRO:HG2	2.50	0.46
1:A:42:SER:HB2	1:A:60:PHE:CD1	2.50	0.46
1:A:196:LEU:C	1:A:198:GLN:H	2.23	0.46
1:C:241:ASN:O	1:C:244:ARG:CA	2.63	0.46
1:A:19:LEU:O	1:A:22:GLY:N	2.39	0.46
1:C:120:LEU:HD12	1:C:124:ARG:NH2	2.30	0.46
1:C:202:ASN:CG	1:C:334:ILE:HG13	2.40	0.46
1:C:313:LYS:O	1:C:313:LYS:HG3	2.15	0.46
1:A:121:THR:O	1:A:122:GLU:HB3	2.14	0.46
1:C:386:VAL:O	1:C:386:VAL:HG12	2.16	0.46
1:A:59:ASN:HB3	5:A:2060:HOH:O	2.16	0.46
1:A:203:GLU:HG3	1:A:333:ILE:O	2.16	0.46
2:B:24:ASN:ND2	2:B:26:TRP:CZ3	2.83	0.46
2:B:64:LEU:O	2:B:65:GLU:CB	2.62	0.46
1:A:11:GLN:CG	1:A:32:TRP:CZ3	2.93	0.46
1:A:313:LYS:O	1:A:313:LYS:HG3	2.16	0.46
1:C:8:MET:HG2	1:C:100:ALA:CB	2.46	0.46
1:A:357:ASN:HD22	1:A:380:VAL:CG2	2.25	0.45
1:A:203:GLU:O	1:A:204:TYR:C	2.58	0.45
1:A:162:ARG:HD2	1:A:167:TRP:CD2	2.51	0.45
1:A:428:ARG:O	1:A:428:ARG:HG3	2.16	0.45
1:C:160:LEU:HD12	1:C:180:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ARG:HD3	1:C:172:GLY:O	2.16	0.45
1:C:59:ASN:O	1:C:60:PHE:C	2.60	0.45
1:A:265:VAL:O	1:A:266:LYS:C	2.58	0.45
1:A:81:ALA:C	1:A:83:SER:N	2.74	0.45
1:A:4:LEU:HD23	1:A:105:PRO:HA	1.99	0.45
1:A:79:TYR:CZ	1:A:140:MET:CE	2.71	0.44
1:A:381:LEU:O	1:A:382:ARG:HB2	2.17	0.44
1:C:229:ARG:NH1	1:C:229:ARG:CG	2.75	0.44
2:D:72:ASP:N	2:D:72:ASP:OD1	2.47	0.44
1:A:414:PHE:CE2	1:A:419:VAL:HG22	2.52	0.44
1:C:240:TRP:CZ3	1:C:247:LEU:N	2.85	0.44
1:A:72:ARG:HA	1:A:75:ILE:HD12	1.98	0.44
1:C:78:ARG:HG2	1:C:79:TYR:CD2	2.53	0.44
1:A:130:THR:O	1:A:130:THR:HG23	2.14	0.44
1:C:42:SER:HB2	1:C:60:PHE:CE1	2.53	0.43
1:C:393:SER:OG	1:C:437:TYR:CD2	2.69	0.43
1:A:243:GLU:C	1:A:245:THR:HG23	2.41	0.43
1:C:68:SER:HA	1:C:69:PRO:HD3	1.76	0.43
1:C:161:LEU:CD1	1:C:177:THR:HG23	2.48	0.43
1:A:370:TYR:O	1:A:371:PRO:C	2.60	0.43
1:C:328:THR:HB	1:C:329:PRO:HD2	2.00	0.43
1:A:242:ALA:C	1:A:244:ARG:H	2.27	0.43
1:C:189:GLN:HB2	1:C:190:PRO:HD2	2.00	0.43
1:A:3:LYS:HG2	1:A:17:THR:OG1	2.16	0.43
1:A:82:LYS:O	1:A:83:SER:HB2	2.16	0.43
1:A:268:GLU:O	1:A:271:GLY:HA3	2.19	0.43
1:A:162:ARG:HD2	1:A:167:TRP:CE2	2.53	0.43
2:B:19:LEU:O	2:B:23:GLN:HG2	2.19	0.43
1:C:65:LEU:HD11	1:C:86:PRO:HA	2.01	0.43
1:C:193[B]:THR:HG22	5:C:2052:HOH:O	2.17	0.43
1:A:311:HIS:ND1	1:A:313:LYS:HB3	2.34	0.42
1:C:162:ARG:HB2	1:C:166:ASP:O	2.17	0.42
1:C:221:GLU:HG2	1:C:232:ALA:HB3	1.99	0.42
1:C:241:ASN:ND2	1:C:245:THR:CG2	2.71	0.42
1:A:75:ILE:CA	1:A:137:PRO:HG3	2.47	0.42
1:C:401:ALA:CB	5:C:2126:HOH:O	2.66	0.42
1:A:49:ARG:HD2	2:B:23:GLN:OE1	2.20	0.42
1:A:113:PRO:HG2	1:A:172:GLY:HA3	2.01	0.42
1:A:144:GLU:OE2	1:A:171:LYS:HE2	2.19	0.42
1:C:120:LEU:HD23	1:C:121:THR:N	2.34	0.42
1:C:121:THR:CG2	1:C:124:ARG:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:CA	1:C:128:VAL:HG23	2.45	0.42
1:C:203:GLU:OE2	1:C:332:ASP:HA	2.18	0.42
1:A:196:LEU:C	1:A:198:GLN:N	2.77	0.42
1:A:268:GLU:CD	1:A:362:LYS:HZ3	2.26	0.42
1:C:259:PHE:CD2	1:C:273:PRO:CG	3.02	0.42
1:A:187:ILE:CG2	1:A:189:GLN:HG3	2.47	0.42
1:C:106:GLU:H	1:C:106:GLU:HG2	1.56	0.42
1:C:174:THR:HA	1:C:175:PRO:HD3	1.83	0.42
1:A:3:LYS:HB2	1:A:3:LYS:HE3	1.58	0.42
2:B:67:SER:HB3	2:D:8:TYR:CE1	2.55	0.42
1:C:207:LEU:HD23	1:C:333:ILE:HD12	2.00	0.42
1:A:189:GLN:C	1:A:191:ASN:N	2.73	0.41
2:B:32:ALA:HB1	2:B:37:ILE:O	2.19	0.41
1:C:72:ARG:HA	1:C:75:ILE:HD12	2.03	0.41
1:C:241:ASN:O	1:C:242:ALA:C	2.64	0.41
1:A:188:ARG:HG2	1:A:193:THR:HB	2.02	0.41
1:C:7:TRP:CZ3	1:C:12:ARG:HB2	2.56	0.41
2:B:40:ALA:O	2:B:44:ASN:CG	2.63	0.41
1:C:250:LEU:HA	1:C:251:PRO:HD3	1.96	0.41
1:C:100:ALA:HA	1:C:249:ARG:HB3	2.02	0.41
1:C:243:GLU:HG3	1:C:245:THR:CG2	2.51	0.41
1:A:112:HIS:HA	1:A:113:PRO:HD2	1.81	0.40
1:C:167:TRP:O	1:C:168[B]:CYS:HB3	2.20	0.40
1:C:32:TRP:C	1:C:34:ALA:N	2.79	0.40
1:C:96:ASP:OD2	1:C:176:THR:HG23	2.21	0.40
1:C:240:TRP:CE3	1:C:246:VAL:C	3.00	0.40
1:C:259:PHE:CD2	1:C:273:PRO:HG2	2.55	0.40
1:C:434:SER:O	1:C:435:ARG:C	2.59	0.40
1:A:75:ILE:HG13	1:A:137:PRO:CB	2.52	0.40
2:D:14:ALA:HB2	2:D:49:PRO:HB3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LYS:NZ	1:A:135:ASP:OD1[7_554]	1.63	0.57
1:A:22:GLY:O	1:A:190:PRO:O[7_554]	2.10	0.10

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	425/446 (95%)	387 (91%)	31 (7%)	7 (2%)	7	6
1	C	392/446 (88%)	365 (93%)	21 (5%)	6 (2%)	8	7
2	B	68/88 (77%)	63 (93%)	5 (7%)	0	100	100
2	D	67/88 (76%)	62 (92%)	4 (6%)	1 (2%)	8	7
All	All	952/1068 (89%)	877 (92%)	61 (6%)	14 (2%)	8	7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	83	SER
1	A	141	ILE
1	C	106	GLU
2	D	25	GLY
1	A	122	GLU
1	A	192	ALA
1	A	244	ARG
1	A	266	LYS
1	C	122	GLU
1	C	126	GLU
1	C	435	ARG
1	C	94	GLY
1	C	170	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	365/380 (96%)	338 (93%)	27 (7%)	13	14
1	C	346/380 (91%)	321 (93%)	25 (7%)	13	14
2	B	66/80 (82%)	63 (96%)	3 (4%)	24	32
2	D	65/80 (81%)	55 (85%)	10 (15%)	2	2
All	All	842/920 (92%)	777 (92%)	65 (8%)	12	13

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	67	ASP
1	A	78	ARG
1	A	83	SER
1	A	114	ILE
1	A	115	MET
1	A	119	LYS
1	A	122	GLU
1	A	124	ARG
1	A	130	THR
1	A	141	ILE
1	A	142	ARG
1	A	151	VAL
1	A	161	LEU
1	A	182	LEU
1	A	193	THR
1	A	208	LEU
1	A	243	GLU
1	A	258	THR
1	A	266	LYS
1	A	270	ASP
1	A	283	MET
1	A	309	ASP
1	A	339	VAL
1	A	393	SER
1	A	427	LEU
1	A	436	GLU
2	B	30	GLU
2	B	43	SER
2	B	65	GLU
1	C	8	MET
1	C	49	ARG
1	C	68	SER

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Mol	Chain	Res	Type
1	C	78	ARG
1	C	91	SER
1	C	101	VAL
1	C	106	GLU
1	C	107	ASP
1	C	124	ARG
1	C	129	LEU
1	C	140	MET
1	C	141	ILE
1	C	148	ARG
1	C	162	ARG
1	C	168[A]	CYS
1	C	168[B]	CYS
1	C	186	GLU
1	C	243	GLU
1	C	245	THR
1	C	258	THR
1	C	366	ILE
1	C	372	ARG
1	C	387	GLN
1	C	412	THR
1	C	413	ASP
2	D	5	GLN
2	D	23	GLN
2	D	31	LEU
2	D	33	LYS
2	D	35	ILE
2	D	37	ILE
2	D	39	GLN
2	D	42	ILE
2	D	84	LEU
2	D	85	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	198	GLN
1	A	357	ASN
1	A	417	ASN
1	C	51	ASN
1	C	241	ASN

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Mol	Chain	Res	Type
2	D	23	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	161:LEU	C	162:ARG	N	0.90

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	431/446 (96%)	0.92	77 (17%) 3 4	25, 44, 87, 115	0
1	C	401/446 (89%)	0.83	56 (13%) 6 7	22, 43, 87, 114	3 (0%)
2	B	71/88 (80%)	0.59	7 (9%) 13 14	29, 42, 67, 83	1 (1%)
2	D	71/88 (80%)	0.78	9 (12%) 8 9	30, 45, 72, 82	0
All	All	974/1068 (91%)	0.85	149 (15%) 5 6	22, 43, 85, 115	4 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	ALA	11.7
1	A	116	ALA	9.3
1	A	265	VAL	9.2
1	A	117	TRP	7.6
1	A	358	ALA	7.3
1	C	120	LEU	6.5
1	C	107	ASP	6.0
1	A	267	TYR	5.9
1	A	113	PRO	5.4
1	A	144	GLU	5.3
1	C	357	ASN	5.3
1	A	266	LYS	5.2
1	A	114	ILE	5.2
1	A	437	TYR	5.2
1	C	163	ILE	5.1
1	A	163	ILE	5.1
1	A	143	GLU	5.0
1	A	193	THR	4.9
1	C	164	GLY	4.8
2	B	72	ASP	4.7
1	A	82	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	264	SER	4.7
1	C	173	ILE	4.6
1	A	135	ASP	4.6
1	C	140	MET	4.6
1	C	434	SER	4.4
1	A	122	GLU	4.4
1	A	132	TYR	4.4
1	C	130	THR	4.3
1	C	437	TYR	4.3
1	C	245	THR	4.3
1	A	136	ILE	4.3
1	C	166	ASP	4.2
1	A	357	ASN	4.2
1	C	171	LYS	4.0
1	C	169	ILE	4.0
1	C	362	LYS	4.0
1	A	118	GLU	3.9
1	A	191	ASN	3.9
1	C	244	ARG	3.9
1	C	126	GLU	3.9
1	C	174	THR	3.9
1	A	147	PHE	3.8
1	A	137	PRO	3.8
1	A	360	LYS	3.8
1	C	435	ARG	3.8
1	C	242	ALA	3.8
2	D	72	ASP	3.8
1	C	228	VAL	3.7
1	A	361	GLY	3.6
1	A	263	SER	3.6
1	A	141	ILE	3.6
1	C	271	GLY	3.6
1	C	161	LEU	3.6
1	A	188	ARG	3.5
1	A	190	PRO	3.5
1	A	80	HIS	3.5
1	A	189	GLN	3.4
1	A	131	ALA	3.3
1	A	151	VAL	3.3
1	C	170	PRO	3.2
1	C	124	ARG	3.2
1	A	192	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	164	GLY	3.2
1	C	167	TRP	3.2
1	A	142	ARG	3.2
2	B	34[A]	LYS	3.2
1	A	146	ASP	3.1
1	C	129	LEU	3.1
1	A	187	ILE	3.1
1	A	244	ARG	3.1
1	A	165	ASN	3.0
1	C	123	ALA	3.0
1	C	127	GLU	3.0
1	A	149	ILE	3.0
1	A	124	ARG	3.0
1	C	125	LEU	2.9
1	A	77	LYS	2.9
1	C	122	GLU	2.9
1	C	277	ARG	2.9
1	A	171	LYS	2.9
1	A	268	GLU	2.9
2	B	48	ASN	2.9
1	A	311	HIS	2.8
1	C	95	ARG	2.8
2	B	35	ILE	2.8
2	D	71	CYS	2.8
1	A	20	ALA	2.8
1	A	270	ASP	2.7
1	A	185	GLY	2.7
1	A	359	SER	2.7
1	A	112	HIS	2.7
1	C	128	VAL	2.7
1	A	121	THR	2.7
1	A	166	ASP	2.7
1	A	269	SER	2.7
1	A	85	GLN	2.7
1	A	21	ASN	2.7
1	C	241	ASN	2.7
2	B	33	LYS	2.7
1	C	148	ARG	2.7
2	D	26	TRP	2.6
1	C	80	HIS	2.6
1	A	256	CYS	2.6
1	A	242	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	108	GLU	2.5
1	A	22	GLY	2.5
1	A	156	GLU	2.5
1	C	70	ILE	2.5
1	C	165	ASN	2.5
1	C	99	GLY	2.5
1	A	412	THR	2.4
1	A	145	ASN	2.4
1	C	436	GLU	2.4
1	A	107	ASP	2.4
1	A	81	ALA	2.4
1	A	154	ALA	2.4
1	A	155	GLN	2.4
2	D	48	ASN	2.3
1	C	34	ALA	2.3
1	A	228	VAL	2.3
1	A	115	MET	2.3
1	C	121	THR	2.3
1	C	155	GLN	2.3
2	B	39	GLN	2.3
2	D	35	ILE	2.3
2	B	71	CYS	2.3
1	A	186	GLU	2.3
1	A	140	MET	2.2
1	C	162	ARG	2.2
1	C	143	GLU	2.2
1	C	37	TYR	2.2
1	A	196	LEU	2.1
1	C	141	ILE	2.1
1	A	227	ASN	2.1
1	C	240	TRP	2.1
1	C	168[A]	CYS	2.1
2	D	29	SER	2.1
1	C	160	LEU	2.1
1	C	413	ASP	2.1
1	C	69	PRO	2.1
1	C	142	ARG	2.1
2	D	38	LYS	2.0
1	A	377	THR	2.0
1	C	81	ALA	2.0
2	D	33	LYS	2.0
1	A	436	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	63	SER	2.0
1	A	225	ALA	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
4	CL	C	1443	1/1	0.89	0.24	72,72,72,72	0
4	CL	A	1441	1/1	0.91	0.23	70,70,70,70	0
4	CL	D	1089	1/1	0.91	0.21	63,63,63,63	0
4	CL	B	1088	1/1	0.93	0.16	53,53,53,53	0
4	CL	B	1089	1/1	0.93	0.20	73,73,73,73	0
3	HG	C	1439	1/1	0.94	0.23	55,55,55,55	1
4	CL	D	1088	1/1	0.95	0.23	66,66,66,66	0
4	CL	A	1442	1/1	0.95	0.20	58,58,58,58	0
4	CL	C	1441	1/1	0.96	0.26	57,57,57,57	0
3	HG	A	1438	1/1	0.96	0.14	78,78,78,78	1
4	CL	A	1440	1/1	0.97	0.15	68,68,68,68	0
3	HG	B	1087	1/1	0.97	0.09	77,77,77,77	1
4	CL	C	1442	1/1	0.97	0.24	66,66,66,66	0
3	HG	C	1438	1/1	0.98	0.10	78,78,78,78	1
3	HG	D	1087	1/1	0.98	0.08	69,69,69,69	1
3	HG	C	1440	1/1	0.99	0.14	40,40,40,40	1
3	HG	A	1439	1/1	0.99	0.14	45,45,45,45	1

6.5 Other polymers [i](#)

There are no such residues in this entry.