



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:05 AM GMT

PDB ID : 4NG2
Title : Crystal structure of LasR LBD-QslA complex from *Pseudomonas aeruginosa*
Authors : Fan, H.; Wu, D.H.; Song, H.
Deposited on : 2013-11-01
Resolution : 2.41 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

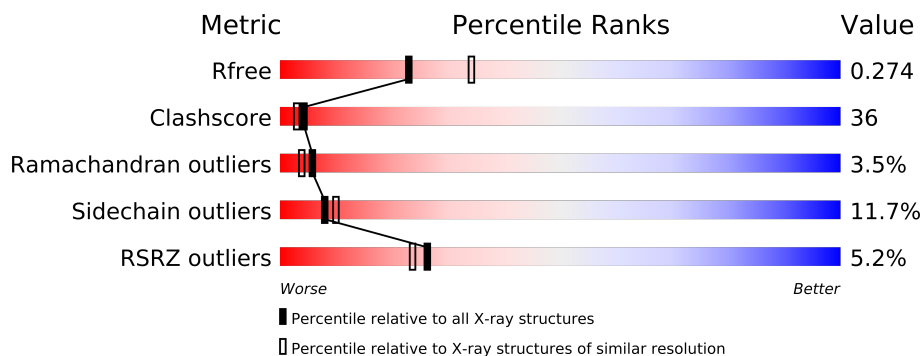
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2496 (2.44-2.40)
Clashscore	79885	3124 (2.44-2.40)
Ramachandran outliers	78287	3067 (2.44-2.40)
Sidechain outliers	78261	3068 (2.44-2.40)
RSRZ outliers	66119	2499 (2.44-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	184	
1	B	184	
1	C	184	
1	D	184	
2	E	113	
2	F	113	
2	G	113	
2	H	113	
2	I	113	
2	J	113	
2	K	113	
2	L	113	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11158 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transcriptional activator protein LasR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1298	834	217	242	5			
1	B	166	Total	C	N	O	S	0	0	0
			1298	834	217	242	5			
1	C	166	Total	C	N	O	S	0	0	0
			1298	834	217	242	5			
1	D	166	Total	C	N	O	S	0	0	0
			1298	834	217	242	5			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP P25084
A	-12	GLY	-	EXPRESSION TAG	UNP P25084
A	-11	SER	-	EXPRESSION TAG	UNP P25084
A	-10	SER	-	EXPRESSION TAG	UNP P25084
A	-9	HIS	-	EXPRESSION TAG	UNP P25084
A	-8	HIS	-	EXPRESSION TAG	UNP P25084
A	-7	HIS	-	EXPRESSION TAG	UNP P25084
A	-6	HIS	-	EXPRESSION TAG	UNP P25084
A	-5	HIS	-	EXPRESSION TAG	UNP P25084
A	-4	HIS	-	EXPRESSION TAG	UNP P25084
A	-3	SER	-	EXPRESSION TAG	UNP P25084
A	-2	GLN	-	EXPRESSION TAG	UNP P25084
A	-1	ASP	-	EXPRESSION TAG	UNP P25084
A	0	PRO	-	EXPRESSION TAG	UNP P25084
B	-13	MET	-	EXPRESSION TAG	UNP P25084
B	-12	GLY	-	EXPRESSION TAG	UNP P25084
B	-11	SER	-	EXPRESSION TAG	UNP P25084
B	-10	SER	-	EXPRESSION TAG	UNP P25084
B	-9	HIS	-	EXPRESSION TAG	UNP P25084
B	-8	HIS	-	EXPRESSION TAG	UNP P25084
B	-7	HIS	-	EXPRESSION TAG	UNP P25084

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP P25084
B	-5	HIS	-	EXPRESSION TAG	UNP P25084
B	-4	HIS	-	EXPRESSION TAG	UNP P25084
B	-3	SER	-	EXPRESSION TAG	UNP P25084
B	-2	GLN	-	EXPRESSION TAG	UNP P25084
B	-1	ASP	-	EXPRESSION TAG	UNP P25084
B	0	PRO	-	EXPRESSION TAG	UNP P25084
C	-13	MET	-	EXPRESSION TAG	UNP P25084
C	-12	GLY	-	EXPRESSION TAG	UNP P25084
C	-11	SER	-	EXPRESSION TAG	UNP P25084
C	-10	SER	-	EXPRESSION TAG	UNP P25084
C	-9	HIS	-	EXPRESSION TAG	UNP P25084
C	-8	HIS	-	EXPRESSION TAG	UNP P25084
C	-7	HIS	-	EXPRESSION TAG	UNP P25084
C	-6	HIS	-	EXPRESSION TAG	UNP P25084
C	-5	HIS	-	EXPRESSION TAG	UNP P25084
C	-4	HIS	-	EXPRESSION TAG	UNP P25084
C	-3	SER	-	EXPRESSION TAG	UNP P25084
C	-2	GLN	-	EXPRESSION TAG	UNP P25084
C	-1	ASP	-	EXPRESSION TAG	UNP P25084
C	0	PRO	-	EXPRESSION TAG	UNP P25084
D	-13	MET	-	EXPRESSION TAG	UNP P25084
D	-12	GLY	-	EXPRESSION TAG	UNP P25084
D	-11	SER	-	EXPRESSION TAG	UNP P25084
D	-10	SER	-	EXPRESSION TAG	UNP P25084
D	-9	HIS	-	EXPRESSION TAG	UNP P25084
D	-8	HIS	-	EXPRESSION TAG	UNP P25084
D	-7	HIS	-	EXPRESSION TAG	UNP P25084
D	-6	HIS	-	EXPRESSION TAG	UNP P25084
D	-5	HIS	-	EXPRESSION TAG	UNP P25084
D	-4	HIS	-	EXPRESSION TAG	UNP P25084
D	-3	SER	-	EXPRESSION TAG	UNP P25084
D	-2	GLN	-	EXPRESSION TAG	UNP P25084
D	-1	ASP	-	EXPRESSION TAG	UNP P25084
D	0	PRO	-	EXPRESSION TAG	UNP P25084

- Molecule 2 is a protein called Uncharacterized protein.

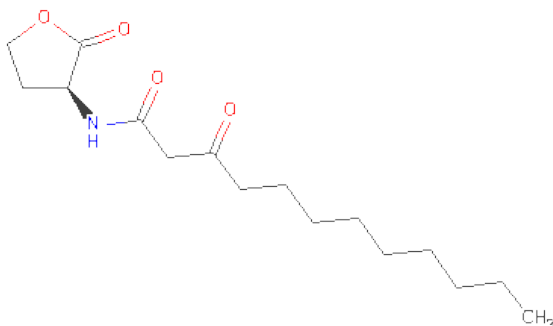
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	94	Total	C	N	O	S	0	0	0
			751	483	133	133	2			
2	F	82	Total	C	N	O	S	0	0	0
			648	417	114	115	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	82	Total	C	N	O	S	0	0	0
			648	417	114	115	2			
2	H	94	Total	C	N	O	S	0	0	0
			751	483	133	133	2			
2	I	94	Total	C	N	O	S	0	0	0
			751	483	133	133	2			
2	J	82	Total	C	N	O	S	0	0	0
			648	417	114	115	2			
2	K	82	Total	C	N	O	S	0	0	0
			648	417	114	115	2			
2	L	94	Total	C	N	O	S	0	0	0
			751	483	133	133	2			

- Molecule 3 is N-3-OXO-DODECANOYL-L-HOMOSERINELACTONE (three-letter code: OHN) (formula: $C_{16}H_{27}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	16	1	4		
3	B	1	Total	C	N	O	0	0
			21	16	1	4		
3	C	1	Total	C	N	O	0	0
			21	16	1	4		
3	D	1	Total	C	N	O	0	0
			21	16	1	4		

- Molecule 4 is water.

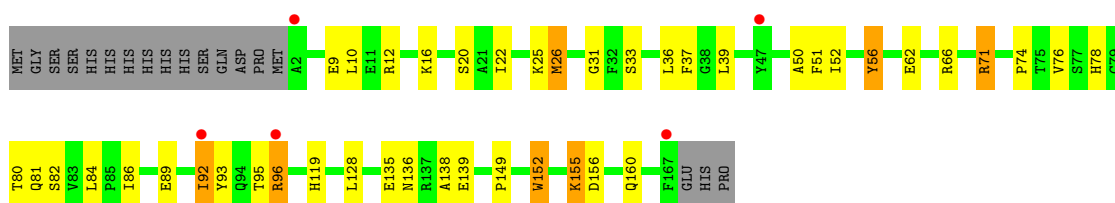
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total 25	O 25	0	0
4	B	39	Total 39	O 39	0	0
4	C	20	Total 20	O 20	0	0
4	D	52	Total 52	O 52	0	0
4	E	29	Total 29	O 29	0	0
4	F	14	Total 14	O 14	0	0
4	G	16	Total 16	O 16	0	0
4	H	11	Total 11	O 11	0	0
4	I	12	Total 12	O 12	0	0
4	J	5	Total 5	O 5	0	0
4	K	30	Total 30	O 30	0	0
4	L	33	Total 33	O 33	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.

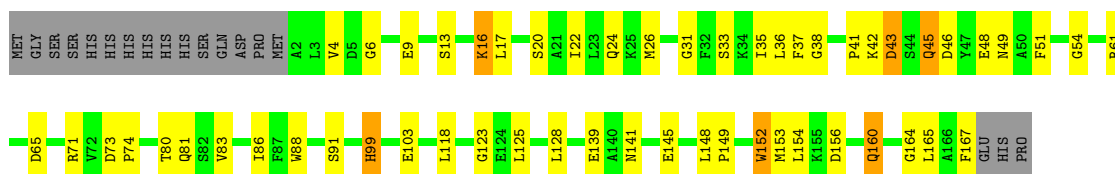
- Molecule 1: Transcriptional activator protein LasR

Chain A:



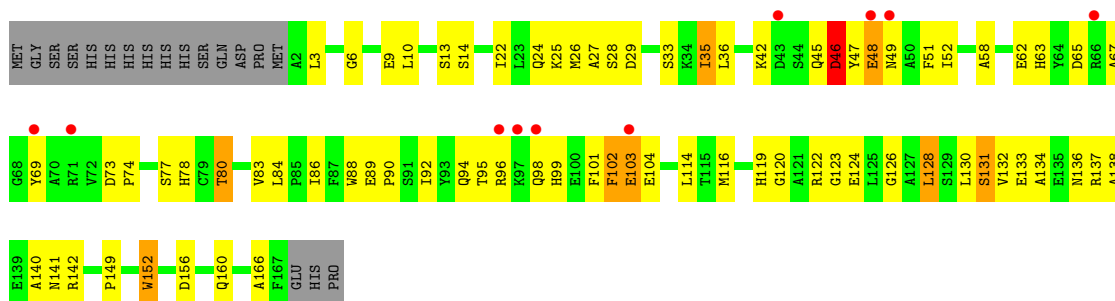
- Molecule 1: Transcriptional activator protein LasR

Chain B:



- Molecule 1: Transcriptional activator protein LasR

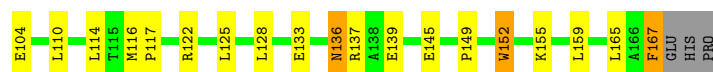
Chain C:



- Molecule 1: Transcriptional activator protein LasR

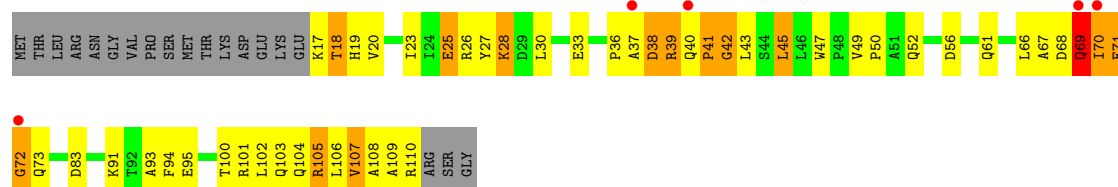
Chain D:





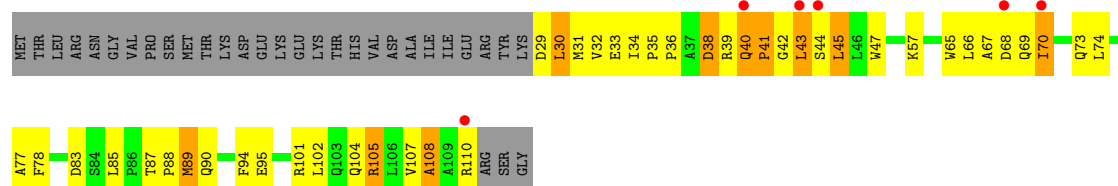
• Molecule 2: Uncharacterized protein

Chain E:



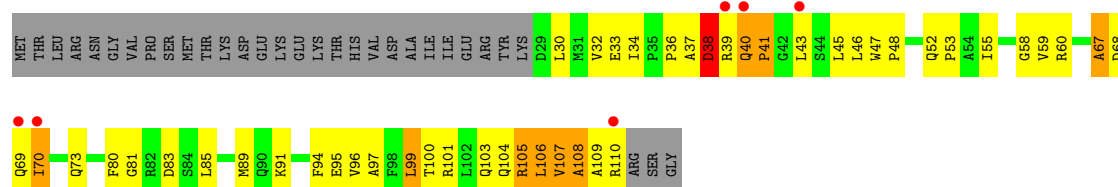
• Molecule 2: Uncharacterized protein

Chain F:



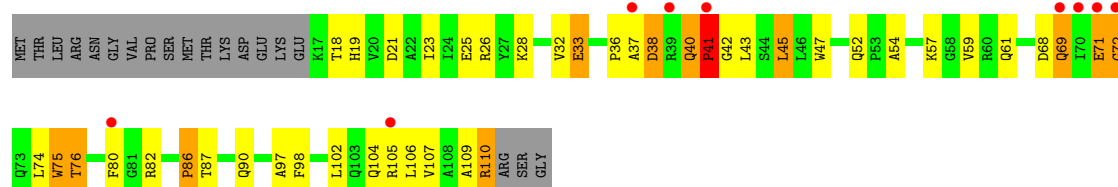
• Molecule 2: Uncharacterized protein

Chain G:



• Molecule 2: Uncharacterized protein

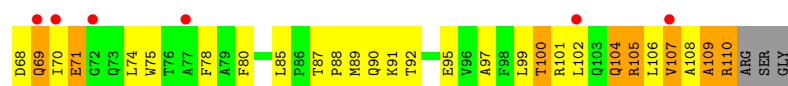
Chain H:



• Molecule 2: Uncharacterized protein

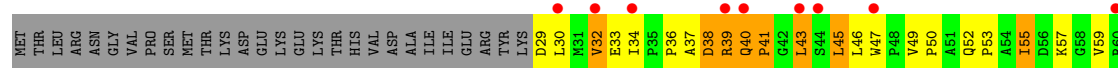
Chain I:





• Molecule 2: Uncharacterized protein

Chain J:



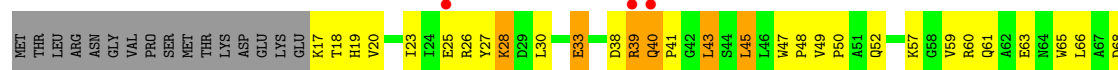
• Molecule 2: Uncharacterized protein

Chain K:



• Molecule 2: Uncharacterized protein

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.51Å 185.89Å 56.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.03 – 2.41 48.03 – 2.41	Depositor EDS
% Data completeness (in resolution range)	93.9 (48.03-2.41) 96.4 (48.03-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.231 , 0.277 0.228 , 0.274	Depositor DCC
R_{free} test set	3260 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 64432 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11158	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/1332	0.56	0/1807
1	B	0.49	0/1332	0.58	0/1807
1	C	0.41	0/1332	0.57	0/1807
1	D	0.55	0/1332	0.66	2/1807 (0.1%)
2	E	0.45	0/770	0.66	0/1049
2	F	0.40	0/665	0.63	0/908
2	G	0.41	0/665	0.70	0/908
2	H	0.52	0/770	0.73	3/1049 (0.3%)
2	I	0.44	0/770	0.62	0/1049
2	J	0.35	0/665	0.58	1/908 (0.1%)
2	K	0.58	0/665	0.74	1/908 (0.1%)
2	L	0.79	0/770	0.77	0/1049
All	All	0.50	0/11068	0.64	7/15056 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	41	PRO	CA-N-CD	-7.00	101.69	111.50
2	H	40	GLN	C-N-CD	5.86	140.71	128.40
2	K	42	GLY	N-CA-C	-5.58	99.14	113.10
2	H	42	GLY	N-CA-C	5.49	126.81	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	J	102	LEU	CA-CB-CG	5.29	127.47	115.30
1	D	110	LEU	CA-CB-CG	-5.03	103.73	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	41	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1298	0	1249	57	0
1	B	1298	0	1249	48	0
1	C	1298	0	1249	87	0
1	D	1298	0	1249	51	0
2	E	751	0	758	76	0
2	F	648	0	650	74	0
2	G	648	0	650	93	0
2	H	751	0	758	67	0
2	I	751	0	758	100	1
2	J	648	0	650	91	0
2	K	648	0	650	37	0
2	L	751	0	758	74	0
3	A	21	0	27	1	0
3	B	21	0	27	3	0
3	C	21	0	27	4	0
3	D	21	0	27	0	0
4	A	25	0	0	21	0
4	B	39	0	0	20	0
4	C	20	0	0	22	1
4	D	52	0	0	14	0
4	E	29	0	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	14	0	0	10	0
4	G	16	0	0	13	0
4	H	11	0	0	10	0
4	I	12	0	0	21	0
4	J	5	0	0	5	0
4	K	30	0	0	2	0
4	L	33	0	0	17	0
All	All	11158	0	10736	780	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (780) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:36:PRO:CB	2:H:41:PRO:HB2	1.36	1.54
2:H:36:PRO:HB3	2:H:41:PRO:CB	1.35	1.52
2:J:30:LEU:HA	4:J:205:HOH:O	1.16	1.33
2:I:63:GLU:HA	4:I:206:HOH:O	1.18	1.31
2:L:39:ARG:HD3	2:L:39:ARG:O	1.36	1.24
2:F:44:SER:HA	4:F:201:HOH:O	1.43	1.17
2:G:34:ILE:HG13	2:G:43:LEU:HD12	1.23	1.15
2:G:36:PRO:HB3	2:G:41:PRO:HB2	1.24	1.15
2:J:101:ARG:HH12	2:J:105:ARG:HB2	1.07	1.14
1:C:49:ASN:ND2	4:C:318:HOH:O	1.81	1.14
2:E:105:ARG:HH11	2:E:105:ARG:HG3	1.00	1.13
2:E:33:GLU:HA	4:E:202:HOH:O	1.48	1.12
2:H:36:PRO:CA	2:H:41:PRO:HB2	1.80	1.12
1:A:81:GLN:NE2	4:A:311:HOH:O	1.82	1.11
2:J:101:ARG:HH22	2:J:105:ARG:HD3	0.95	1.10
2:H:36:PRO:CB	2:H:41:PRO:CB	2.08	1.09
2:H:38:ASP:OD1	4:H:203:HOH:O	1.70	1.09
2:L:17:LYS:N	4:L:220:HOH:O	1.85	1.09
2:E:100:THR:C	4:E:209:HOH:O	1.88	1.08
2:E:26:ARG:CG	4:E:221:HOH:O	2.00	1.08
2:E:101:ARG:N	4:E:209:HOH:O	1.87	1.08
2:E:36:PRO:HA	2:E:41:PRO:HB2	1.36	1.07
2:G:39:ARG:N	4:G:202:HOH:O	1.85	1.07
2:F:105:ARG:HG2	2:F:105:ARG:HH11	1.17	1.07
2:G:105:ARG:HB3	2:G:105:ARG:HH11	1.20	1.06
1:A:92:ILE:HG23	4:A:321:HOH:O	1.53	1.05
1:C:88:TRP:HB2	4:C:313:HOH:O	1.56	1.05
2:E:39:ARG:HG3	2:E:107:VAL:HB	1.39	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:26:ARG:NH1	4:H:210:HOH:O	1.87	1.04
2:I:105:ARG:HB2	4:I:210:HOH:O	1.57	1.04
2:F:34:ILE:H	2:F:43:LEU:HD12	1.22	1.04
2:G:34:ILE:H	2:G:43:LEU:HB3	1.23	1.04
2:G:39:ARG:HE	2:G:108:ALA:HA	1.19	1.03
2:K:105:ARG:HH11	2:K:105:ARG:CB	1.70	1.03
2:J:105:ARG:HH11	2:J:105:ARG:HG2	0.90	1.03
2:E:36:PRO:HB3	2:E:41:PRO:HG2	1.38	1.03
2:H:105:ARG:HG3	4:H:203:HOH:O	1.58	1.03
2:I:105:ARG:HH11	2:I:105:ARG:HB2	1.21	1.03
4:B:308:HOH:O	2:H:18:THR:HB	1.56	1.03
2:I:105:ARG:N	4:I:210:HOH:O	1.83	1.02
2:E:26:ARG:N	4:E:221:HOH:O	1.92	1.02
2:J:87:THR:HG22	2:J:89:MET:H	1.21	1.02
2:E:26:ARG:HG2	4:E:221:HOH:O	1.57	1.02
2:K:105:ARG:HH11	2:K:105:ARG:HB3	1.20	1.02
1:A:66:ARG:NH2	4:A:322:HOH:O	1.90	1.01
2:J:32:VAL:O	2:J:43:LEU:HD11	1.59	1.01
1:A:92:ILE:N	4:A:321:HOH:O	1.84	1.00
2:G:32:VAL:O	2:G:43:LEU:HD22	1.62	1.00
2:J:105:ARG:NH1	2:J:105:ARG:HG2	1.70	0.99
1:A:92:ILE:CB	4:A:321:HOH:O	2.09	0.99
2:G:39:ARG:NE	2:G:108:ALA:HA	1.78	0.98
2:L:73:GLN:HA	2:L:73:GLN:OE1	1.62	0.98
2:I:105:ARG:CB	4:I:210:HOH:O	2.08	0.98
2:E:100:THR:HG22	4:E:209:HOH:O	1.63	0.97
2:L:40:GLN:HG3	2:L:41:PRO:HD2	1.45	0.97
2:I:62:ALA:O	4:I:206:HOH:O	1.81	0.97
1:A:89:GLU:O	4:A:321:HOH:O	1.82	0.96
1:D:145:GLU:OE2	4:D:338:HOH:O	1.84	0.96
2:G:106:LEU:HG	2:H:106:LEU:HD21	1.45	0.96
1:C:24:GLN:OE1	4:C:317:HOH:O	1.84	0.96
2:L:52:GLN:NE2	4:L:210:HOH:O	1.96	0.96
2:J:32:VAL:HG23	2:J:45:LEU:HB3	1.47	0.95
2:E:43:LEU:O	4:E:202:HOH:O	1.84	0.95
2:K:105:ARG:CG	2:K:105:ARG:HH11	1.81	0.94
2:I:71:GLU:HG3	2:J:107:VAL:HG22	1.46	0.94
2:E:105:ARG:NH1	2:E:105:ARG:HG3	1.76	0.94
2:J:29:ASP:O	4:J:205:HOH:O	1.84	0.94
2:J:101:ARG:NH2	2:J:105:ARG:HD3	1.81	0.94
1:D:24:GLN:OE1	4:D:305:HOH:O	1.85	0.94
1:D:80:THR:HG22	1:D:125:LEU:HD21	1.50	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:45:GLN:O	4:C:314:HOH:O	1.86	0.93
2:J:39:ARG:HG2	2:J:108:ALA:HA	1.50	0.93
2:L:57:LYS:HD3	4:L:223:HOH:O	1.67	0.93
1:B:13:SER:O	4:B:319:HOH:O	1.84	0.93
2:F:83:ASP:CB	4:F:213:HOH:O	2.15	0.93
2:F:83:ASP:HB2	4:F:213:HOH:O	1.69	0.93
2:J:55:ILE:HG13	2:J:97:ALA:HB2	1.52	0.92
2:L:57:LYS:CG	4:L:223:HOH:O	2.16	0.92
2:F:43:LEU:O	4:F:201:HOH:O	1.85	0.92
2:G:34:ILE:HG13	2:G:43:LEU:CD1	1.99	0.92
2:J:34:ILE:H	2:J:43:LEU:HD22	1.35	0.91
2:G:40:GLN:OE1	4:G:215:HOH:O	1.87	0.91
2:E:56:ASP:OD1	4:E:227:HOH:O	1.87	0.91
2:F:43:LEU:HD22	2:F:44:SER:N	1.84	0.91
1:B:33:SER:OG	4:B:315:HOH:O	1.89	0.91
1:C:141:ASN:ND2	4:C:316:HOH:O	1.98	0.91
2:G:105:ARG:CB	2:G:105:ARG:HH11	1.84	0.91
2:E:104:GLN:OE1	4:E:210:HOH:O	1.89	0.90
2:G:105:ARG:HB3	2:G:105:ARG:NH1	1.86	0.90
2:G:46:LEU:O	4:G:216:HOH:O	1.89	0.90
2:F:83:ASP:OD2	4:F:213:HOH:O	1.90	0.89
2:H:36:PRO:HB3	2:H:41:PRO:CG	2.01	0.89
2:G:34:ILE:CG1	2:G:43:LEU:HD12	2.02	0.88
1:D:117:PRO:O	4:D:324:HOH:O	1.91	0.88
2:H:26:ARG:CZ	4:H:210:HOH:O	2.19	0.88
1:C:141:ASN:OD1	4:C:316:HOH:O	1.89	0.88
1:A:39:LEU:O	4:A:324:HOH:O	1.90	0.88
2:E:105:ARG:CG	2:E:105:ARG:HH11	1.86	0.87
2:G:34:ILE:H	2:G:43:LEU:CB	1.88	0.87
2:H:38:ASP:OD2	4:H:203:HOH:O	1.93	0.87
1:B:152:TRP:HZ3	2:G:83:ASP:OD2	1.58	0.86
2:H:26:ARG:NH2	4:H:210:HOH:O	2.09	0.86
2:H:36:PRO:CA	2:H:41:PRO:CB	2.48	0.85
2:F:105:ARG:HH11	2:F:105:ARG:CG	1.87	0.85
2:G:34:ILE:HB	2:G:43:LEU:HB2	1.59	0.85
1:D:48:GLU:HG3	4:D:311:HOH:O	1.76	0.85
1:D:48:GLU:OE2	4:D:311:HOH:O	1.93	0.85
2:J:101:ARG:NH1	2:J:105:ARG:HB2	1.91	0.84
2:H:33:GLU:H	2:H:52:GLN:NE2	1.75	0.84
2:H:25:GLU:O	2:H:28:LYS:HE3	1.77	0.84
1:B:164:GLY:N	4:B:323:HOH:O	2.09	0.84
2:I:55:ILE:CG2	4:I:204:HOH:O	2.25	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:52:GLN:NE2	4:I:204:HOH:O	2.11	0.84
1:B:71:ARG:NH2	4:B:335:HOH:O	1.82	0.84
2:L:61:GLN:NE2	4:L:208:HOH:O	2.10	0.84
2:F:36:PRO:HB3	2:F:41:PRO:HB2	1.58	0.83
1:A:71:ARG:HH11	1:A:71:ARG:CG	1.91	0.83
1:A:71:ARG:HH11	1:A:71:ARG:HG2	1.43	0.83
1:A:78:HIS:CD2	1:A:86:ILE:HB	2.12	0.83
2:L:70:ILE:HG23	2:L:71:GLU:N	1.92	0.83
2:K:105:ARG:HB3	2:K:105:ARG:NH1	1.94	0.83
2:L:66:LEU:O	2:L:69:GLN:HG2	1.79	0.82
2:L:69:GLN:HA	2:L:70:ILE:O	1.80	0.82
2:I:34:ILE:O	2:I:42:GLY:HA2	1.78	0.82
1:B:48:GLU:OE2	4:B:335:HOH:O	1.98	0.82
1:A:92:ILE:CG1	4:A:321:HOH:O	2.26	0.81
1:A:96:ARG:HD3	1:A:96:ARG:C	1.99	0.81
1:C:141:ASN:CG	4:C:316:HOH:O	2.19	0.81
1:A:96:ARG:HD3	1:A:96:ARG:O	1.80	0.81
2:G:73:GLN:O	4:G:211:HOH:O	1.97	0.81
2:L:39:ARG:HD3	2:L:39:ARG:C	2.01	0.81
2:J:36:PRO:HA	2:J:41:PRO:HB2	1.60	0.81
2:L:60:ARG:NH2	4:L:230:HOH:O	2.13	0.80
2:J:105:ARG:HH11	2:J:105:ARG:CG	1.83	0.80
2:I:66:LEU:HD12	4:I:206:HOH:O	1.80	0.80
2:L:69:GLN:CA	2:L:70:ILE:O	2.29	0.80
1:C:24:GLN:HE22	1:D:25:LYS:NZ	1.79	0.80
2:K:34:ILE:HD12	2:K:43:LEU:HD23	1.63	0.80
2:G:43:LEU:HD21	2:G:45:LEU:HB3	1.63	0.80
2:I:33:GLU:H	2:I:52:GLN:HE21	1.27	0.79
2:G:36:PRO:CB	2:G:41:PRO:HB2	2.10	0.79
2:L:70:ILE:HG23	2:L:71:GLU:H	1.47	0.79
2:E:20:VAL:C	4:E:205:HOH:O	2.21	0.79
2:I:36:PRO:HA	2:I:41:PRO:HB2	1.65	0.79
2:G:32:VAL:O	2:G:43:LEU:CD2	2.30	0.79
2:G:99:LEU:O	2:H:74:LEU:HD23	1.83	0.78
1:C:46:ASP:OD1	4:C:319:HOH:O	2.01	0.78
2:F:85:LEU:HD13	2:F:94:PHE:HB2	1.66	0.78
1:B:152:TRP:CZ3	2:G:83:ASP:OD2	2.35	0.78
2:E:39:ARG:O	2:E:41:PRO:HG3	1.83	0.78
1:B:16:LYS:HE2	1:B:165:LEU:O	1.84	0.77
1:B:41:PRO:O	4:B:310:HOH:O	2.02	0.77
2:I:18:THR:HG22	2:I:19:HIS:N	1.99	0.77
2:L:48:PRO:O	4:L:205:HOH:O	2.03	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:73:ASP:O	4:B:311:HOH:O	2.01	0.77
1:D:167:PHE:CA	4:D:344:HOH:O	2.31	0.77
2:H:36:PRO:HB3	2:H:41:PRO:HB2	0.77	0.77
2:L:33:GLU:H	2:L:52:GLN:HE22	1.33	0.77
2:K:73:GLN:HE22	2:L:103:GLN:HE22	1.29	0.77
2:E:20:VAL:O	4:E:205:HOH:O	2.01	0.77
2:K:38:ASP:OD2	2:K:105:ARG:HG3	1.85	0.76
1:C:9:GLU:OE1	4:C:309:HOH:O	2.02	0.76
1:C:102:PHE:HD1	1:C:102:PHE:O	1.67	0.76
2:L:68:ASP:OD1	4:L:215:HOH:O	2.01	0.76
2:G:39:ARG:CA	4:G:202:HOH:O	2.24	0.76
2:G:59:VAL:HG23	2:G:97:ALA:HB1	1.68	0.76
2:E:33:GLU:H	2:E:52:GLN:HE21	1.31	0.76
1:D:167:PHE:CB	4:D:344:HOH:O	2.33	0.76
2:I:57:LYS:HD2	2:I:85:LEU:HD21	1.65	0.76
2:E:36:PRO:HA	2:E:41:PRO:CB	2.14	0.76
2:I:105:ARG:CB	2:I:105:ARG:HH11	1.96	0.75
2:G:39:ARG:C	4:G:202:HOH:O	2.24	0.75
2:J:34:ILE:N	2:J:43:LEU:HD22	2.02	0.75
2:F:33:GLU:OE2	4:F:201:HOH:O	2.04	0.75
2:H:36:PRO:CB	2:H:41:PRO:HB3	2.13	0.75
2:I:101:ARG:NH1	4:I:210:HOH:O	2.19	0.75
2:F:43:LEU:O	2:F:43:LEU:HD13	1.87	0.75
2:F:105:ARG:HG2	2:F:105:ARG:NH1	1.94	0.75
2:J:30:LEU:CA	4:J:205:HOH:O	1.95	0.75
2:J:34:ILE:HB	2:J:43:LEU:HB3	1.68	0.74
2:H:59:VAL:HG23	2:H:97:ALA:HB1	1.68	0.74
1:D:4:VAL:HG23	4:L:205:HOH:O	1.87	0.74
2:G:38:ASP:HA	4:G:209:HOH:O	1.85	0.74
2:I:52:GLN:CD	4:I:204:HOH:O	2.25	0.74
2:J:102:LEU:O	2:J:106:LEU:HB2	1.88	0.74
4:B:308:HOH:O	2:H:18:THR:CB	2.21	0.74
2:J:33:GLU:HA	2:J:43:LEU:HD21	1.70	0.74
2:E:36:PRO:CB	2:E:41:PRO:HG2	2.18	0.73
2:H:36:PRO:HA	2:H:41:PRO:HB2	1.67	0.73
1:A:33:SER:OG	4:A:305:HOH:O	2.06	0.73
2:I:23:ILE:O	2:I:26:ARG:O	2.06	0.73
2:E:26:ARG:CA	4:E:221:HOH:O	2.34	0.73
2:J:36:PRO:CA	2:J:41:PRO:HB2	2.19	0.73
1:D:167:PHE:N	4:D:344:HOH:O	2.22	0.72
1:C:132:VAL:O	4:C:307:HOH:O	2.05	0.72
2:L:18:THR:HG22	2:L:19:HIS:N	2.04	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:74:LEU:HB2	2:J:103:GLN:HG3	1.71	0.72
2:J:33:GLU:HA	2:J:43:LEU:CD2	2.19	0.72
2:I:18:THR:HG22	2:I:19:HIS:H	1.54	0.72
2:G:73:GLN:HE21	2:H:43:LEU:HD11	1.55	0.72
2:I:26:ARG:O	2:I:27:TYR:HB2	1.90	0.72
2:H:104:GLN:OE1	4:H:205:HOH:O	2.08	0.72
1:C:88:TRP:O	4:C:313:HOH:O	2.07	0.71
2:F:43:LEU:HD21	2:F:45:LEU:HB2	1.71	0.71
2:J:43:LEU:HD12	2:J:45:LEU:HB2	1.70	0.71
2:F:66:LEU:O	4:F:214:HOH:O	2.06	0.71
1:A:51:PHE:CB	4:A:324:HOH:O	2.37	0.71
2:G:107:VAL:HG22	2:H:71:GLU:HG3	1.71	0.71
2:E:68:ASP:OD1	4:E:223:HOH:O	2.09	0.71
2:L:57:LYS:HG3	4:L:228:HOH:O	1.90	0.71
2:F:43:LEU:C	2:F:43:LEU:HD13	2.11	0.71
1:D:45:GLN:HA	1:D:45:GLN:NE2	2.06	0.70
1:C:25:LYS:HZ2	1:D:24:GLN:HE22	1.36	0.70
2:I:41:PRO:CB	2:I:104:GLN:HE21	2.05	0.70
2:G:60:ARG:NH1	4:G:214:HOH:O	2.10	0.70
1:A:139:GLU:OE2	2:E:18:THR:HG21	1.91	0.70
2:H:36:PRO:HA	2:H:41:PRO:CB	2.20	0.70
1:A:92:ILE:CA	4:A:321:HOH:O	2.19	0.70
2:H:38:ASP:CG	4:H:203:HOH:O	2.08	0.70
1:D:40:LEU:HD22	1:D:44:SER:HB3	1.74	0.70
2:G:36:PRO:HB3	2:G:41:PRO:CB	2.14	0.70
2:G:105:ARG:CG	2:G:105:ARG:HH11	2.04	0.69
2:L:68:ASP:O	2:L:69:GLN:C	2.30	0.69
2:J:37:ALA:H	2:J:41:PRO:CB	2.06	0.69
2:E:101:ARG:HH12	2:E:105:ARG:HB2	1.57	0.69
2:I:63:GLU:CA	4:I:206:HOH:O	1.99	0.69
4:G:215:HOH:O	2:H:71:GLU:O	2.10	0.69
1:C:25:LYS:NZ	4:C:306:HOH:O	2.26	0.69
1:C:45:GLN:HB3	4:C:314:HOH:O	1.91	0.69
1:B:48:GLU:CD	4:B:335:HOH:O	2.31	0.69
2:J:37:ALA:H	2:J:41:PRO:HB3	1.58	0.69
2:I:70:ILE:HD12	2:I:70:ILE:H	1.56	0.69
2:G:95:GLU:CD	2:H:82:ARG:HH12	1.95	0.69
2:G:43:LEU:C	2:G:43:LEU:HD23	2.14	0.68
2:E:41:PRO:CB	2:E:104:GLN:HE21	2.06	0.68
1:A:81:GLN:CD	4:A:311:HOH:O	2.23	0.68
2:J:32:VAL:C	2:J:43:LEU:HD11	2.13	0.68
2:J:52:GLN:O	2:J:55:ILE:HG22	1.92	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:106:LEU:O	4:E:212:HOH:O	2.10	0.68
1:C:25:LYS:NZ	1:D:24:GLN:HE22	1.91	0.68
2:J:63:GLU:HA	2:J:66:LEU:HB2	1.76	0.68
1:D:167:PHE:HB2	4:D:344:HOH:O	1.93	0.68
2:L:39:ARG:CD	2:L:39:ARG:O	2.29	0.67
2:K:105:ARG:CG	2:K:105:ARG:NH1	2.46	0.67
1:C:137:ARG:CZ	1:C:137:ARG:HB2	2.23	0.67
2:I:41:PRO:HB2	2:I:104:GLN:HE21	1.59	0.67
1:D:136:ASN:ND2	1:D:139:GLU:H	1.91	0.67
1:C:156:ASP:O	1:C:160:GLN:HG2	1.95	0.67
2:J:32:VAL:CG2	2:J:45:LEU:HB3	2.24	0.67
1:A:92:ILE:CG2	4:A:321:HOH:O	2.12	0.66
2:J:34:ILE:H	2:J:43:LEU:CD2	2.07	0.66
1:B:9:GLU:HB3	1:B:22:ILE:HD13	1.76	0.66
2:G:70:ILE:O	2:G:70:ILE:HG23	1.95	0.66
1:C:58:ALA:O	1:C:62:GLU:HG2	1.95	0.66
1:C:45:GLN:CA	4:C:314:HOH:O	2.43	0.66
1:D:149:PRO:HG2	2:L:45:LEU:HG	1.78	0.66
1:B:20:SER:O	4:B:333:HOH:O	2.13	0.66
2:K:34:ILE:CD1	2:K:43:LEU:HD23	2.25	0.66
2:F:33:GLU:HA	2:F:43:LEU:CD1	2.26	0.66
2:L:38:ASP:C	2:L:40:GLN:H	1.99	0.65
2:I:52:GLN:OE1	4:I:204:HOH:O	2.14	0.65
2:I:102:LEU:O	2:I:106:LEU:HB2	1.96	0.65
2:K:105:ARG:NH1	2:K:105:ARG:HG2	2.11	0.65
1:A:25:LYS:NZ	4:A:307:HOH:O	1.93	0.65
1:B:45:GLN:HE21	1:B:45:GLN:H	1.44	0.65
2:F:34:ILE:H	2:F:43:LEU:CD1	2.05	0.65
2:G:43:LEU:HD21	2:G:45:LEU:CB	2.27	0.65
2:J:87:THR:HB	2:J:90:GLN:HG2	1.79	0.65
1:D:45:GLN:HE21	1:D:45:GLN:HA	1.61	0.65
1:B:139:GLU:OE1	4:B:308:HOH:O	2.14	0.65
1:A:51:PHE:HB3	4:A:324:HOH:O	1.97	0.65
1:A:149:PRO:HG2	2:E:45:LEU:HG	1.79	0.65
2:E:39:ARG:O	2:E:41:PRO:CG	2.45	0.64
1:D:45:GLN:C	1:D:47:TYR:H	2.00	0.64
1:B:48:GLU:OE1	4:B:335:HOH:O	2.13	0.64
2:K:29:ASP:OD2	4:K:213:HOH:O	2.15	0.64
1:D:45:GLN:O	1:D:47:TYR:N	2.31	0.64
1:C:33:SER:OG	4:C:305:HOH:O	2.15	0.64
1:A:155:LYS:NZ	4:F:213:HOH:O	2.28	0.64
2:K:73:GLN:NE2	2:L:103:GLN:HE22	1.95	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:31:GLY:HA3	2:H:23:ILE:HD13	1.80	0.64
2:L:69:GLN:HA	2:L:70:ILE:C	2.15	0.63
2:F:85:LEU:CD1	2:F:94:PHE:HB2	2.28	0.63
2:G:39:ARG:O	2:G:41:PRO:HB3	1.98	0.63
1:C:134:ALA:CB	1:C:140:ALA:HB2	2.28	0.63
2:L:18:THR:CG2	2:L:19:HIS:N	2.61	0.63
2:L:33:GLU:HG2	4:L:210:HOH:O	1.99	0.63
2:I:101:ARG:HD2	2:I:101:ARG:O	1.98	0.63
2:L:70:ILE:CG2	2:L:71:GLU:N	2.61	0.63
2:I:22:ALA:O	4:I:205:HOH:O	2.16	0.62
2:J:38:ASP:OD2	2:J:105:ARG:HG3	2.00	0.62
2:E:69:GLN:C	2:E:71:GLU:H	2.02	0.62
2:F:43:LEU:HD23	2:F:45:LEU:HD13	1.81	0.62
2:L:57:LYS:CD	4:L:223:HOH:O	2.24	0.62
2:G:107:VAL:HG22	2:H:71:GLU:HB2	1.81	0.62
1:C:152:TRP:HZ3	2:J:83:ASP:OD2	1.83	0.62
1:A:160:GLN:NE2	4:A:303:HOH:O	2.32	0.62
2:L:38:ASP:OD2	2:L:105:ARG:HD3	1.99	0.61
2:E:61:GLN:NE2	4:E:211:HOH:O	2.33	0.61
2:J:39:ARG:HD3	2:J:39:ARG:N	2.15	0.61
2:L:26:ARG:O	2:L:27:TYR:HB2	2.00	0.61
2:F:43:LEU:CD2	2:F:45:LEU:HD13	2.30	0.61
2:L:73:GLN:CA	2:L:73:GLN:OE1	2.45	0.61
2:L:18:THR:HG22	2:L:20:VAL:H	1.64	0.61
1:B:42:LYS:HG3	1:B:123:GLY:HA3	1.83	0.61
2:F:87:THR:HG22	2:F:89:MET:N	2.15	0.61
1:B:149:PRO:HG2	2:H:45:LEU:HG	1.81	0.61
1:C:69:TYR:HD2	1:C:101:PHE:CD2	2.18	0.61
2:F:33:GLU:HA	2:F:43:LEU:HD11	1.83	0.61
2:E:43:LEU:HD11	2:F:73:GLN:NE2	2.16	0.61
2:I:69:GLN:HB3	2:I:70:ILE:HD12	1.83	0.60
2:G:34:ILE:CB	2:G:43:LEU:HB2	2.28	0.60
2:J:39:ARG:HG2	2:J:108:ALA:CA	2.27	0.60
1:D:48:GLU:CG	4:D:311:HOH:O	2.42	0.60
2:G:37:ALA:O	4:G:209:HOH:O	2.16	0.60
2:I:43:LEU:HD11	2:J:73:GLN:OE1	2.02	0.60
2:I:41:PRO:HB2	2:I:104:GLN:NE2	2.16	0.60
1:C:152:TRP:CZ3	2:J:83:ASP:OD2	2.55	0.60
2:I:99:LEU:O	2:J:74:LEU:HD23	2.02	0.60
2:I:38:ASP:HA	4:I:203:HOH:O	2.01	0.60
2:G:34:ILE:N	2:G:43:LEU:HB3	2.05	0.60
2:E:101:ARG:HD3	4:E:210:HOH:O	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:41:PRO:HA	2:H:104:GLN:HE21	1.67	0.59
2:G:73:GLN:NE2	2:H:43:LEU:HD11	2.16	0.59
2:I:106:LEU:O	2:I:106:LEU:HD23	2.03	0.59
2:L:49:VAL:HG22	2:L:89:MET:HG2	1.83	0.59
1:C:10:LEU:HD13	1:C:22:ILE:HG22	1.84	0.59
2:F:87:THR:HG22	2:F:89:MET:H	1.66	0.59
2:J:34:ILE:N	2:J:43:LEU:HD13	2.17	0.59
2:G:104:GLN:OE1	4:G:205:HOH:O	2.16	0.59
1:B:61:ARG:HD2	4:B:302:HOH:O	2.02	0.59
2:G:68:ASP:O	2:G:68:ASP:OD1	2.20	0.59
2:E:41:PRO:HB3	2:E:104:GLN:HE21	1.67	0.59
1:C:45:GLN:CB	4:C:314:HOH:O	2.50	0.59
1:C:67:ALA:HB3	1:C:69:TYR:HE1	1.68	0.59
1:C:45:GLN:O	1:C:47:TYR:N	2.36	0.59
1:B:160:GLN:O	4:B:323:HOH:O	2.17	0.59
1:C:58:ALA:HB2	4:C:310:HOH:O	2.02	0.59
2:G:39:ARG:HE	2:G:108:ALA:CA	2.06	0.59
1:A:78:HIS:HD2	1:A:86:ILE:CG2	2.16	0.59
2:F:89:MET:HA	2:F:89:MET:HE3	1.84	0.59
2:G:85:LEU:HD13	2:G:94:PHE:HB2	1.85	0.59
2:F:36:PRO:CB	2:F:41:PRO:HB2	2.33	0.58
2:I:43:LEU:HD11	2:J:73:GLN:CD	2.24	0.58
1:C:77:SER:HA	1:C:80:THR:HG23	1.84	0.58
2:I:36:PRO:HB3	2:I:41:PRO:HG2	1.85	0.58
1:D:145:GLU:HG3	4:D:338:HOH:O	2.03	0.58
2:J:85:LEU:CD1	2:J:94:PHE:HB2	2.34	0.58
2:E:23:ILE:N	4:E:205:HOH:O	1.91	0.58
2:L:57:LYS:HG3	4:L:223:HOH:O	1.95	0.58
2:I:62:ALA:O	2:I:66:LEU:HG	2.04	0.58
2:E:70:ILE:O	2:E:71:GLU:O	2.20	0.58
1:A:74:PRO:HG2	1:A:93:TYR:CD1	2.38	0.58
2:I:70:ILE:HD12	2:I:70:ILE:N	2.19	0.58
2:G:43:LEU:HD23	2:G:45:LEU:N	2.18	0.58
2:I:87:THR:HB	2:I:88:PRO:HD2	1.86	0.57
2:L:17:LYS:HE3	2:L:25:GLU:OE1	2.03	0.57
1:B:152:TRP:HZ3	2:G:83:ASP:CG	2.07	0.57
2:I:55:ILE:HG21	4:I:204:HOH:O	1.98	0.57
2:I:26:ARG:O	2:I:27:TYR:CB	2.52	0.57
2:F:34:ILE:N	2:F:43:LEU:HD12	2.05	0.57
1:C:24:GLN:HE22	1:D:25:LYS:HZ2	1.50	0.57
1:C:149:PRO:HG2	2:I:45:LEU:HG	1.86	0.57
2:K:38:ASP:OD2	2:K:105:ARG:CG	2.51	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:25:LYS:NZ	1:D:24:GLN:NE2	2.52	0.57
2:E:23:ILE:HB	4:E:205:HOH:O	2.05	0.57
1:C:133:GLU:HG2	4:C:303:HOH:O	2.05	0.57
2:L:70:ILE:C	2:L:71:GLU:HG2	2.24	0.57
2:L:110:ARG:NH2	4:L:229:HOH:O	2.37	0.57
1:D:63:HIS:HE1	1:D:104:GLU:OE1	1.88	0.57
2:G:34:ILE:CD1	2:G:43:LEU:HD12	2.35	0.56
1:B:6:GLY:HA3	1:B:26:MET:SD	2.44	0.56
1:C:42:LYS:HA	1:C:123:GLY:O	2.05	0.56
2:E:30:LEU:HB3	2:E:47:TRP:O	2.05	0.56
2:J:101:ARG:HH12	2:J:105:ARG:CB	1.98	0.56
2:J:101:ARG:HH22	2:J:105:ARG:CD	1.90	0.56
2:G:101:ARG:HH12	2:G:105:ARG:HD3	1.69	0.56
2:I:102:LEU:O	2:I:106:LEU:CB	2.53	0.56
1:B:36:LEU:C	1:B:36:LEU:HD23	2.26	0.56
2:I:34:ILE:CD1	2:I:97:ALA:HA	2.35	0.56
2:F:30:LEU:HD12	2:F:47:TRP:O	2.05	0.56
2:E:26:ARG:CB	4:E:221:HOH:O	2.38	0.56
1:C:152:TRP:HZ3	2:J:83:ASP:CG	2.09	0.56
1:A:50:ALA:O	1:A:52:ILE:HD12	2.05	0.56
1:A:119:HIS:ND1	4:A:319:HOH:O	2.33	0.56
2:J:49:VAL:HB	2:J:50:PRO:HD2	1.88	0.56
2:J:96:VAL:O	2:J:100:THR:HB	2.05	0.56
2:L:38:ASP:C	2:L:40:GLN:N	2.59	0.56
1:D:36:LEU:C	1:D:36:LEU:HD23	2.26	0.56
2:F:43:LEU:HD23	2:F:45:LEU:HD22	1.87	0.56
1:D:4:VAL:HG21	2:L:49:VAL:HG13	1.88	0.56
1:D:45:GLN:C	1:D:47:TYR:N	2.59	0.56
2:G:30:LEU:CD2	2:I:80:PHE:HE1	2.18	0.56
4:B:308:HOH:O	2:H:21:ASP:OD2	2.18	0.55
2:E:69:GLN:O	2:E:71:GLU:N	2.39	0.55
1:A:62:GLU:HB3	4:A:322:HOH:O	2.05	0.55
2:J:43:LEU:HD23	2:J:43:LEU:O	2.06	0.55
2:L:68:ASP:C	2:L:69:GLN:O	2.43	0.55
1:A:16:LYS:HD3	1:A:51:PHE:HE1	1.72	0.55
2:L:49:VAL:HB	2:L:50:PRO:HD2	1.88	0.55
2:H:54:ALA:HB2	2:H:90:GLN:HE21	1.71	0.55
4:G:215:HOH:O	2:H:72:GLY:HA2	2.06	0.55
1:B:31:GLY:HA3	2:H:23:ILE:CD1	2.36	0.55
2:G:95:GLU:OE1	2:H:82:ARG:NH1	2.37	0.55
2:I:108:ALA:O	2:I:109:ALA:HB2	2.07	0.55
1:C:3:LEU:HD11	2:I:27:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:6:GLY:HA3	1:C:26:MET:SD	2.47	0.55
2:I:110:ARG:H	2:I:110:ARG:CZ	2.19	0.55
1:C:94:GLN:O	1:C:99:HIS:NE2	2.41	0.55
1:C:48:GLU:HG2	1:C:65:ASP:HB3	1.89	0.54
2:G:107:VAL:HG22	2:H:71:GLU:CG	2.36	0.54
2:L:59:VAL:O	2:L:63:GLU:HG3	2.08	0.54
2:I:41:PRO:CB	2:I:104:GLN:NE2	2.70	0.54
1:C:98:GLN:O	1:C:101:PHE:HB3	2.07	0.54
2:I:18:THR:CG2	2:I:19:HIS:N	2.68	0.54
2:J:70:ILE:O	2:J:70:ILE:HG23	2.08	0.54
2:I:18:THR:CG2	2:I:19:HIS:H	2.21	0.54
1:B:80:THR:HG22	1:B:125:LEU:HD21	1.88	0.54
2:G:70:ILE:O	2:G:70:ILE:CG2	2.56	0.54
1:A:155:LYS:HD2	1:A:155:LYS:C	2.27	0.54
2:I:75:TRP:CD2	2:J:96:VAL:HG22	2.43	0.54
1:D:4:VAL:HG21	2:L:49:VAL:CG1	2.39	0.53
2:J:67:ALA:O	2:J:68:ASP:C	2.45	0.53
2:H:75:TRP:CD1	2:H:76:THR:N	2.76	0.53
1:A:78:HIS:CD2	1:A:86:ILE:CB	2.90	0.53
1:C:152:TRP:HZ3	2:J:83:ASP:OD1	1.91	0.53
2:E:91:LYS:O	2:E:95:GLU:HG3	2.08	0.53
1:C:136:ASN:ND2	1:C:138:ALA:HB3	2.23	0.53
2:F:44:SER:CA	4:F:201:HOH:O	2.24	0.53
2:F:43:LEU:CD2	2:F:45:LEU:N	2.71	0.53
2:J:34:ILE:HB	2:J:43:LEU:CB	2.37	0.53
2:G:85:LEU:CD1	2:G:94:PHE:HB2	2.38	0.53
2:I:33:GLU:H	2:I:52:GLN:NE2	2.01	0.53
1:C:86:ILE:HD11	1:C:92:ILE:HG21	1.91	0.53
1:C:86:ILE:O	1:C:86:ILE:HG23	2.08	0.53
2:G:89:MET:SD	2:J:89:MET:HE2	2.49	0.53
2:K:69:GLN:NE2	2:K:69:GLN:HA	2.23	0.53
2:I:34:ILE:HD11	2:I:97:ALA:HA	1.90	0.53
2:L:47:TRP:CD1	2:L:48:PRO:HD2	2.44	0.53
2:G:39:ARG:NH1	2:G:110:ARG:HD2	2.23	0.53
2:E:37:ALA:HB3	2:E:104:GLN:HB3	1.91	0.53
2:G:107:VAL:C	2:G:109:ALA:H	2.13	0.52
1:A:31:GLY:HA3	2:E:23:ILE:HG13	1.91	0.52
2:G:107:VAL:O	2:G:109:ALA:N	2.42	0.52
4:B:308:HOH:O	2:H:21:ASP:CG	2.48	0.52
2:L:18:THR:HG22	2:L:20:VAL:N	2.25	0.52
1:B:86:ILE:O	1:B:86:ILE:HG23	2.10	0.52
1:A:152:TRP:HZ3	2:F:83:ASP:OD2	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:87:THR:HG23	2:K:88:PRO:HD2	1.91	0.52
2:G:40:GLN:NE2	2:G:110:ARG:HH22	2.08	0.52
2:I:36:PRO:CB	2:I:41:PRO:HG2	2.38	0.52
1:C:27:ALA:HB2	1:C:35:ILE:HD13	1.91	0.52
2:F:87:THR:HG23	2:F:88:PRO:HD2	1.91	0.52
1:C:95:THR:O	1:C:99:HIS:CD2	2.62	0.52
1:A:71:ARG:CG	1:A:71:ARG:NH1	2.60	0.52
2:J:49:VAL:HB	2:J:50:PRO:CD	2.39	0.51
1:D:114:LEU:HD23	1:D:114:LEU:N	2.24	0.51
2:E:103:GLN:HE22	2:F:73:GLN:NE2	2.08	0.51
2:I:36:PRO:HA	2:I:41:PRO:CB	2.39	0.51
2:H:33:GLU:H	2:H:52:GLN:HE22	1.55	0.51
2:F:87:THR:HB	2:F:90:GLN:HG2	1.91	0.51
2:J:46:LEU:HB3	4:J:204:HOH:O	2.09	0.51
2:E:83:ASP:CB	2:K:50:PRO:HG2	2.41	0.51
2:K:95:GLU:OE1	2:L:75:TRP:HZ3	1.93	0.51
2:K:42:GLY:O	2:K:43:LEU:HB3	2.11	0.51
2:H:110:ARG:H	2:H:110:ARG:HD3	1.76	0.51
2:E:41:PRO:HB3	2:E:104:GLN:NE2	2.26	0.51
1:B:38:GLY:HA2	1:B:51:PHE:O	2.10	0.51
2:F:39:ARG:NH1	2:F:110:ARG:HG3	2.25	0.51
1:B:61:ARG:NH2	1:B:65:ASP:OD2	2.44	0.51
2:E:38:ASP:HB2	2:E:108:ALA:HB2	1.92	0.51
2:G:39:ARG:NH1	2:G:110:ARG:HB2	2.26	0.50
2:L:68:ASP:O	2:L:69:GLN:O	2.29	0.50
2:K:59:VAL:O	2:K:63:GLU:HG3	2.11	0.50
1:C:58:ALA:CB	4:C:310:HOH:O	2.59	0.50
1:C:24:GLN:HE22	1:D:25:LYS:HZ3	1.56	0.50
1:A:78:HIS:CE1	1:A:82:SER:HB3	2.45	0.50
2:I:99:LEU:HD11	2:J:78:PHE:CG	2.47	0.50
2:I:105:ARG:HB2	2:I:105:ARG:NH1	2.06	0.50
2:F:43:LEU:HD22	2:F:45:LEU:N	2.26	0.50
1:A:92:ILE:HD13	4:A:321:HOH:O	2.11	0.50
2:H:41:PRO:HD2	2:H:41:PRO:O	2.11	0.50
2:G:39:ARG:O	2:G:41:PRO:CB	2.60	0.50
2:J:39:ARG:HG3	2:J:110:ARG:CZ	2.42	0.50
1:C:63:HIS:HD1	1:C:63:HIS:C	2.15	0.50
1:D:159:LEU:HD12	1:D:159:LEU:O	2.12	0.50
2:I:55:ILE:HG22	4:I:204:HOH:O	2.02	0.50
2:I:95:GLU:O	2:I:99:LEU:HB2	2.10	0.50
2:E:68:ASP:CG	4:E:223:HOH:O	2.49	0.50
1:C:69:TYR:HB3	1:C:101:PHE:HE2	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:68:ASP:O	2:I:69:GLN:O	2.30	0.50
2:E:23:ILE:CB	4:E:205:HOH:O	2.60	0.50
1:C:120:GLY:HA3	1:C:124:GLU:OE1	2.12	0.50
2:G:58:GLY:HA2	2:G:94:PHE:CE2	2.47	0.49
1:C:35:ILE:HG13	1:C:36:LEU:N	2.27	0.49
2:K:95:GLU:HB3	2:L:75:TRP:HZ3	1.77	0.49
2:J:37:ALA:H	2:J:41:PRO:HB2	1.77	0.49
1:A:25:LYS:O	1:A:25:LYS:HD2	2.12	0.49
1:A:50:ALA:HB3	1:A:52:ILE:HD11	1.93	0.49
1:C:138:ALA:O	1:C:142:ARG:HG3	2.12	0.49
2:E:38:ASP:HB2	2:E:108:ALA:CB	2.42	0.49
2:I:17:LYS:HG3	2:I:17:LYS:O	2.10	0.49
1:C:83:VAL:HG12	1:C:119:HIS:HD2	1.78	0.49
2:J:34:ILE:H	2:J:43:LEU:HD13	1.78	0.49
2:J:106:LEU:C	2:J:106:LEU:HD23	2.33	0.49
2:L:33:GLU:N	2:L:52:GLN:HE22	2.08	0.49
2:E:25:GLU:O	2:E:28:LYS:HG3	2.12	0.49
2:H:37:ALA:HB3	2:H:104:GLN:HB3	1.93	0.49
2:J:39:ARG:O	2:J:40:GLN:C	2.50	0.49
2:J:52:GLN:HB3	2:J:53:PRO:HD3	1.95	0.49
2:I:36:PRO:CA	2:I:41:PRO:HG2	2.43	0.49
2:G:67:ALA:O	2:G:68:ASP:C	2.51	0.49
2:G:43:LEU:C	2:G:43:LEU:CD2	2.82	0.49
2:L:69:GLN:CA	2:L:70:ILE:C	2.80	0.49
2:L:71:GLU:HB3	4:L:219:HOH:O	2.12	0.49
2:H:109:ALA:O	2:H:110:ARG:C	2.52	0.49
2:F:45:LEU:HG	2:K:46:LEU:CD2	2.43	0.48
2:E:102:LEU:O	2:E:106:LEU:HD12	2.13	0.48
1:D:136:ASN:C	1:D:136:ASN:HD22	2.16	0.48
2:G:39:ARG:HG3	2:G:108:ALA:CA	2.43	0.48
2:I:41:PRO:HB3	2:I:104:GLN:HG2	1.96	0.48
2:G:107:VAL:HG22	2:H:71:GLU:CB	2.43	0.48
1:C:102:PHE:CD1	1:C:102:PHE:C	2.87	0.48
1:D:45:GLN:HE21	1:D:45:GLN:CA	2.22	0.48
1:D:96:ARG:O	1:D:96:ARG:HD2	2.13	0.48
2:F:32:VAL:O	2:F:43:LEU:HD11	2.13	0.48
2:L:68:ASP:O	2:L:70:ILE:O	2.30	0.48
1:A:152:TRP:HZ3	2:F:83:ASP:CG	2.16	0.48
2:G:43:LEU:CD2	2:G:45:LEU:CB	2.92	0.48
1:B:148:LEU:N	1:B:149:PRO:CD	2.76	0.48
2:L:40:GLN:HB3	2:L:104:GLN:HG2	1.96	0.48
1:C:102:PHE:C	1:C:102:PHE:HD1	2.17	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:152:TRP:HZ3	2:K:83:ASP:CG	2.17	0.48
2:J:63:GLU:OE2	2:J:101:ARG:NE	2.35	0.47
2:I:85:LEU:N	2:I:85:LEU:HD23	2.29	0.47
2:H:68:ASP:O	2:H:69:GLN:C	2.52	0.47
1:B:24:GLN:NE2	4:B:333:HOH:O	2.44	0.47
1:D:10:LEU:HD13	1:D:22:ILE:HG22	1.95	0.47
2:I:105:ARG:HH11	2:I:105:ARG:CG	2.26	0.47
2:I:39:ARG:O	2:I:41:PRO:N	2.47	0.47
1:C:67:ALA:HB3	1:C:69:TYR:CE1	2.47	0.47
2:I:66:LEU:CG	4:I:206:HOH:O	2.62	0.47
2:F:38:ASP:OD2	2:F:105:ARG:HG3	2.14	0.47
2:H:25:GLU:O	2:H:28:LYS:HG2	2.14	0.47
1:C:3:LEU:N	1:C:3:LEU:HD12	2.30	0.47
1:D:149:PRO:O	1:D:152:TRP:HD1	1.97	0.47
2:H:19:HIS:NE2	2:H:23:ILE:HD11	2.29	0.47
1:B:81:GLN:NE2	4:B:307:HOH:O	2.48	0.47
2:I:49:VAL:HG22	2:I:89:MET:HG2	1.96	0.47
1:C:90:PRO:HB3	1:C:102:PHE:HE2	1.79	0.47
1:C:51:PHE:CG	1:C:166:ALA:HB2	2.50	0.47
1:D:167:PHE:C	4:D:344:HOH:O	2.53	0.47
2:E:69:GLN:C	2:E:71:GLU:N	2.67	0.47
2:F:39:ARG:HH11	2:F:110:ARG:HG3	1.80	0.47
1:C:116:MET:HE3	1:C:128:LEU:HD13	1.97	0.47
2:L:61:GLN:NE2	4:L:221:HOH:O	2.47	0.46
2:G:37:ALA:C	4:G:209:HOH:O	2.52	0.46
2:I:66:LEU:CD1	4:I:206:HOH:O	2.51	0.46
2:J:39:ARG:NH1	2:J:110:ARG:HD2	2.31	0.46
2:J:36:PRO:HA	2:J:41:PRO:O	2.15	0.46
2:G:55:ILE:HG23	2:G:97:ALA:HB2	1.98	0.46
2:K:56:ASP:OD1	4:K:229:HOH:O	2.20	0.46
2:G:89:MET:CE	2:J:89:MET:HE2	2.44	0.46
2:E:19:HIS:O	4:E:205:HOH:O	2.21	0.46
1:C:58:ALA:N	4:C:310:HOH:O	2.36	0.46
2:L:19:HIS:CE1	2:L:23:ILE:HD13	2.50	0.46
1:C:42:LYS:HB2	1:C:123:GLY:HA3	1.98	0.46
1:D:94:GLN:NE2	4:D:307:HOH:O	2.48	0.46
2:I:101:ARG:HH12	2:I:105:ARG:NH1	2.14	0.46
2:I:71:GLU:HG2	2:I:71:GLU:H	1.40	0.46
1:C:35:ILE:HD12	1:C:130:LEU:HG	1.97	0.46
2:K:95:GLU:OE1	2:L:75:TRP:CZ3	2.68	0.46
1:B:88:TRP:CE2	3:B:201:OHN:H5C2	2.51	0.46
2:I:70:ILE:CD1	2:I:70:ILE:H	2.27	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:39:ARG:NH1	2:L:39:ARG:O	2.30	0.46
2:E:26:ARG:O	2:E:27:TYR:HB2	2.15	0.46
2:K:87:THR:HB	2:K:90:GLN:HG3	1.96	0.46
2:K:70:ILE:HG23	2:K:70:ILE:O	2.15	0.46
1:A:9:GLU:HB3	1:A:22:ILE:HD13	1.97	0.46
2:I:63:GLU:HG3	2:I:101:ARG:NE	2.31	0.46
2:L:39:ARG:C	2:L:39:ARG:CD	2.72	0.46
2:E:101:ARG:HH22	2:E:105:ARG:NH1	2.14	0.46
2:J:91:LYS:O	2:J:95:GLU:HG3	2.15	0.46
2:F:39:ARG:HG3	2:F:108:ALA:HA	1.97	0.46
2:H:38:ASP:OD2	2:H:105:ARG:HG3	2.15	0.46
2:G:106:LEU:HD11	2:H:102:LEU:HD22	1.96	0.46
1:C:89:GLU:OE2	4:C:316:HOH:O	2.21	0.46
2:I:52:GLN:N	2:I:53:PRO:CD	2.79	0.46
1:D:16:LYS:O	1:D:20:SER:HB2	2.15	0.46
2:G:103:GLN:OE1	2:H:72:GLY:O	2.33	0.46
2:E:41:PRO:O	2:E:42:GLY:C	2.54	0.46
1:B:83:VAL:HG21	2:G:81:GLY:HA2	1.97	0.46
2:K:34:ILE:HD12	2:K:43:LEU:CD2	2.41	0.46
2:L:30:LEU:HB3	2:L:47:TRP:O	2.16	0.46
2:J:85:LEU:HD11	2:J:94:PHE:HB2	1.96	0.46
2:E:17:LYS:CE	2:E:25:GLU:HG3	2.45	0.46
2:I:54:ALA:HB2	2:I:90:GLN:HE21	1.81	0.46
2:K:87:THR:HB	2:K:90:GLN:CG	2.46	0.45
1:B:88:TRP:CZ2	3:B:201:OHN:H5C2	2.51	0.45
2:K:87:THR:CG2	2:K:88:PRO:HD2	2.46	0.45
2:H:33:GLU:H	2:H:52:GLN:HE21	1.60	0.45
3:B:201:OHN:H172	3:B:201:OHN:H202	1.70	0.45
2:K:75:TRP:CG	2:L:96:VAL:HG13	2.51	0.45
2:F:70:ILE:O	2:F:70:ILE:HG23	2.16	0.45
1:A:78:HIS:CD2	1:A:86:ILE:CG2	2.98	0.45
2:J:43:LEU:CD1	2:J:45:LEU:HB2	2.42	0.45
1:C:73:ASP:OD2	3:C:201:OHN:H101	2.17	0.45
2:E:107:VAL:C	2:E:109:ALA:H	2.20	0.45
2:J:33:GLU:OE2	2:J:43:LEU:HD21	2.17	0.45
2:F:39:ARG:CG	2:F:108:ALA:HA	2.47	0.45
2:K:57:LYS:HE3	2:K:61:GLN:OE1	2.16	0.45
2:L:69:GLN:C	2:L:70:ILE:O	2.55	0.45
2:I:74:LEU:HG	2:J:99:LEU:HD22	1.97	0.45
2:F:29:ASP:C	2:F:31:MET:H	2.19	0.45
2:J:38:ASP:C	2:J:39:ARG:HD3	2.37	0.45
1:B:45:GLN:NE2	1:B:45:GLN:H	2.11	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:136:ASN:HD21	1:A:138:ALA:HB3	1.81	0.45
2:I:59:VAL:HG22	2:I:101:ARG:HB2	1.99	0.45
2:H:32:VAL:HG22	2:H:45:LEU:O	2.17	0.45
2:I:91:LYS:O	2:I:95:GLU:HG3	2.17	0.45
1:C:136:ASN:HD22	1:C:138:ALA:H	1.64	0.45
1:A:78:HIS:NE2	1:A:86:ILE:HB	2.31	0.44
1:A:12:ARG:O	1:D:12:ARG:HG2	2.17	0.44
2:I:66:LEU:C	2:I:68:ASP:H	2.20	0.44
2:I:34:ILE:HG21	2:I:100:THR:HG22	1.98	0.44
2:F:39:ARG:NE	2:F:108:ALA:CB	2.80	0.44
1:C:116:MET:CE	1:C:128:LEU:HD13	2.47	0.44
2:I:37:ALA:H	2:I:41:PRO:CG	2.30	0.44
2:F:39:ARG:CD	2:F:108:ALA:HA	2.46	0.44
2:F:101:ARG:HD2	2:F:104:GLN:OE1	2.18	0.44
1:B:26:MET:HE3	1:B:154:LEU:CD1	2.48	0.44
2:E:49:VAL:HB	2:E:50:PRO:HD2	2.00	0.44
2:K:95:GLU:HB3	2:L:75:TRP:CZ3	2.51	0.44
1:A:10:LEU:HD13	1:A:22:ILE:HG22	1.99	0.44
2:F:35:PRO:HA	2:F:36:PRO:HD3	1.81	0.44
2:F:43:LEU:CD2	2:F:45:LEU:HD22	2.47	0.44
2:J:95:GLU:O	2:J:99:LEU:HB2	2.18	0.44
2:H:40:GLN:HG3	2:H:107:VAL:HG12	2.00	0.44
2:J:33:GLU:HA	2:J:43:LEU:HD22	1.99	0.44
1:A:152:TRP:CZ3	2:F:83:ASP:OD2	2.70	0.44
1:C:9:GLU:HB3	1:C:22:ILE:HD13	1.99	0.44
2:J:37:ALA:HB3	2:J:104:GLN:HB3	1.99	0.44
2:I:66:LEU:HB2	4:I:206:HOH:O	2.17	0.44
2:G:43:LEU:CD2	2:G:45:LEU:N	2.80	0.44
1:C:51:PHE:CD2	1:C:166:ALA:HB2	2.52	0.44
2:G:73:GLN:HB3	4:H:208:HOH:O	2.18	0.43
2:F:39:ARG:HG3	2:F:108:ALA:N	2.31	0.43
1:C:152:TRP:HB2	2:J:80:PHE:CZ	2.53	0.43
2:G:33:GLU:HA	2:G:43:LEU:HD22	2.00	0.43
1:D:136:ASN:HD21	1:D:139:GLU:H	1.64	0.43
1:C:84:LEU:HD21	2:J:77:ALA:HA	1.99	0.43
2:E:101:ARG:CA	4:E:209:HOH:O	2.49	0.43
2:G:106:LEU:HG	2:H:106:LEU:CD2	2.31	0.43
1:C:78:HIS:CD2	1:C:86:ILE:HB	2.53	0.43
1:D:114:LEU:HD23	1:D:114:LEU:H	1.82	0.43
2:H:86:PRO:HG2	2:H:87:THR:H	1.84	0.43
1:A:36:LEU:HD23	1:A:37:PHE:N	2.33	0.43
1:B:35:ILE:O	1:B:54:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:91:LYS:O	2:G:94:PHE:HB3	2.19	0.43
2:I:109:ALA:O	2:I:110:ARG:C	2.57	0.43
2:I:110:ARG:NH1	2:I:110:ARG:H	2.17	0.43
2:G:68:ASP:C	2:G:68:ASP:OD1	2.57	0.43
2:G:96:VAL:HG22	2:H:75:TRP:CD2	2.54	0.43
2:F:43:LEU:C	2:F:43:LEU:HD22	2.36	0.43
2:F:45:LEU:HD12	2:F:45:LEU:HA	1.60	0.43
2:F:39:ARG:HG2	2:F:108:ALA:HB2	2.01	0.43
2:F:78:PHE:CZ	2:F:95:GLU:HG2	2.54	0.43
2:L:66:LEU:HD13	2:L:105:ARG:HG3	1.99	0.43
2:E:71:GLU:OE2	4:E:218:HOH:O	2.21	0.43
2:I:99:LEU:HD23	2:I:99:LEU:HA	1.71	0.43
2:G:34:ILE:HD13	2:G:100:THR:HG21	2.01	0.43
2:G:39:ARG:HG3	2:G:108:ALA:N	2.34	0.43
2:I:55:ILE:HB	4:I:204:HOH:O	2.19	0.43
2:K:68:ASP:HB2	2:K:71:GLU:CG	2.48	0.43
2:G:47:TRP:HA	2:G:48:PRO:HD3	1.83	0.43
1:D:48:GLU:HG2	1:D:65:ASP:O	2.18	0.42
2:I:39:ARG:O	2:I:41:PRO:CD	2.66	0.42
2:E:100:THR:CB	4:E:209:HOH:O	2.65	0.42
2:E:41:PRO:CB	2:E:104:GLN:NE2	2.77	0.42
2:G:105:ARG:HG2	2:G:105:ARG:HH11	1.83	0.42
1:B:152:TRP:HB2	2:G:80:PHE:CZ	2.55	0.42
2:L:75:TRP:CD1	2:L:75:TRP:C	2.88	0.42
2:I:105:ARG:CA	4:I:210:HOH:O	2.32	0.42
2:L:40:GLN:HE21	2:L:40:GLN:HB2	1.64	0.42
2:J:103:GLN:HB3	2:J:103:GLN:HE21	1.58	0.42
1:C:69:TYR:CD2	1:C:101:PHE:CD2	3.03	0.42
2:E:47:TRP:CZ2	2:E:93:ALA:HA	2.54	0.42
1:D:89:GLU:O	1:D:92:ILE:HG12	2.19	0.42
2:G:52:GLN:N	2:G:53:PRO:CD	2.82	0.42
2:E:33:GLU:H	2:E:52:GLN:NE2	2.05	0.42
2:L:25:GLU:O	2:L:28:LYS:HB3	2.20	0.42
2:F:39:ARG:HG3	2:F:107:VAL:HG12	2.02	0.42
1:C:69:TYR:OH	1:C:104:GLU:OE1	2.31	0.42
2:G:30:LEU:HD23	2:I:80:PHE:HE1	1.83	0.42
2:J:45:LEU:HD12	2:J:47:TRP:HE3	1.84	0.42
2:I:39:ARG:HG3	2:I:107:VAL:HG13	2.01	0.42
2:E:66:LEU:C	2:E:68:ASP:H	2.22	0.42
1:B:26:MET:HE3	1:B:154:LEU:HD13	2.01	0.42
2:E:72:GLY:HA2	2:F:40:GLN:OE1	2.19	0.42
1:B:149:PRO:O	1:B:152:TRP:HD1	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:39:ARG:HG3	2:F:108:ALA:CA	2.50	0.42
1:C:73:ASP:OD1	1:C:74:PRO:HD2	2.20	0.42
1:B:37:PHE:CE2	1:B:118:LEU:HD11	2.55	0.42
1:B:46:ASP:OD2	1:B:49:ASN:HB2	2.19	0.42
2:L:101:ARG:HD2	2:L:101:ARG:HA	1.81	0.42
1:D:116:MET:HA	1:D:117:PRO:HD3	1.95	0.42
2:K:57:LYS:O	2:K:61:GLN:HB2	2.20	0.42
2:H:105:ARG:NH2	4:H:201:HOH:O	2.06	0.42
1:A:62:GLU:HB3	1:A:66:ARG:HH21	1.85	0.42
2:J:107:VAL:C	2:J:109:ALA:H	2.23	0.42
1:D:152:TRP:CZ3	2:K:83:ASP:OD2	2.73	0.42
1:B:153:MET:O	1:B:154:LEU:C	2.59	0.42
1:C:52:ILE:HD11	3:C:201:OHN:H162	2.02	0.42
2:E:101:ARG:HD2	2:E:101:ARG:HA	1.80	0.41
2:E:39:ARG:O	2:E:41:PRO:CD	2.67	0.41
1:C:88:TRP:CZ3	1:C:131:SER:HB2	2.55	0.41
2:L:40:GLN:CG	2:L:41:PRO:HD2	2.33	0.41
2:J:107:VAL:O	2:J:109:ALA:N	2.52	0.41
2:J:55:ILE:O	2:J:59:VAL:HG23	2.20	0.41
2:K:42:GLY:O	2:K:43:LEU:CB	2.68	0.41
2:J:29:ASP:C	4:J:205:HOH:O	2.43	0.41
1:C:103:GLU:HG2	1:C:104:GLU:N	2.35	0.41
1:C:48:GLU:OE2	1:C:65:ASP:O	2.37	0.41
2:H:57:LYS:O	2:H:61:GLN:HB2	2.20	0.41
1:A:84:LEU:CD2	2:F:77:ALA:HA	2.50	0.41
2:F:43:LEU:HD22	2:F:44:SER:CA	2.50	0.41
2:E:71:GLU:HG3	2:F:107:VAL:HG22	2.03	0.41
2:E:101:ARG:NH1	2:E:105:ARG:HB2	2.32	0.41
1:A:92:ILE:HG12	4:A:321:HOH:O	2.08	0.41
1:C:10:LEU:HD13	1:C:22:ILE:CG2	2.51	0.41
1:C:126:GLY:HA2	3:C:201:OHN:H212	2.01	0.41
1:A:76:VAL:HG13	3:A:201:OHN:H201	2.02	0.41
2:I:69:GLN:HB3	2:I:70:ILE:H	1.48	0.41
2:F:65:TRP:CE3	2:F:74:LEU:HD13	2.56	0.41
2:E:94:PHE:CD1	2:E:94:PHE:C	2.94	0.41
2:K:52:GLN:N	2:K:53:PRO:CD	2.84	0.41
1:A:51:PHE:HB2	4:A:324:HOH:O	2.13	0.41
2:I:34:ILE:HD12	2:I:97:ALA:HA	2.03	0.41
1:A:74:PRO:HG2	1:A:93:TYR:CE1	2.55	0.41
2:F:69:GLN:NE2	4:F:207:HOH:O	2.53	0.41
2:H:98:PHE:CD1	2:H:98:PHE:C	2.94	0.41
2:H:36:PRO:HA	2:H:41:PRO:CA	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:39:ARG:CG	2:G:108:ALA:HB2	2.50	0.41
2:G:39:ARG:CZ	2:G:110:ARG:HB2	2.51	0.41
2:E:41:PRO:O	2:E:43:LEU:N	2.54	0.41
2:J:45:LEU:HA	2:J:45:LEU:HD22	1.85	0.41
2:H:45:LEU:HD12	2:H:45:LEU:HA	1.85	0.41
2:E:69:GLN:HB3	2:E:70:ILE:H	1.48	0.41
2:F:39:ARG:HE	2:F:108:ALA:CB	2.33	0.41
1:A:10:LEU:HD22	1:A:26:MET:CE	2.51	0.41
2:F:69:GLN:O	2:F:70:ILE:C	2.59	0.41
1:A:36:LEU:HD12	1:A:56:TYR:CD2	2.56	0.41
1:B:99:HIS:CE1	4:B:337:HOH:O	2.74	0.41
1:B:141:ASN:O	1:B:145:GLU:HB2	2.20	0.41
2:I:34:ILE:CD1	2:I:55:ILE:HG23	2.51	0.41
2:I:78:PHE:CG	2:J:99:LEU:HD11	2.56	0.41
2:F:39:ARG:NE	2:F:108:ALA:HA	2.36	0.41
2:F:42:GLY:O	2:F:43:LEU:HB3	2.20	0.40
2:F:43:LEU:HD21	2:F:45:LEU:N	2.36	0.40
1:B:17:LEU:C	1:B:17:LEU:HD23	2.42	0.40
2:G:39:ARG:O	2:G:41:PRO:N	2.54	0.40
3:C:201:OHN:H152	3:C:201:OHN:H182	1.31	0.40
2:F:34:ILE:HA	2:F:35:PRO:HD2	1.84	0.40
2:J:105:ARG:NH1	2:J:105:ARG:CG	2.54	0.40
2:H:102:LEU:HA	2:H:102:LEU:HD23	1.92	0.40
2:I:92:THR:HA	2:I:95:GLU:HG3	2.03	0.40
1:D:16:LYS:HE2	1:D:165:LEU:O	2.21	0.40
2:F:74:LEU:HD21	2:F:102:LEU:HD11	2.02	0.40
1:C:29:ASP:OD1	4:C:302:HOH:O	2.21	0.40
2:L:43:LEU:HD23	2:L:43:LEU:HA	1.92	0.40
2:G:107:VAL:HA	2:H:71:GLU:HG3	2.03	0.40
2:L:65:TRP:O	4:L:219:HOH:O	2.22	0.40
1:B:73:ASP:HA	1:B:74:PRO:HD3	1.90	0.40
2:I:106:LEU:HD23	2:I:106:LEU:C	2.41	0.40
1:D:133:GLU:HG3	4:D:301:HOH:O	2.22	0.40
2:J:34:ILE:H	2:J:43:LEU:CG	2.34	0.40
2:L:38:ASP:OD2	2:L:105:ARG:HG2	2.22	0.40
2:I:99:LEU:CD1	2:J:78:PHE:CG	3.05	0.40
1:C:63:HIS:ND1	1:C:63:HIS:C	2.75	0.40
1:A:136:ASN:ND2	1:A:138:ALA:HB3	2.37	0.40

All (1) 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	Distance(Å)	Clash(Å)
2:I:36:PRO:O	4:C:318:HOH:O[1_554]	1.92	0.28

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	164/184 (89%)	158 (96%)	6 (4%)	0	100	100
1	B	164/184 (89%)	157 (96%)	6 (4%)	1 (1%)	33	46
1	C	164/184 (89%)	154 (94%)	9 (6%)	1 (1%)	33	46
1	D	164/184 (89%)	158 (96%)	4 (2%)	2 (1%)	19	25
2	E	92/113 (81%)	75 (82%)	9 (10%)	8 (9%)	1	0
2	F	80/113 (71%)	66 (82%)	9 (11%)	5 (6%)	2	1
2	G	80/113 (71%)	64 (80%)	10 (12%)	6 (8%)	2	0
2	H	92/113 (81%)	75 (82%)	12 (13%)	5 (5%)	3	1
2	I	92/113 (81%)	73 (79%)	13 (14%)	6 (6%)	2	0
2	J	80/113 (71%)	55 (69%)	18 (22%)	7 (9%)	1	0
2	K	80/113 (71%)	75 (94%)	2 (2%)	3 (4%)	5	3
2	L	92/113 (81%)	85 (92%)	4 (4%)	3 (3%)	6	4
All	All	1344/1640 (82%)	1195 (89%)	102 (8%)	47 (4%)	6	4

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	46	ASP
1	D	47	TYR
2	E	41	PRO
2	E	42	GLY
2	E	69	GLN
2	E	70	ILE
2	E	71	GLU
2	F	41	PRO
2	F	67	ALA

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Mol	Chain	Res	Type
2	F	70	ILE
2	G	41	PRO
2	H	41	PRO
2	H	69	GLN
2	I	69	GLN
2	I	109	ALA
2	J	41	PRO
2	J	67	ALA
2	J	108	ALA
2	L	70	ILE
1	D	46	ASP
2	E	40	GLN
2	F	108	ALA
2	G	38	ASP
2	G	108	ALA
2	H	38	ASP
2	K	43	LEU
2	K	69	GLN
2	G	67	ALA
2	J	68	ASP
2	L	69	GLN
2	L	72	GLY
1	B	43	ASP
2	E	67	ALA
2	E	72	GLY
2	G	107	VAL
2	I	67	ALA
2	I	104	GLN
2	J	40	GLN
2	J	104	GLN
2	G	40	GLN
2	I	40	GLN
2	I	41	PRO
2	J	69	GLN
2	K	70	ILE
2	F	40	GLN
2	H	86	PRO
2	H	72	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	132/151 (87%)	119 (90%)	13 (10%)	12	16
1	B	132/151 (87%)	120 (91%)	12 (9%)	14	19
1	C	132/151 (87%)	117 (89%)	15 (11%)	8	11
1	D	132/151 (87%)	122 (92%)	10 (8%)	19	28
2	E	78/95 (82%)	67 (86%)	11 (14%)	5	6
2	F	67/95 (70%)	59 (88%)	8 (12%)	8	9
2	G	67/95 (70%)	61 (91%)	6 (9%)	14	20
2	H	78/95 (82%)	70 (90%)	8 (10%)	10	15
2	I	78/95 (82%)	63 (81%)	15 (19%)	2	2
2	J	67/95 (70%)	55 (82%)	12 (18%)	2	2
2	K	67/95 (70%)	61 (91%)	6 (9%)	14	20
2	L	78/95 (82%)	64 (82%)	14 (18%)	2	2
All	All	1108/1364 (81%)	978 (88%)	130 (12%)	8	10

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	26	MET
1	A	56	TYR
1	A	71	ARG
1	A	80	THR
1	A	92	ILE
1	A	95	THR
1	A	96	ARG
1	A	128	LEU
1	A	135	GLU
1	A	152	TRP
1	A	155	LYS
1	A	156	ASP
1	B	4	VAL
1	B	16	LYS

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Mol	Chain	Res	Type
1	B	43	ASP
1	B	45	GLN
1	B	91	SER
1	B	99	HIS
1	B	103	GLU
1	B	128	LEU
1	B	152	TRP
1	B	156	ASP
1	B	160	GLN
1	B	167	PHE
1	C	13	SER
1	C	14	SER
1	C	28	SER
1	C	35	ILE
1	C	46	ASP
1	C	48	GLU
1	C	80	THR
1	C	96	ARG
1	C	102	PHE
1	C	103	GLU
1	C	114	LEU
1	C	122	ARG
1	C	128	LEU
1	C	131	SER
1	C	152	TRP
1	D	12	ARG
1	D	20	SER
1	D	44	SER
1	D	122	ARG
1	D	128	LEU
1	D	136	ASN
1	D	137	ARG
1	D	152	TRP
1	D	155	LYS
1	D	167	PHE
2	E	18	THR
2	E	25	GLU
2	E	28	LYS
2	E	38	ASP
2	E	39	ARG
2	E	45	LEU
2	E	69	GLN

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Mol	Chain	Res	Type
2	E	73	GLN
2	E	105	ARG
2	E	107	VAL
2	E	110	ARG
2	F	30	LEU
2	F	38	ASP
2	F	43	LEU
2	F	45	LEU
2	F	57	LYS
2	F	68	ASP
2	F	89	MET
2	F	105	ARG
2	G	38	ASP
2	G	69	GLN
2	G	70	ILE
2	G	99	LEU
2	G	105	ARG
2	G	106	LEU
2	H	33	GLU
2	H	45	LEU
2	H	47	TRP
2	H	71	GLU
2	H	75	TRP
2	H	76	THR
2	H	80	PHE
2	H	110	ARG
2	I	17	LYS
2	I	25	GLU
2	I	26	ARG
2	I	28	LYS
2	I	31	MET
2	I	33	GLU
2	I	38	ASP
2	I	39	ARG
2	I	44	SER
2	I	45	LEU
2	I	71	GLU
2	I	100	THR
2	I	105	ARG
2	I	107	VAL
2	I	110	ARG
2	J	32	VAL

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Mol	Chain	Res	Type
2	J	38	ASP
2	J	39	ARG
2	J	43	LEU
2	J	45	LEU
2	J	55	ILE
2	J	57	LYS
2	J	68	ASP
2	J	69	GLN
2	J	100	THR
2	J	103	GLN
2	J	105	ARG
2	K	39	ARG
2	K	57	LYS
2	K	68	ASP
2	K	85	LEU
2	K	105	ARG
2	K	110	ARG
2	L	28	LYS
2	L	33	GLU
2	L	39	ARG
2	L	40	GLN
2	L	43	LEU
2	L	45	LEU
2	L	69	GLN
2	L	70	ILE
2	L	71	GLU
2	L	73	GLN
2	L	75	TRP
2	L	89	MET
2	L	105	ARG
2	L	110	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	99	HIS
1	A	136	ASN
1	B	24	GLN
1	B	45	GLN
1	B	136	ASN
1	C	24	GLN

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Mol	Chain	Res	Type
1	C	119	HIS
1	C	136	ASN
1	D	24	GLN
1	D	45	GLN
1	D	63	HIS
1	D	136	ASN
2	E	52	GLN
2	E	73	GLN
2	F	73	GLN
2	G	40	GLN
2	G	73	GLN
2	H	52	GLN
2	H	90	GLN
2	H	104	GLN
2	I	52	GLN
2	I	90	GLN
2	J	73	GLN
2	J	103	GLN
2	K	69	GLN
2	K	73	GLN
2	L	40	GLN
2	L	52	GLN
2	L	90	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	OHN	A	201	-	21,21,21	1.49	3 (14%)	25,25,25	2.53	4 (16%)
3	OHN	B	201	-	21,21,21	1.50	2 (9%)	25,25,25	1.76	4 (16%)
3	OHN	C	201	-	21,21,21	1.53	2 (9%)	25,25,25	1.69	4 (16%)
3	OHN	D	201	-	21,21,21	1.37	2 (9%)	25,25,25	1.54	3 (12%)

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
3	OHN	A	201	-	-	0/17/27/27	0/1/1/1
3	OHN	B	201	-	-	0/17/27/27	0/1/1/1
3	OHN	C	201	-	-	0/17/27/27	0/1/1/1
3	OHN	D	201	-	-	0/17/27/27	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	OHN	C8-N7	5.76	1.45	1.34
3	B	201	OHN	C8-N7	5.69	1.45	1.34
3	A	201	OHN	C8-N7	5.63	1.45	1.34
3	D	201	OHN	C8-N7	5.09	1.44	1.34
3	D	201	OHN	OAP-C4	-2.77	1.38	1.46
3	B	201	OHN	OAP-C4	-2.58	1.39	1.46
3	C	201	OHN	OAP-C4	-2.50	1.39	1.46
3	A	201	OHN	C1-C2	-2.20	1.46	1.52
3	A	201	OHN	OAP-C4	-2.20	1.40	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	OHN	OAP-C2-C1	-10.55	102.94	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	OHN	OAP-C2-C1	-5.75	106.35	110.43
3	D	201	OHN	OAP-C2-C1	-4.63	107.14	110.43
3	B	201	OHN	OAP-C2-O6	4.37	126.38	121.40
3	A	201	OHN	OAP-C2-O6	4.33	126.34	121.40
3	B	201	OHN	OAP-C2-C1	-3.95	107.63	110.43
3	B	201	OHN	C10-C8-N7	3.64	121.02	116.00
3	C	201	OHN	OAP-C2-O6	3.63	125.54	121.40
3	B	201	OHN	O9-C8-C10	-3.29	117.12	121.43
3	D	201	OHN	OAP-C2-O6	2.84	124.64	121.40
3	A	201	OHN	C4-OAP-C2	-2.81	108.12	110.52
3	D	201	OHN	C14-C13-C11	-2.65	107.96	114.86
3	A	201	OHN	C14-C13-C11	-2.50	108.33	114.86
3	C	201	OHN	C10-C8-N7	2.35	119.24	116.00
3	C	201	OHN	O9-C8-C10	-2.28	118.44	121.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	166/184 (90%)	0.05	5 (3%) 48 45	22, 47, 77, 104	0
1	B	166/184 (90%)	-0.04	0 100 100	21, 39, 70, 102	0
1	C	166/184 (90%)	0.35	10 (6%) 21 18	26, 54, 97, 134	0
1	D	166/184 (90%)	-0.08	4 (2%) 56 53	17, 34, 69, 161	0
2	E	94/113 (83%)	0.16	5 (5%) 25 23	25, 45, 95, 130	0
2	F	82/113 (72%)	0.33	6 (7%) 15 13	27, 46, 109, 157	0
2	G	82/113 (72%)	0.54	6 (7%) 15 13	35, 55, 106, 144	0
2	H	94/113 (83%)	0.47	9 (9%) 8 7	32, 58, 108, 174	0
2	I	94/113 (83%)	0.69	8 (8%) 11 9	32, 60, 104, 182	0
2	J	82/113 (72%)	1.14	12 (14%) 3 2	43, 73, 120, 181	0
2	K	82/113 (72%)	0.00	1 (1%) 75 75	19, 31, 64, 189	0
2	L	94/113 (83%)	-0.03	6 (6%) 19 17	22, 36, 89, 179	0
All	All	1368/1640 (83%)	0.24	72 (5%) 26 23	17, 46, 99, 189	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	70	ILE	9.9
2	J	44	SER	9.4
2	J	40	GLN	8.9
2	I	70	ILE	8.4
2	J	110	ARG	7.6
2	G	43	LEU	6.5
2	F	44	SER	6.2
2	L	70	ILE	5.9
2	H	72	GLY	5.9
2	I	40	GLN	5.4
2	H	69	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
2	J	70	ILE	5.1
2	F	40	GLN	5.1
2	J	30	LEU	5.1
2	I	72	GLY	4.8
2	K	69	GLN	4.8
2	J	69	GLN	4.6
2	G	69	GLN	4.5
2	E	70	ILE	4.4
2	I	42	GLY	4.4
2	F	43	LEU	4.3
2	E	40	GLN	4.3
1	C	96	ARG	4.0
2	J	43	LEU	3.9
1	D	48	GLU	3.8
1	C	49	ASN	3.6
1	C	69	TYR	3.5
2	J	39	ARG	3.4
2	G	40	GLN	3.4
2	I	102	LEU	3.4
2	G	39	ARG	3.3
2	H	39	ARG	3.3
2	F	110	ARG	3.3
2	H	71	GLU	3.3
2	E	72	GLY	3.2
2	G	70	ILE	3.1
2	L	40	GLN	3.1
2	H	80	PHE	3.1
2	L	39	ARG	3.1
1	D	96	ARG	3.1
1	C	97	LYS	3.0
1	D	49	ASN	2.9
2	I	69	GLN	2.9
2	L	69	GLN	2.9
2	F	68	ASP	2.7
2	I	77	ALA	2.7
2	G	110	ARG	2.7
2	I	107	VAL	2.7
1	A	47	TYR	2.6
1	A	92	ILE	2.6
2	E	69	GLN	2.5
1	C	103	GLU	2.5
1	D	43	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	70	ILE	2.4
2	J	60	ARG	2.4
2	J	34	ILE	2.3
2	H	105	ARG	2.3
1	C	43	ASP	2.3
1	A	167	PHE	2.3
2	J	32	VAL	2.2
2	H	37	ALA	2.2
1	C	48	GLU	2.2
1	C	98	GLN	2.2
1	A	96	ARG	2.2
1	C	71	ARG	2.2
2	L	25	GLU	2.2
2	L	72	GLY	2.2
1	C	66	ARG	2.1
1	A	2	ALA	2.1
2	H	41	PRO	2.1
2	E	37	ALA	2.1
2	J	47	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	OHN	B	201	21/21	0.18	1.90	29,37,41,45	0
3	OHN	C	201	21/21	0.24	1.64	46,54,59,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	OHN	A	201	21/21	0.19	0.80	29,38,42,45	0
3	OHN	D	201	21/21	0.15	0.36	19,28,32,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.