Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2021 – 11:32 PM EDT

PDB ID	:	3E74
Title	:	Crystal structure of E. coli allantoinase with iron ions at the metal center
Authors	:	Kim, K.
Deposited on	:	2008-08-17
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

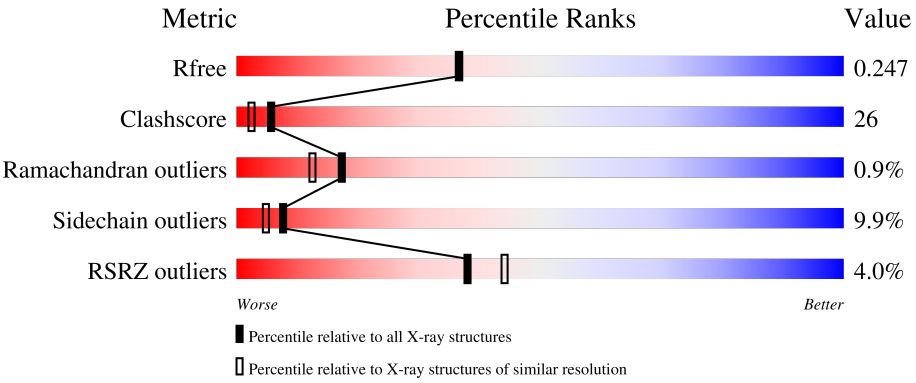
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	473	3% 53% 30% 7% 9%
1	B	473	3% 61% 26% • 8%
1	C	473	3% 61% 24% 5% 10%
1	D	473	6% 55% 29% 7% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14068 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 Allantoinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	Se	0	0	0
			3290	2073	569	625	11	12			
1	B	433	Total	C	N	O	S	Se	0	0	0
			3329	2098	576	632	11	12			
1	C	428	Total	C	N	O	S	Se	0	0	0
			3286	2071	568	624	11	12			
1	D	429	Total	C	N	O	S	Se	0	0	0
			3290	2073	569	625	11	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP P77671
A	-18	GLY	-	expression tag	UNP P77671
A	-17	SER	-	expression tag	UNP P77671
A	-16	SER	-	expression tag	UNP P77671
A	-15	HIS	-	expression tag	UNP P77671
A	-14	HIS	-	expression tag	UNP P77671
A	-13	HIS	-	expression tag	UNP P77671
A	-12	HIS	-	expression tag	UNP P77671
A	-11	HIS	-	expression tag	UNP P77671
A	-10	SER	-	expression tag	UNP P77671
A	-9	SER	-	expression tag	UNP P77671
A	-8	GLY	-	expression tag	UNP P77671
A	-7	GLU	-	expression tag	UNP P77671
A	-6	ASN	-	expression tag	UNP P77671
A	-5	LEU	-	expression tag	UNP P77671
A	-4	TYR	-	expression tag	UNP P77671
A	-3	PHE	-	expression tag	UNP P77671
A	-2	GLN	-	expression tag	UNP P77671
A	-1	GLY	-	expression tag	UNP P77671
A	0	HIS	-	expression tag	UNP P77671
A	262	ILE	VAL	engineered mutation	UNP P77671

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MSE	-	expression tag	UNP P77671
B	-18	GLY	-	expression tag	UNP P77671
B	-17	SER	-	expression tag	UNP P77671
B	-16	SER	-	expression tag	UNP P77671
B	-15	HIS	-	expression tag	UNP P77671
B	-14	HIS	-	expression tag	UNP P77671
B	-13	HIS	-	expression tag	UNP P77671
B	-12	HIS	-	expression tag	UNP P77671
B	-11	HIS	-	expression tag	UNP P77671
B	-10	SER	-	expression tag	UNP P77671
B	-9	SER	-	expression tag	UNP P77671
B	-8	GLY	-	expression tag	UNP P77671
B	-7	GLU	-	expression tag	UNP P77671
B	-6	ASN	-	expression tag	UNP P77671
B	-5	LEU	-	expression tag	UNP P77671
B	-4	TYR	-	expression tag	UNP P77671
B	-3	PHE	-	expression tag	UNP P77671
B	-2	GLN	-	expression tag	UNP P77671
B	-1	GLY	-	expression tag	UNP P77671
B	0	HIS	-	expression tag	UNP P77671
B	262	ILE	VAL	engineered mutation	UNP P77671
C	-19	MSE	-	expression tag	UNP P77671
C	-18	GLY	-	expression tag	UNP P77671
C	-17	SER	-	expression tag	UNP P77671
C	-16	SER	-	expression tag	UNP P77671
C	-15	HIS	-	expression tag	UNP P77671
C	-14	HIS	-	expression tag	UNP P77671
C	-13	HIS	-	expression tag	UNP P77671
C	-12	HIS	-	expression tag	UNP P77671
C	-11	HIS	-	expression tag	UNP P77671
C	-10	SER	-	expression tag	UNP P77671
C	-9	SER	-	expression tag	UNP P77671
C	-8	GLY	-	expression tag	UNP P77671
C	-7	GLU	-	expression tag	UNP P77671
C	-6	ASN	-	expression tag	UNP P77671
C	-5	LEU	-	expression tag	UNP P77671
C	-4	TYR	-	expression tag	UNP P77671
C	-3	PHE	-	expression tag	UNP P77671
C	-2	GLN	-	expression tag	UNP P77671
C	-1	GLY	-	expression tag	UNP P77671
C	0	HIS	-	expression tag	UNP P77671
C	262	ILE	VAL	engineered mutation	UNP P77671

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MSE	-	expression tag	UNP P77671
D	-18	GLY	-	expression tag	UNP P77671
D	-17	SER	-	expression tag	UNP P77671
D	-16	SER	-	expression tag	UNP P77671
D	-15	HIS	-	expression tag	UNP P77671
D	-14	HIS	-	expression tag	UNP P77671
D	-13	HIS	-	expression tag	UNP P77671
D	-12	HIS	-	expression tag	UNP P77671
D	-11	HIS	-	expression tag	UNP P77671
D	-10	SER	-	expression tag	UNP P77671
D	-9	SER	-	expression tag	UNP P77671
D	-8	GLY	-	expression tag	UNP P77671
D	-7	GLU	-	expression tag	UNP P77671
D	-6	ASN	-	expression tag	UNP P77671
D	-5	LEU	-	expression tag	UNP P77671
D	-4	TYR	-	expression tag	UNP P77671
D	-3	PHE	-	expression tag	UNP P77671
D	-2	GLN	-	expression tag	UNP P77671
D	-1	GLY	-	expression tag	UNP P77671
D	0	HIS	-	expression tag	UNP P77671
D	262	ILE	VAL	engineered mutation	UNP P77671

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	232	Total O 232 232	0	0
3	B	255	Total O 255 255	0	0
3	C	219	Total O 219 219	0	0

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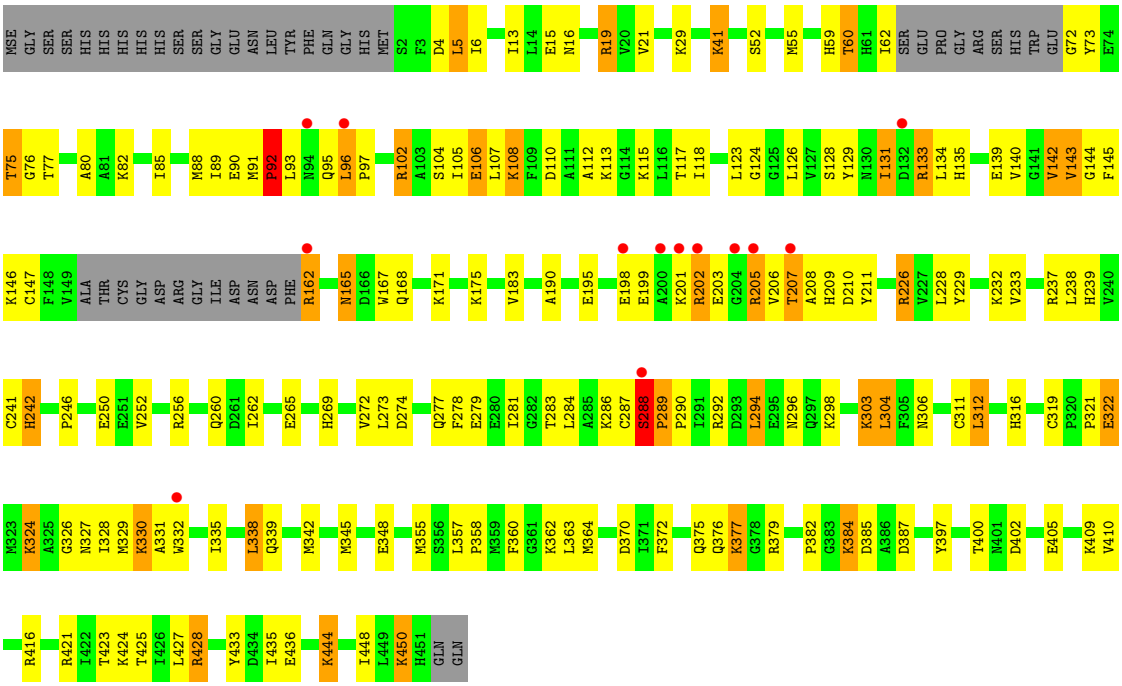
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	159	Total	O	0	0
			159	159		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

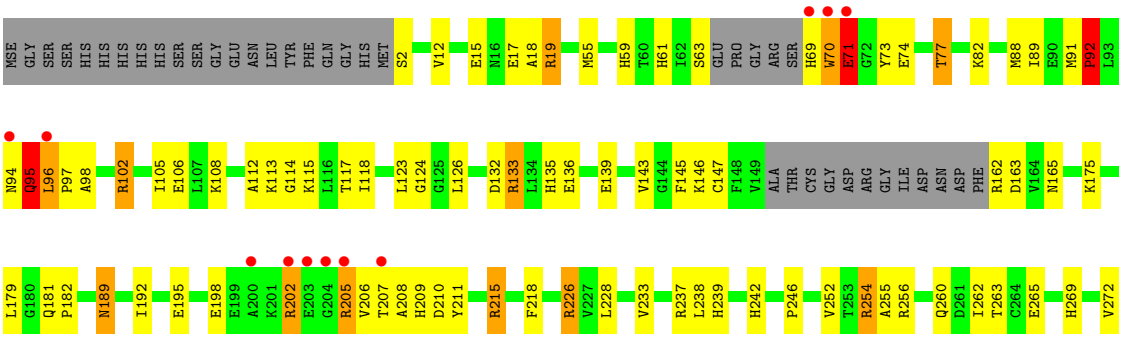
• Molecule 1: Allantoinase

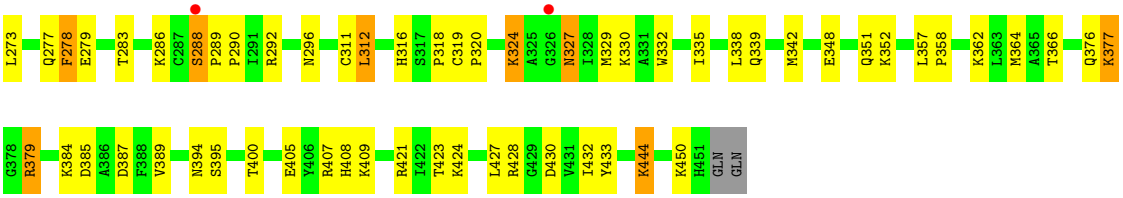
Chain A:



• Molecule 1: Allantoinase

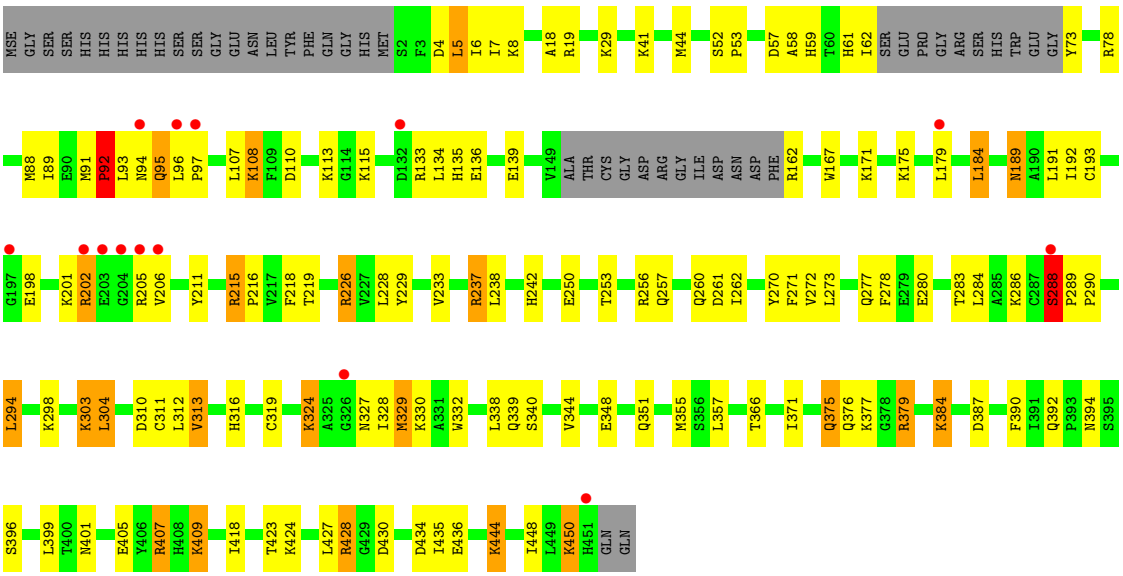
Chain B:





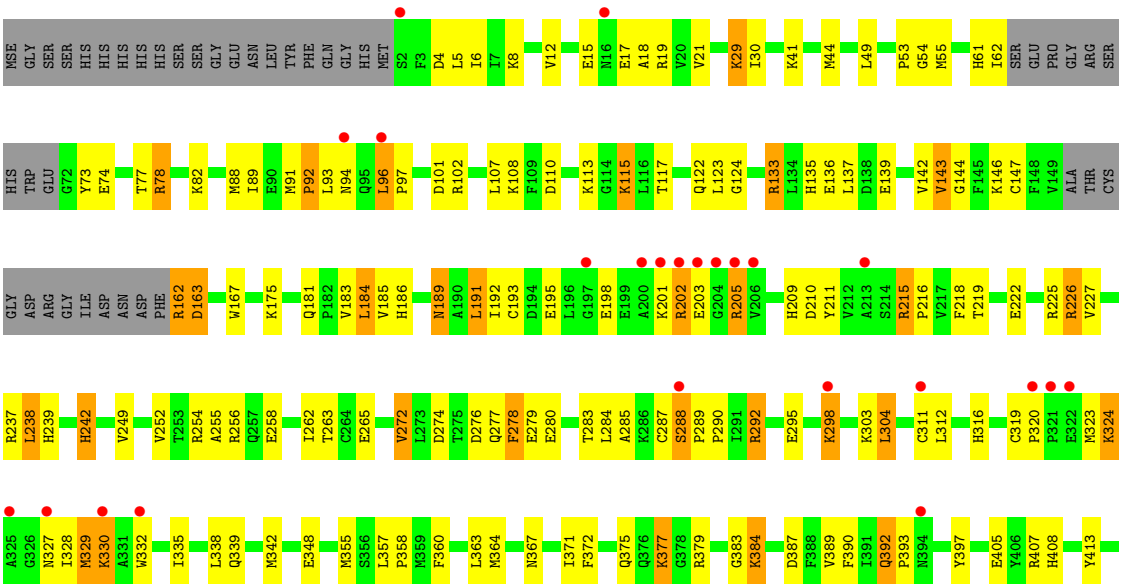
• Molecule 1: Allantoinase

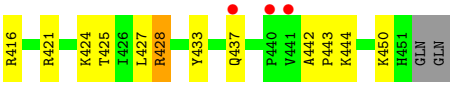
Chain C:



• Molecule 1: Allantoinase

Chain D:




R416
R421
K424
T425
I426
L427
R428
Y433
Q437
P440
V441
A442
P443
K444
K450
H461
GLN
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.68Å 92.45Å 168.43Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 42.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	79.3 (50.00-2.10) 97.2 (42.49-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.240 0.210 , 0.247	Depositor DCC
R_{free} test set	14820 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14068	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.45	0/3323	0.76	2/4467 (0.0%)
1	B	0.46	0/3365	0.76	0/4525
1	C	0.44	0/3319	0.77	1/4462 (0.0%)
1	D	0.42	0/3323	0.73	1/4467 (0.0%)
All	All	0.44	0/13330	0.75	4/17921 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	238	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	289	PRO	N-CA-C	-5.53	97.72	112.10
1	C	288	SER	C-N-CD	5.50	139.94	128.40
1	A	288	SER	C-N-CD	5.18	139.28	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3290	0	3271	213	0
1	B	3329	0	3299	153	0
1	C	3286	0	3268	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3290	0	3271	192	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	232	0	0	12	0
3	B	255	0	0	5	0
3	C	219	0	0	5	0
3	D	159	0	0	10	0
All	All	14068	0	13109	671	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (671) 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:D:320:PRO:HG2	1:D:323:MSE:HG3	1.33	1.09
1:A:77:THR:HG22	1:A:117:THR:HB	1.34	1.06
1:B:102:ARG:HB2	1:B:102:ARG:HH11	1.18	1.01
1:D:272:VAL:HG22	1:D:416:ARG:HH22	1.23	1.00
1:D:320:PRO:HD2	1:D:323:MSE:HE2	1.41	0.98
1:A:77:THR:HG21	1:A:117:THR:H	1.28	0.97
1:B:77:THR:HG23	1:B:117:THR:HB	1.46	0.96
1:D:216:PRO:O	1:D:219:THR:HG22	1.64	0.96
1:A:205:ARG:HH11	1:A:205:ARG:HB2	1.30	0.96
1:D:108:LYS:HZ1	1:D:122:GLN:HE22	1.05	0.96
1:C:95:GLN:H	1:C:95:GLN:HE21	1.03	0.95
1:D:108:LYS:NZ	1:D:122:GLN:HE22	1.65	0.95
1:D:238:LEU:HB3	1:D:262:ILE:HG22	1.49	0.94
1:C:351:GLN:HE22	1:C:394:ASN:H	1.13	0.94
1:A:312:LEU:HD21	1:A:345:MSE:HE2	1.49	0.92
1:C:95:GLN:H	1:C:95:GLN:NE2	1.67	0.92
1:D:215:ARG:HG3	1:D:215:ARG:HH11	1.33	0.92
1:B:351:GLN:HE22	1:B:394:ASN:H	1.15	0.90
1:D:203:GLU:HB2	1:D:205:ARG:HD3	1.53	0.90
1:B:77:THR:HG21	1:B:117:THR:H	1.37	0.88
1:A:205:ARG:HH11	1:A:205:ARG:CB	1.86	0.88
1:B:423:THR:O	1:B:424:LYS:HD2	1.73	0.88
1:C:44:MSE:HE3	1:C:424:LYS:NZ	1.88	0.87
1:A:77:THR:HG23	1:A:118:ILE:HG12	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:HG21	1:A:117:THR:N	1.88	0.87
1:A:288:SER:HB3	1:A:289:PRO:HD3	1.57	0.86
1:D:91:MSE:SE	1:D:146:KCX:HG2	2.25	0.85
1:D:201:LYS:HE2	1:D:330:LYS:HE2	1.57	0.84
1:A:339:GLN:HE22	1:A:405:GLU:H	1.22	0.84
1:B:288:SER:HB3	1:B:289:PRO:HD3	1.59	0.82
1:C:5:LEU:HD22	1:C:6:ILE:N	1.95	0.81
1:B:324:LYS:HE3	1:B:332:TRP:O	1.79	0.81
1:C:198:GLU:O	1:C:202:ARG:HD3	1.80	0.81
1:D:342:MSE:HE2	1:D:342:MSE:HA	1.61	0.81
1:A:162:ARG:N	1:A:162:ARG:NE	2.28	0.81
1:A:400:THR:HG22	1:A:402:ASP:H	1.45	0.80
1:B:77:THR:CG2	1:B:117:THR:H	1.95	0.80
1:B:71:GLU:HG3	1:B:318:PRO:HG3	1.63	0.80
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.45	0.79
1:A:4:ASP:HA	1:A:41:LYS:HD3	1.65	0.79
1:A:165:ASN:ND2	1:A:168:GLN:H	1.80	0.79
1:A:327:ASN:H	1:A:330:LYS:CE	1.95	0.79
1:D:342:MSE:HE1	1:D:364:MSE:CG	2.13	0.79
1:A:113:LYS:HD2	3:A:680:HOH:O	1.81	0.78
1:B:70:TRP:HB2	1:B:320:PRO:HG3	1.65	0.78
1:C:407:ARG:HH11	1:C:407:ARG:HB2	1.48	0.78
1:A:91:MSE:SE	1:A:146:KCX:HG2	2.33	0.78
1:A:226:ARG:HE	1:D:226:ARG:HE	1.29	0.78
1:B:207:THR:HB	1:B:210:ASP:OD2	1.84	0.78
1:D:295:GLU:O	1:D:298:LYS:HG3	1.84	0.78
1:A:342:MSE:HE1	1:A:364:MSE:CG	2.14	0.78
1:B:206:VAL:HG23	1:B:329:MSE:HG2	1.64	0.78
1:C:29:LYS:HE2	1:C:376:GLN:NE2	1.99	0.77
1:D:133:ARG:HG2	1:D:133:ARG:HH11	1.47	0.77
1:A:326:GLY:HA3	1:A:330:LYS:HE3	1.66	0.77
1:A:377:LYS:HE3	1:A:385:ASP:OD2	1.84	0.77
1:C:226:ARG:HG2	1:C:226:ARG:HH11	1.49	0.77
1:C:19:ARG:HG2	1:C:19:ARG:HH11	1.49	0.77
1:C:324:LYS:HE3	1:C:332:TRP:O	1.85	0.77
1:A:312:LEU:HD22	1:A:364:MSE:HE1	1.66	0.77
1:B:377:LYS:HE3	1:B:385:ASP:OD2	1.85	0.77
1:C:44:MSE:HE3	1:C:424:LYS:HZ3	1.50	0.76
1:C:201:LYS:HD2	1:C:329:MSE:HG2	1.68	0.76
1:A:62:ILE:HG12	1:A:88:MSE:HE1	1.68	0.76
1:D:288:SER:HB2	1:D:289:PRO:HD3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:CD	1:A:379:ARG:HD3	2.06	0.75
1:D:96:LEU:HB2	1:D:97:PRO:CD	2.16	0.75
1:A:135:HIS:O	1:A:139:GLU:HG3	1.87	0.75
1:A:72:GLY:HA3	3:A:678:HOH:O	1.86	0.74
1:B:88:MSE:HE2	1:B:118:ILE:HD11	1.68	0.74
1:A:228:LEU:HD22	1:A:262:ILE:HD13	1.68	0.74
1:D:237:ARG:NH2	1:D:371:ILE:O	2.21	0.74
1:B:430:ASP:HB2	1:B:444:LYS:NZ	2.02	0.73
1:D:342:MSE:HE1	1:D:364:MSE:SE	2.38	0.73
1:D:17:GLU:OE2	1:D:19:ARG:HD2	1.88	0.73
1:A:162:ARG:N	1:A:162:ARG:HE	1.86	0.73
1:D:226:ARG:HG2	1:D:226:ARG:HH11	1.52	0.73
1:B:339:GLN:HE22	1:B:405:GLU:H	1.37	0.73
1:A:273:LEU:HA	1:A:277:GLN:NE2	2.04	0.73
1:D:215:ARG:HH11	1:D:215:ARG:CG	2.02	0.73
1:A:232:LYS:HD3	1:A:260:GLN:HG2	1.71	0.73
1:A:327:ASN:H	1:A:330:LYS:HE3	1.52	0.73
1:A:326:GLY:CA	1:A:330:LYS:HE3	2.19	0.73
1:A:250:GLU:HG3	1:A:303:LYS:NZ	2.03	0.72
1:A:60:THR:HG21	1:A:88:MSE:HB2	1.72	0.72
1:D:73:TYR:O	1:D:77:THR:HG22	1.90	0.72
1:A:274:ASP:H	1:A:277:GLN:HE21	1.37	0.72
1:A:342:MSE:HA	1:A:342:MSE:HE2	1.70	0.72
1:A:312:LEU:CD2	1:A:345:MSE:HE2	2.20	0.72
1:B:102:ARG:HH12	1:B:136:GLU:HG2	1.55	0.72
1:C:5:LEU:HD22	1:C:6:ILE:H	1.55	0.71
1:A:284:LEU:HD11	1:A:410:VAL:HG22	1.71	0.71
1:C:201:LYS:HD2	1:C:329:MSE:CG	2.21	0.71
1:C:288:SER:HB3	1:C:289:PRO:CD	2.20	0.71
1:A:423:THR:HG22	1:A:424:LYS:HD3	1.72	0.71
1:D:272:VAL:CG2	1:D:416:ARG:HH22	2.02	0.71
1:A:96:LEU:HB2	1:A:97:PRO:HD2	1.70	0.71
1:C:95:GLN:HE21	1:C:95:GLN:N	1.84	0.71
1:A:77:THR:CG2	1:A:117:THR:HB	2.19	0.70
1:D:312:LEU:HD23	1:D:363:LEU:HB3	1.72	0.70
1:B:226:ARG:HH11	1:B:226:ARG:HG2	1.56	0.70
1:B:206:VAL:HG21	1:B:327:ASN:CG	2.12	0.70
1:D:5:LEU:CD1	1:D:44:MSE:HE3	2.22	0.69
1:C:250:GLU:HG3	1:C:303:LYS:NZ	2.07	0.69
1:D:324:LYS:HE3	1:D:332:TRP:O	1.92	0.69
1:B:61:HIS:HD1	1:B:94:ASN:ND2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LYS:HD2	1:D:433:TYR:CE1	2.28	0.69
1:B:207:THR:HG23	1:B:279:GLU:OE1	1.93	0.69
1:A:205:ARG:HB3	1:A:210:ASP:CG	2.13	0.68
1:B:342:MSE:HE2	1:B:389:VAL:HG11	1.75	0.68
1:A:324:LYS:HE2	1:A:332:TRP:O	1.91	0.68
1:B:77:THR:HG23	1:B:117:THR:CB	2.20	0.68
1:A:207:THR:HG22	1:A:209:HIS:N	2.08	0.68
1:C:238:LEU:HB3	1:C:262:ILE:HD12	1.76	0.68
1:D:115:LYS:HD2	1:D:115:LYS:N	2.09	0.68
1:B:288:SER:O	1:B:289:PRO:C	2.30	0.68
1:D:444:LYS:HE3	3:D:532:HOH:O	1.94	0.68
1:A:207:THR:HG23	1:A:279:GLU:OE1	1.94	0.68
1:A:327:ASN:N	1:A:330:LYS:HE3	2.09	0.68
1:D:146:KCX:HZ	1:D:186:HIS:HB2	1.58	0.68
1:D:272:VAL:HG22	1:D:416:ARG:NH2	2.04	0.67
1:A:288:SER:HB3	1:A:289:PRO:CD	2.25	0.67
1:A:377:LYS:HE2	1:A:387:ASP:OD2	1.93	0.67
1:B:73:TYR:O	1:B:77:THR:HB	1.94	0.67
1:B:206:VAL:HG23	1:B:329:MSE:CG	2.25	0.67
1:C:189:ASN:HD22	1:C:192:ILE:H	1.43	0.67
1:B:102:ARG:O	1:B:106:GLU:HG3	1.95	0.67
1:B:254:ARG:HG3	1:B:255:ALA:N	2.09	0.67
1:B:288:SER:HB3	1:B:289:PRO:CD	2.25	0.67
1:A:207:THR:HG22	1:A:209:HIS:H	1.60	0.66
1:D:189:ASN:HD22	1:D:192:ILE:H	1.40	0.66
1:B:342:MSE:CE	1:B:389:VAL:HG11	2.26	0.66
1:D:5:LEU:HD11	1:D:44:MSE:HE3	1.76	0.66
1:D:108:LYS:NZ	1:D:122:GLN:NE2	2.42	0.66
1:C:44:MSE:HE2	1:C:390:PHE:CE2	2.31	0.66
1:C:250:GLU:HG3	1:C:303:LYS:HZ1	1.58	0.66
1:C:407:ARG:HD2	3:C:687:HOH:O	1.96	0.66
1:C:57:ASP:OD1	1:C:313:VAL:HG22	1.96	0.66
1:D:276:ASP:O	1:D:280:GLU:HG3	1.96	0.66
1:D:252:VAL:O	1:D:256:ARG:HG3	1.95	0.66
1:D:55:MSE:SE	1:D:342:MSE:HE3	2.47	0.65
1:A:96:LEU:HB2	1:A:97:PRO:CD	2.26	0.65
1:A:102:ARG:HD2	1:A:106:GLU:OE2	1.95	0.65
1:A:423:THR:O	1:A:424:LYS:HD2	1.97	0.65
1:B:63:SER:HB2	1:B:71:GLU:N	2.10	0.65
1:B:377:LYS:HE2	1:B:387:ASP:OD2	1.97	0.65
1:C:96:LEU:HB2	1:C:97:PRO:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:TYR:OH	1:C:289:PRO:HG2	1.96	0.65
1:A:339:GLN:HE22	1:A:405:GLU:N	1.95	0.65
1:C:304:LEU:HD13	1:C:355:MSE:HE1	1.79	0.65
1:D:54:GLY:HA2	1:D:389:VAL:HG23	1.78	0.64
1:A:165:ASN:C	1:A:165:ASN:HD22	2.01	0.64
1:C:272:VAL:HG12	1:C:348:GLU:HG2	1.80	0.64
1:A:370:ASP:OD1	1:A:379:ARG:NH2	2.28	0.64
1:A:55:MSE:SE	1:A:342:MSE:HE3	2.47	0.64
1:B:102:ARG:HH11	1:B:102:ARG:CB	2.02	0.64
1:C:226:ARG:HG2	1:C:226:ARG:NH1	2.12	0.64
1:A:250:GLU:HG3	1:A:303:LYS:HZ3	1.63	0.63
1:C:193:CYS:SG	1:C:215:ARG:NH1	2.71	0.63
1:D:96:LEU:HB2	1:D:97:PRO:HD2	1.81	0.63
1:D:201:LYS:HE2	1:D:330:LYS:CE	2.29	0.63
1:A:85:ILE:HD12	1:A:338:LEU:CD2	2.28	0.63
1:A:272:VAL:CG2	1:A:348:GLU:HG3	2.29	0.63
1:B:283:THR:O	1:B:324:LYS:HE2	1.99	0.63
1:D:189:ASN:ND2	1:D:192:ILE:H	1.97	0.63
1:A:274:ASP:N	1:A:277:GLN:HE21	1.97	0.63
1:A:316:HIS:CG	1:A:338:LEU:HB2	2.34	0.63
1:B:444:LYS:NZ	3:B:878:HOH:O	2.32	0.63
1:C:4:ASP:HA	1:C:41:LYS:HD3	1.80	0.63
1:A:102:ARG:NH1	1:A:140:VAL:HG23	2.14	0.62
1:A:239:HIS:HE1	1:A:265:GLU:OE1	1.82	0.62
1:B:61:HIS:HB2	1:B:316:HIS:O	1.99	0.62
1:B:319:CYS:HB2	1:B:332:TRP:CZ3	2.34	0.62
1:B:145:PHE:CE1	1:B:181:GLN:HG2	2.34	0.62
1:D:288:SER:HB2	1:D:289:PRO:CD	2.29	0.62
1:A:105:ILE:O	1:A:108:LYS:HB3	1.99	0.62
1:C:215:ARG:HG3	1:C:215:ARG:HH11	1.65	0.62
1:D:328:ILE:HD12	1:D:328:ILE:H	1.63	0.62
1:B:102:ARG:HB2	1:B:102:ARG:NH1	2.03	0.62
1:D:226:ARG:HG2	1:D:226:ARG:NH1	2.15	0.62
1:A:228:LEU:CD2	1:A:262:ILE:HD13	2.29	0.62
1:D:19:ARG:HG3	1:D:21:VAL:HG13	1.82	0.62
1:A:339:GLN:NE2	1:A:405:GLU:H	1.96	0.61
1:A:29:LYS:HE2	1:A:385:ASP:OD1	2.00	0.61
1:B:430:ASP:HB2	1:B:444:LYS:HZ1	1.64	0.61
1:A:400:THR:HG22	1:A:402:ASP:N	2.15	0.61
1:B:102:ARG:HB3	3:B:899:HOH:O	1.99	0.61
1:D:142:VAL:HG12	1:D:144:GLY:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:THR:HG22	1:A:424:LYS:CD	2.31	0.60
1:D:203:GLU:HB2	1:D:205:ARG:CD	2.29	0.60
1:D:427:LEU:HD13	1:D:428:ARG:HB2	1.81	0.60
1:B:252:VAL:O	1:B:256:ARG:HG3	2.00	0.60
1:D:4:ASP:HA	1:D:41:LYS:HD3	1.83	0.60
1:A:312:LEU:HD23	1:A:345:MSE:HG3	1.82	0.60
1:C:29:LYS:HE2	1:C:376:GLN:HE21	1.65	0.60
1:A:238:LEU:HD13	1:A:238:LEU:C	2.22	0.60
1:C:423:THR:O	1:C:424:LYS:HD2	2.01	0.60
1:A:165:ASN:HD21	1:A:168:GLN:H	1.50	0.60
1:D:198:GLU:O	1:D:202:ARG:HD3	2.00	0.60
1:A:59:HIS:CG	1:A:91:MSE:HE3	2.36	0.60
1:A:342:MSE:HE1	1:A:364:MSE:SE	2.51	0.60
1:D:272:VAL:HG23	1:D:348:GLU:HG3	1.84	0.60
1:D:375:GLN:O	1:D:384:LYS:HE2	2.01	0.60
1:A:450:LYS:HE2	3:A:620:HOH:O	2.01	0.60
1:C:351:GLN:HE22	1:C:394:ASN:N	1.93	0.60
1:B:15:GLU:CD	1:B:379:ARG:HE	2.05	0.60
1:D:183:VAL:HG13	1:D:238:LEU:HD23	1.84	0.59
1:C:238:LEU:HB3	1:C:262:ILE:CD1	2.31	0.59
1:B:239:HIS:HD2	1:B:263:THR:OG1	1.85	0.59
1:C:288:SER:O	1:C:290:PRO:N	2.36	0.59
1:B:366:THR:HG23	1:B:379:ARG:HD3	1.85	0.59
1:C:189:ASN:ND2	1:C:192:ILE:HG13	2.16	0.59
1:D:162:ARG:HG2	1:D:162:ARG:HH11	1.67	0.59
1:D:437:GLN:O	1:D:437:GLN:HG2	2.03	0.59
1:B:182:PRO:HB3	1:B:237:ARG:HG2	1.84	0.59
1:D:239:HIS:HD2	1:D:263:THR:OG1	1.86	0.59
1:C:351:GLN:NE2	1:C:394:ASN:H	1.94	0.59
1:A:77:THR:CG2	1:A:117:THR:H	2.09	0.59
1:A:95:GLN:O	1:A:96:LEU:O	2.20	0.59
1:D:255:ALA:HB3	1:D:262:ILE:HD11	1.83	0.59
1:A:88:MSE:HE2	1:A:90:GLU:HB2	1.85	0.58
1:A:19:ARG:HD3	1:A:21:VAL:HG13	1.86	0.58
1:A:342:MSE:HE1	1:A:364:MSE:HG3	1.85	0.58
1:C:288:SER:O	1:C:289:PRO:C	2.38	0.58
1:D:53:PRO:O	1:D:387:ASP:O	2.21	0.58
1:A:77:THR:HG22	1:A:117:THR:CB	2.23	0.58
1:A:206:VAL:HA	1:A:329:MSE:HG2	1.86	0.58
1:A:96:LEU:HA	3:A:682:HOH:O	2.04	0.58
1:A:233:VAL:HG11	1:D:218:PHE:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLN:OE1	1:A:262:ILE:HD11	2.03	0.58
1:B:73:TYR:CE2	1:B:112:ALA:HB2	2.39	0.58
1:C:62:ILE:HD11	1:C:88:MSE:SE	2.54	0.58
1:B:91:MSE:SE	1:B:146:KCX:HE3	2.53	0.57
1:D:328:ILE:HD12	1:D:328:ILE:N	2.19	0.57
1:A:85:ILE:HD12	1:A:338:LEU:HD23	1.86	0.57
1:A:274:ASP:OD1	1:A:277:GLN:HG3	2.05	0.57
1:A:427:LEU:HD23	1:A:444:LYS:HD2	1.85	0.57
1:D:205:ARG:HB3	1:D:210:ASP:CG	2.24	0.57
1:A:207:THR:CG2	1:A:209:HIS:H	2.18	0.57
1:D:133:ARG:HG2	1:D:133:ARG:NH1	2.15	0.57
1:A:62:ILE:CG1	1:A:88:MSE:HE1	2.35	0.57
1:B:237:ARG:HG3	1:B:238:LEU:N	2.20	0.57
1:D:49:LEU:HD13	1:D:390:PHE:HB3	1.87	0.57
1:A:211:TYR:CE1	1:A:286:LYS:HE3	2.39	0.57
1:A:283:THR:HG22	1:A:328:ILE:HD13	1.86	0.57
1:B:133:ARG:HG2	1:B:133:ARG:HH11	1.69	0.57
1:A:312:LEU:CD2	1:A:364:MSE:HE1	2.35	0.57
1:B:198:GLU:O	1:B:202:ARG:HD3	2.05	0.57
1:B:206:VAL:CG2	1:B:327:ASN:HB2	2.34	0.57
1:D:407:ARG:HB3	3:D:557:HOH:O	2.04	0.57
1:B:272:VAL:CG1	1:B:348:GLU:HG3	2.35	0.56
1:D:288:SER:CB	1:D:289:PRO:HD3	2.35	0.56
1:C:277:GLN:HA	1:C:280:GLU:HG2	1.87	0.56
1:C:428:ARG:HG2	1:C:428:ARG:HH11	1.70	0.56
1:D:342:MSE:HE1	1:D:364:MSE:HG3	1.87	0.56
1:A:19:ARG:HD3	1:A:21:VAL:CG1	2.35	0.56
1:A:92:PRO:HG2	1:A:93:LEU:H	1.70	0.56
1:D:29:LYS:HD2	1:D:30:ILE:O	2.05	0.56
1:C:19:ARG:HG2	1:C:19:ARG:NH1	2.15	0.56
1:D:97:PRO:HG3	1:D:107:LEU:HD12	1.86	0.56
1:D:249:VAL:HG11	1:D:303:LYS:HG3	1.87	0.56
1:A:232:LYS:HD3	1:A:260:GLN:CG	2.36	0.56
1:B:432:ILE:CG2	1:B:444:LYS:HE2	2.36	0.56
1:C:260:GLN:HG2	1:C:262:ILE:HG12	1.86	0.56
1:D:397:TYR:HB3	1:D:421:ARG:NH1	2.21	0.56
1:B:207:THR:HG22	1:B:210:ASP:H	1.71	0.56
1:C:58:ALA:HA	1:C:89:ILE:HB	1.88	0.56
1:A:327:ASN:H	1:A:330:LYS:HE2	1.67	0.56
1:C:189:ASN:ND2	1:C:192:ILE:H	2.03	0.56
1:C:5:LEU:HD11	1:C:7:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:HH11	1:A:428:ARG:HG2	1.71	0.55
1:C:206:VAL:HB	1:C:327:ASN:HD22	1.71	0.55
1:D:162:ARG:HD2	1:D:162:ARG:N	2.21	0.55
1:A:327:ASN:N	1:A:330:LYS:CE	2.67	0.55
1:D:249:VAL:HG11	1:D:303:LYS:CG	2.37	0.55
1:D:339:GLN:HE22	1:D:405:GLU:N	2.05	0.55
1:A:60:THR:CG2	1:A:88:MSE:HB2	2.36	0.55
1:A:205:ARG:HB2	1:A:205:ARG:NH1	2.12	0.55
1:D:242:HIS:ND1	1:D:289:PRO:HG2	2.22	0.55
1:D:272:VAL:CG2	1:D:348:GLU:HG3	2.37	0.55
1:D:407:ARG:HH11	1:D:407:ARG:HG2	1.69	0.55
1:C:316:HIS:CG	1:C:338:LEU:HB2	2.41	0.55
1:A:238:LEU:HD12	1:A:262:ILE:HG23	1.89	0.55
1:B:316:HIS:CG	1:B:338:LEU:HB2	2.41	0.55
1:C:256:ARG:NH2	1:C:310:ASP:OD2	2.39	0.55
1:D:82:LYS:HD2	1:D:433:TYR:CZ	2.41	0.55
1:B:207:THR:HG22	1:B:209:HIS:N	2.22	0.55
1:B:430:ASP:HB2	1:B:444:LYS:HZ3	1.71	0.55
1:C:167:TRP:CZ2	1:C:171:LYS:HD3	2.42	0.54
1:D:201:LYS:CE	1:D:330:LYS:HE2	2.31	0.54
1:C:135:HIS:HD2	1:C:139:GLU:OE2	1.90	0.54
1:C:366:THR:HG23	1:C:379:ARG:HD3	1.88	0.54
1:A:377:LYS:NZ	1:A:448:ILE:HD11	2.21	0.54
1:C:430:ASP:HB2	1:C:444:LYS:HE2	1.90	0.54
1:A:89:ILE:HG22	1:A:123:LEU:HG	1.89	0.54
1:A:190:ALA:HB3	3:A:635:HOH:O	2.07	0.54
1:B:206:VAL:HG21	1:B:327:ASN:CB	2.38	0.54
1:C:44:MSE:HE2	1:C:390:PHE:HE2	1.71	0.54
1:A:226:ARG:NE	1:D:226:ARG:HE	2.03	0.54
1:B:82:LYS:HG3	1:B:433:TYR:CZ	2.42	0.54
1:A:288:SER:O	1:A:289:PRO:C	2.43	0.54
1:A:324:LYS:CE	1:A:332:TRP:O	2.54	0.54
1:B:239:HIS:HE1	1:B:265:GLU:OE1	1.91	0.54
1:B:288:SER:O	1:B:290:PRO:N	2.41	0.54
1:D:225:ARG:NH1	3:D:520:HOH:O	2.36	0.54
1:A:75:THR:HG22	1:A:76:GLY:N	2.23	0.54
1:B:206:VAL:HG21	1:B:327:ASN:HB2	1.89	0.54
1:D:254:ARG:O	1:D:258:GLU:HG3	2.08	0.54
1:B:319:CYS:HB2	1:B:332:TRP:CE3	2.44	0.53
1:D:413:TYR:O	1:D:416:ARG:HB3	2.09	0.53
1:D:319:CYS:HB2	1:D:323:MSE:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:HD22	1:A:6:ILE:N	2.24	0.53
1:B:195:GLU:HG3	1:C:167:TRP:CG	2.44	0.53
1:B:206:VAL:O	1:B:206:VAL:HG22	2.08	0.53
1:C:423:THR:HA	1:C:435:ILE:HB	1.89	0.53
1:A:167:TRP:HB2	1:D:191:LEU:HD13	1.91	0.53
1:D:327:ASN:HD21	1:D:330:LYS:HD3	1.74	0.53
1:A:342:MSE:HE1	1:A:364:MSE:HB3	1.90	0.53
1:C:94:ASN:HB3	1:C:95:GLN:NE2	2.24	0.53
1:A:207:THR:HB	1:A:210:ASP:OD2	2.09	0.52
1:A:397:TYR:CG	1:A:421:ARG:NH1	2.77	0.52
1:C:237:ARG:NH2	1:C:371:ILE:O	2.38	0.52
1:D:256:ARG:HG2	1:D:262:ILE:HG13	1.92	0.52
1:A:16:ASN:HB3	1:B:15:GLU:OE2	2.09	0.52
1:A:77:THR:CG2	1:A:118:ILE:H	2.23	0.52
1:A:238:LEU:HD13	1:A:239:HIS:N	2.23	0.52
1:A:284:LEU:HD11	1:A:410:VAL:CG2	2.39	0.52
1:A:102:ARG:NE	3:A:679:HOH:O	2.43	0.52
1:A:133:ARG:HG2	1:A:133:ARG:HH11	1.74	0.52
1:D:54:GLY:HA2	1:D:389:VAL:CG2	2.39	0.52
1:D:108:LYS:HZ1	1:D:122:GLN:NE2	1.89	0.52
1:D:239:HIS:HE1	1:D:265:GLU:OE1	1.93	0.52
1:C:133:ARG:O	1:C:136:GLU:HB2	2.09	0.52
1:C:303:LYS:HE2	3:C:689:HOH:O	2.10	0.52
1:B:63:SER:CB	1:B:71:GLU:N	2.72	0.52
1:A:202:ARG:HH11	1:A:202:ARG:HG2	1.75	0.52
1:D:288:SER:O	1:D:289:PRO:C	2.43	0.52
1:A:102:ARG:CZ	3:A:579:HOH:O	2.57	0.52
1:B:327:ASN:ND2	1:B:330:LYS:H	2.08	0.52
1:A:202:ARG:HG2	1:A:202:ARG:NH1	2.24	0.52
1:B:189:ASN:ND2	1:B:192:ILE:H	2.08	0.51
1:A:59:HIS:CD2	1:A:91:MSE:HE3	2.45	0.51
1:A:110:ASP:HA	1:A:113:LYS:HD3	1.92	0.51
1:C:401:ASN:ND2	3:C:598:HOH:O	2.42	0.51
1:D:342:MSE:HE1	1:D:364:MSE:HB3	1.93	0.51
1:D:215:ARG:CG	1:D:215:ARG:NH1	2.67	0.51
1:A:80:ALA:HA	1:A:338:LEU:HD22	1.91	0.51
1:A:319:CYS:HG	1:A:332:TRP:HE3	1.57	0.51
1:B:215:ARG:HH11	1:B:215:ARG:CG	2.18	0.51
1:D:316:HIS:CG	1:D:338:LEU:HB2	2.46	0.51
1:C:327:ASN:OD1	1:C:330:LYS:HD3	2.11	0.51
1:D:202:ARG:HD3	1:D:202:ARG:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HD12	1:A:175:LYS:HG2	1.92	0.51
1:A:421:ARG:NH2	1:A:435:ILE:HD11	2.26	0.51
1:A:129:TYR:HE1	1:A:162:ARG:HD2	1.74	0.51
1:C:59:HIS:CG	1:C:91:MSE:HE3	2.46	0.51
1:A:384:LYS:HE3	1:B:17:GLU:OE2	2.11	0.51
1:C:96:LEU:CB	1:C:97:PRO:HD3	2.40	0.51
1:C:434:ASP:OD1	1:C:436:GLU:HB2	2.10	0.51
1:D:209:HIS:HD2	1:D:279:GLU:OE1	1.94	0.51
1:D:428:ARG:HG2	3:D:576:HOH:O	2.10	0.50
1:A:342:MSE:HE1	1:A:364:MSE:CB	2.42	0.50
1:D:283:THR:O	1:D:324:LYS:HE2	2.12	0.50
1:D:339:GLN:HE22	1:D:405:GLU:H	1.58	0.50
1:A:126:LEU:HB3	1:A:147:CYS:HB3	1.94	0.50
1:B:162:ARG:NE	1:B:162:ARG:HA	2.26	0.50
1:D:304:LEU:HD21	1:D:363:LEU:HD13	1.94	0.50
1:D:428:ARG:HG2	1:D:428:ARG:HH11	1.76	0.50
1:B:189:ASN:HD22	1:B:192:ILE:H	1.59	0.50
1:B:395:SER:OG	1:B:421:ARG:HD2	2.10	0.50
1:C:284:LEU:HD23	1:C:324:LYS:HG2	1.93	0.50
1:D:135:HIS:O	1:D:139:GLU:HG3	2.11	0.50
1:A:195:GLU:HG3	1:D:167:TRP:CG	2.47	0.50
1:C:110:ASP:O	1:C:113:LYS:HB2	2.11	0.50
1:D:319:CYS:HB3	1:D:332:TRP:CZ3	2.46	0.50
1:A:294:LEU:HD22	1:A:298:LYS:CD	2.42	0.50
1:A:428:ARG:HG2	3:A:571:HOH:O	2.12	0.50
1:C:6:ILE:HG22	1:C:8:LYS:HD2	1.93	0.50
1:B:256:ARG:HG2	1:B:262:ILE:HG12	1.94	0.50
1:B:71:GLU:HG3	1:B:318:PRO:CG	2.36	0.49
1:B:357:LEU:N	1:B:358:PRO:HD2	2.27	0.49
1:C:377:LYS:NZ	1:C:448:ILE:HD11	2.27	0.49
1:B:269:HIS:CG	1:B:335:ILE:HD12	2.47	0.49
1:B:272:VAL:HG12	1:B:348:GLU:HG3	1.93	0.49
1:C:184:LEU:N	1:C:184:LEU:HD23	2.27	0.49
1:C:201:LYS:HD2	1:C:329:MSE:HG3	1.94	0.49
1:D:407:ARG:HG2	1:D:407:ARG:NH1	2.27	0.49
1:A:124:GLY:O	1:A:145:PHE:HA	2.12	0.49
1:A:198:GLU:O	1:A:202:ARG:HB2	2.11	0.49
1:B:59:HIS:CG	1:B:91:MSE:HE3	2.47	0.49
1:C:44:MSE:HE3	1:C:424:LYS:HZ2	1.69	0.49
1:B:226:ARG:HG2	1:B:226:ARG:NH1	2.26	0.49
1:A:131:ILE:HD12	1:A:131:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:HIS:HD2	1:A:279:GLU:OE1	1.95	0.49
1:D:143:VAL:CG2	1:D:372:PHE:O	2.60	0.49
1:B:77:THR:HG21	1:B:117:THR:N	2.16	0.49
1:B:82:LYS:HG3	1:B:433:TYR:CE1	2.47	0.49
1:B:273:LEU:HA	1:B:277:GLN:OE1	2.12	0.49
1:C:409:LYS:HD2	1:C:409:LYS:N	2.26	0.49
1:D:320:PRO:CD	1:D:323:MSE:HE2	2.29	0.49
1:A:269:HIS:HD2	3:A:472:HOH:O	1.94	0.49
1:C:175:LYS:HE2	1:C:179:LEU:HD11	1.95	0.49
1:C:407:ARG:HB2	1:C:407:ARG:NH1	2.21	0.49
1:D:107:LEU:HD13	1:D:107:LEU:C	2.32	0.49
1:A:92:PRO:HG2	1:A:93:LEU:HD13	1.95	0.49
1:D:328:ILE:H	1:D:328:ILE:CD1	2.25	0.49
1:D:330:LYS:HD2	1:D:330:LYS:N	2.28	0.49
1:A:102:ARG:NH1	1:A:102:ARG:HB2	2.28	0.49
1:D:146:KCX:HD2	1:D:147:CYS:N	2.27	0.49
1:D:288:SER:CB	1:D:289:PRO:CD	2.91	0.49
1:B:162:ARG:HA	1:B:162:ARG:HE	1.77	0.48
1:C:211:TYR:CE1	1:C:286:LYS:HE3	2.47	0.48
1:C:229:TYR:O	1:C:233:VAL:HG23	2.13	0.48
1:D:96:LEU:CB	1:D:97:PRO:CD	2.89	0.48
1:A:5:LEU:CD2	1:A:6:ILE:N	2.75	0.48
1:D:185:VAL:HG11	1:D:227:VAL:HG21	1.95	0.48
1:D:319:CYS:SG	1:D:324:LYS:HD3	2.52	0.48
1:D:392:GLN:NE2	1:D:393:PRO:O	2.46	0.48
1:A:376:GLN:NE2	3:A:548:HOH:O	2.45	0.48
1:B:77:THR:CG2	1:B:117:THR:HB	2.32	0.48
1:B:96:LEU:O	1:B:98:ALA:N	2.47	0.48
1:C:339:GLN:HE22	1:C:405:GLU:H	1.62	0.48
1:D:162:ARG:HG2	1:D:162:ARG:NH1	2.29	0.48
1:D:342:MSE:HE1	1:D:364:MSE:CB	2.43	0.48
1:B:70:TRP:HA	1:B:70:TRP:CE3	2.48	0.48
1:B:376:GLN:C	1:B:377:LYS:HD2	2.33	0.48
1:C:201:LYS:CE	1:C:329:MSE:HG3	2.44	0.48
1:C:206:VAL:HB	1:C:327:ASN:ND2	2.28	0.48
1:D:205:ARG:HG2	1:D:205:ARG:HH11	1.78	0.48
1:A:96:LEU:CB	1:A:97:PRO:CD	2.92	0.48
1:A:286:LYS:NZ	1:A:331:ALA:O	2.47	0.48
1:D:397:TYR:CG	1:D:421:ARG:NH1	2.82	0.48
1:A:416:ARG:HG2	1:A:416:ARG:HH11	1.78	0.48
1:A:382:PRO:O	1:B:19:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ILE:HG22	1:B:123:LEU:HG	1.95	0.47
1:A:143:VAL:HG22	1:A:372:PHE:O	2.14	0.47
1:A:102:ARG:O	1:A:106:GLU:HB2	2.14	0.47
1:B:132:ASP:OD2	1:B:133:ARG:HD3	2.14	0.47
1:B:145:PHE:HE1	1:B:181:GLN:HG2	1.76	0.47
1:B:233:VAL:HG11	1:C:218:PHE:CD2	2.50	0.47
1:C:107:LEU:C	1:C:107:LEU:HD13	2.35	0.47
1:D:62:ILE:CD1	1:D:88:MSE:HE1	2.44	0.47
1:A:283:THR:CG2	1:A:328:ILE:HD13	2.44	0.47
1:C:328:ILE:HG12	3:C:640:HOH:O	2.14	0.47
1:D:215:ARG:HB3	1:D:290:PRO:HG3	1.96	0.47
1:A:284:LEU:CD1	1:A:410:VAL:HG22	2.41	0.47
1:B:2:SER:HB3	3:B:829:HOH:O	2.14	0.47
1:A:77:THR:HG21	1:A:118:ILE:H	1.79	0.47
1:A:427:LEU:O	1:A:444:LYS:HE3	2.14	0.47
1:B:94:ASN:OD1	1:B:95:GLN:NE2	2.48	0.47
1:B:133:ARG:HG2	1:B:133:ARG:NH1	2.29	0.47
1:B:260:GLN:HG2	1:B:262:ILE:HG23	1.96	0.47
1:C:61:HIS:HB2	1:C:316:HIS:O	2.15	0.47
1:D:74:GLU:HA	3:D:546:HOH:O	2.14	0.47
1:D:319:CYS:HG	1:D:332:TRP:HE3	1.63	0.47
1:A:15:GLU:OE2	1:A:379:ARG:HD3	2.14	0.47
1:A:133:ARG:HG2	1:A:133:ARG:NH1	2.30	0.47
1:A:304:LEU:HD13	1:A:355:MSE:HE1	1.96	0.47
1:A:319:CYS:HB3	1:A:332:TRP:CZ3	2.50	0.46
1:D:5:LEU:HG	1:D:6:ILE:N	2.30	0.46
1:D:407:ARG:HG3	1:D:408:HIS:CD2	2.51	0.46
1:D:425:THR:HB	1:D:433:TYR:HB3	1.95	0.46
1:A:13:ILE:HD12	1:A:52:SER:HB2	1.96	0.46
1:B:211:TYR:CE1	1:B:286:LYS:HE3	2.50	0.46
1:A:250:GLU:HG3	1:A:303:LYS:HZ1	1.79	0.46
1:A:294:LEU:HD22	1:A:298:LYS:HD3	1.97	0.46
1:B:339:GLN:HE22	1:B:405:GLU:N	2.09	0.46
1:A:73:TYR:CE2	1:A:112:ALA:HB2	2.51	0.46
1:A:183:VAL:HG13	1:A:238:LEU:HD23	1.97	0.46
1:A:199:GLU:HG2	1:A:203:GLU:OE2	2.15	0.46
1:D:29:LYS:HD2	1:D:30:ILE:C	2.36	0.46
1:D:339:GLN:NE2	1:D:405:GLU:H	2.14	0.46
1:A:435:ILE:HG23	1:A:436:GLU:HG3	1.98	0.46
1:D:93:LEU:O	1:D:94:ASN:HB2	2.16	0.46
1:D:252:VAL:HG12	1:D:256:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TRP:CZ2	1:A:171:LYS:HD3	2.51	0.46
1:A:195:GLU:HG3	1:D:167:TRP:CD1	2.51	0.46
1:B:278:PHE:HD1	1:B:278:PHE:O	1.99	0.46
1:C:215:ARG:HB3	1:C:290:PRO:HG3	1.97	0.46
1:C:253:THR:O	1:C:257:GLN:HG3	2.16	0.46
1:D:442:ALA:HB1	1:D:443:PRO:HD2	1.97	0.46
1:A:252:VAL:O	1:A:256:ARG:HG3	2.16	0.46
1:B:226:ARG:HE	1:C:226:ARG:HH21	1.64	0.46
1:B:423:THR:C	1:B:424:LYS:HD2	2.35	0.46
1:D:82:LYS:HG2	1:D:339:GLN:CD	2.36	0.46
1:D:201:LYS:HD2	1:D:329:MSE:HG3	1.98	0.46
1:D:367:ASN:O	1:D:371:ILE:HG13	2.16	0.46
1:B:207:THR:CG2	1:B:208:ALA:N	2.79	0.45
1:A:77:THR:CG2	1:A:118:ILE:N	2.80	0.45
1:B:105:ILE:HG13	1:B:108:LYS:NZ	2.30	0.45
1:B:206:VAL:HG21	1:B:327:ASN:ND2	2.30	0.45
1:D:89:ILE:HG22	1:D:123:LEU:HG	1.97	0.45
1:D:312:LEU:HG	1:D:364:MSE:HE1	1.98	0.45
1:B:379:ARG:HB3	1:B:384:LYS:HG3	1.97	0.45
1:D:77:THR:HG23	1:D:117:THR:HB	1.98	0.45
1:C:57:ASP:OD1	1:C:313:VAL:CG2	2.65	0.45
1:A:357:LEU:N	1:A:358:PRO:HD2	2.31	0.45
1:B:255:ALA:HB3	1:B:262:ILE:CD1	2.46	0.45
1:D:319:CYS:HB2	1:D:323:MSE:HE3	1.99	0.45
1:D:74:GLU:O	1:D:78:ARG:HB2	2.16	0.45
1:D:298:LYS:HD2	1:D:298:LYS:C	2.37	0.45
1:D:427:LEU:HD13	1:D:427:LEU:C	2.36	0.45
1:A:226:ARG:HG2	1:A:226:ARG:HH11	1.80	0.45
1:B:246:PRO:HD2	1:B:296:ASN:ND2	2.31	0.45
1:C:273:LEU:HA	1:C:277:GLN:OE1	2.17	0.45
1:C:327:ASN:HD21	1:C:329:MSE:CB	2.30	0.45
1:A:102:ARG:HB2	1:A:102:ARG:HH11	1.81	0.45
1:A:107:LEU:C	1:A:107:LEU:HD13	2.37	0.45
1:C:201:LYS:HE3	1:C:329:MSE:HG3	1.99	0.45
1:C:216:PRO:HG2	1:C:219:THR:HG23	1.99	0.45
1:A:206:VAL:HA	1:A:329:MSE:CG	2.47	0.45
1:B:269:HIS:CD2	1:B:335:ILE:HD12	2.52	0.45
1:D:107:LEU:HD13	1:D:107:LEU:O	2.17	0.45
1:D:304:LEU:HD13	1:D:355:MSE:HE1	1.98	0.45
1:B:432:ILE:HG21	1:B:444:LYS:HE2	1.98	0.44
1:C:134:LEU:HD12	1:C:175:LYS:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:CG2	3:A:460:HOH:O	2.65	0.44
1:B:278:PHE:CD1	1:B:278:PHE:C	2.89	0.44
1:C:59:HIS:N	1:C:313:VAL:CG2	2.81	0.44
1:C:288:SER:HB3	1:C:289:PRO:HD2	1.99	0.44
1:C:215:ARG:HG2	1:C:290:PRO:HD3	1.98	0.44
1:D:201:LYS:HD2	1:D:329:MSE:CG	2.47	0.44
1:A:246:PRO:HD2	1:A:296:ASN:ND2	2.32	0.44
1:B:74:GLU:HG3	1:B:115:LYS:HG3	1.99	0.44
1:D:312:LEU:CD2	1:D:363:LEU:HB3	2.44	0.44
1:B:77:THR:CG2	1:B:117:THR:CB	2.92	0.44
1:D:77:THR:HG21	1:D:117:THR:H	1.82	0.44
1:D:357:LEU:N	1:D:358:PRO:HD2	2.33	0.44
1:B:312:LEU:HD12	1:B:312:LEU:HA	1.82	0.44
1:D:189:ASN:HD21	1:D:191:LEU:HB3	1.83	0.44
1:B:145:PHE:CD1	1:B:181:GLN:HG2	2.53	0.44
1:C:202:ARG:NH1	1:C:202:ARG:HG2	2.33	0.44
1:D:427:LEU:HD11	1:D:428:ARG:NH2	2.33	0.44
1:A:277:GLN:O	1:A:281:ILE:HG13	2.18	0.44
1:B:15:GLU:CD	1:B:379:ARG:NE	2.71	0.44
1:B:63:SER:HB2	1:B:71:GLU:H	1.80	0.44
1:B:70:TRP:HB3	1:B:408:HIS:HE1	1.82	0.44
1:B:272:VAL:HG11	1:B:348:GLU:HG3	1.99	0.44
1:B:427:LEU:HD23	1:B:444:LYS:HD2	1.99	0.44
1:C:93:LEU:HB3	1:C:162:ARG:HD2	1.99	0.44
1:D:284:LEU:HD12	1:D:324:LYS:HG2	2.00	0.44
1:C:52:SER:OG	1:C:53:PRO:HD2	2.18	0.44
1:C:211:TYR:CZ	1:C:286:LYS:HE3	2.52	0.44
1:C:384:LYS:HD2	1:C:384:LYS:N	2.32	0.44
1:A:321:PRO:HG2	1:A:322:GLU:OE2	2.18	0.43
1:B:96:LEU:HB3	1:B:97:PRO:CD	2.48	0.43
1:C:327:ASN:ND2	1:C:329:MSE:HB2	2.32	0.43
1:D:162:ARG:HB2	1:D:163:ASP:H	1.53	0.43
1:A:92:PRO:HG2	1:A:93:LEU:CD1	2.48	0.43
1:A:102:ARG:NH1	1:A:140:VAL:CG2	2.81	0.43
1:A:205:ARG:HH11	1:A:205:ARG:CG	2.30	0.43
1:D:5:LEU:HD13	1:D:44:MSE:HE3	1.97	0.43
1:A:92:PRO:HG2	1:A:93:LEU:N	2.33	0.43
1:B:126:LEU:HB3	1:B:147:CYS:HB3	2.01	0.43
1:B:215:ARG:HB3	1:B:290:PRO:HG3	2.00	0.43
1:D:397:TYR:CB	1:D:421:ARG:NH1	2.81	0.43
1:A:428:ARG:HH11	1:A:428:ARG:CG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:THR:O	1:C:286:LYS:HB3	2.18	0.43
1:D:29:LYS:HD3	1:D:383:GLY:HA2	2.01	0.43
1:D:184:LEU:N	1:D:184:LEU:HD23	2.34	0.43
1:D:292:ARG:HG3	3:D:621:HOH:O	2.18	0.43
1:A:41:LYS:H	1:A:41:LYS:HD2	1.82	0.43
1:A:288:SER:O	1:A:290:PRO:N	2.51	0.43
1:D:287:CYS:HB3	1:D:335:ILE:HG13	1.99	0.43
1:A:229:TYR:O	1:A:232:LYS:HB3	2.19	0.43
1:B:113:LYS:HD2	1:B:114:GLY:N	2.33	0.43
1:B:175:LYS:HE2	1:B:179:LEU:HG	2.01	0.43
1:B:424:LYS:HD3	3:B:708:HOH:O	2.18	0.43
1:C:428:ARG:HH11	1:C:428:ARG:CG	2.32	0.43
1:D:392:GLN:HE21	1:D:392:GLN:C	2.22	0.43
1:A:128:SER:HB2	1:A:168:GLN:NE2	2.34	0.42
1:A:167:TRP:CG	1:D:195:GLU:HG3	2.54	0.42
1:A:198:GLU:O	1:A:202:ARG:HD3	2.19	0.42
1:A:273:LEU:HA	1:A:277:GLN:HE22	1.78	0.42
1:B:55:MSE:HG3	1:B:364:MSE:O	2.19	0.42
1:B:61:HIS:HD1	1:B:94:ASN:HD22	1.65	0.42
1:D:61:HIS:HB2	1:D:316:HIS:O	2.19	0.42
1:A:304:LEU:HD21	1:A:363:LEU:HD13	2.01	0.42
1:A:425:THR:HB	1:A:433:TYR:HB3	2.00	0.42
1:B:195:GLU:HG3	1:C:167:TRP:CD1	2.54	0.42
1:D:15:GLU:OE2	1:D:379:ARG:NE	2.45	0.42
1:D:428:ARG:HH11	1:D:428:ARG:CG	2.32	0.42
1:A:112:ALA:O	1:A:115:LYS:HB2	2.19	0.42
1:B:228:LEU:HD23	1:B:238:LEU:HD23	2.02	0.42
1:D:205:ARG:HB3	1:D:210:ASP:OD2	2.19	0.42
1:A:203:GLU:HB2	1:A:205:ARG:HD3	2.02	0.42
1:A:370:ASP:CG	1:A:379:ARG:HH22	2.21	0.42
1:B:63:SER:HB2	1:B:71:GLU:CA	2.48	0.42
1:B:215:ARG:HG3	1:B:215:ARG:NH1	2.22	0.42
1:B:218:PHE:CD2	1:C:233:VAL:HG11	2.55	0.42
1:C:73:TYR:N	3:C:554:HOH:O	2.52	0.42
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.81	0.42
1:B:63:SER:HB2	1:B:71:GLU:C	2.39	0.42
1:B:143:VAL:C	1:B:181:GLN:NE2	2.73	0.42
1:A:75:THR:CG2	1:A:76:GLY:N	2.82	0.42
1:B:61:HIS:ND1	1:B:94:ASN:ND2	2.64	0.42
1:C:377:LYS:CE	1:C:387:ASP:OD2	2.67	0.42
1:D:184:LEU:HD22	1:D:239:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:TYR:HD1	1:D:329:MSE:HE1	1.84	0.42
1:B:77:THR:CG2	1:B:117:THR:N	2.74	0.42
1:B:165:ASN:CG	1:C:191:LEU:HD21	2.40	0.42
1:C:261:ASP:O	1:C:262:ILE:HD13	2.19	0.42
1:D:73:TYR:O	1:D:77:THR:CG2	2.66	0.42
1:A:142:VAL:HG13	1:A:144:GLY:H	1.84	0.42
1:A:269:HIS:CD2	1:A:269:HIS:H	2.37	0.42
1:C:277:GLN:HA	1:C:280:GLU:CG	2.49	0.42
1:D:124:GLY:N	1:D:142:VAL:HG11	2.35	0.42
1:A:327:ASN:OD1	1:A:330:LYS:HG3	2.20	0.41
1:B:255:ALA:HB3	1:B:262:ILE:HD11	2.02	0.41
1:C:18:ALA:HB2	1:C:357:LEU:HB2	2.02	0.41
1:A:142:VAL:CG1	1:A:144:GLY:H	2.33	0.41
1:A:207:THR:CG2	1:A:208:ALA:N	2.83	0.41
1:B:69:HIS:N	1:B:320:PRO:HD3	2.34	0.41
1:C:59:HIS:N	1:C:313:VAL:HG21	2.35	0.41
1:C:319:CYS:SG	1:C:324:LYS:HD3	2.60	0.41
1:D:225:ARG:NH1	3:D:480:HOH:O	2.47	0.41
1:A:286:LYS:HD3	1:A:328:ILE:HG23	2.03	0.41
1:B:206:VAL:CG2	1:B:329:MSE:HG2	2.42	0.41
1:C:424:LYS:HE2	1:C:434:ASP:OD2	2.19	0.41
1:D:255:ALA:HB3	1:D:262:ILE:CD1	2.49	0.41
1:A:237:ARG:HD3	3:A:569:HOH:O	2.20	0.41
1:B:278:PHE:O	1:B:278:PHE:CD1	2.73	0.41
1:D:360:PHE:O	1:D:364:MSE:HG2	2.21	0.41
1:D:377:LYS:HD2	1:D:377:LYS:N	2.36	0.41
1:A:82:LYS:HG3	1:A:433:TYR:CZ	2.55	0.41
1:A:242:HIS:ND1	1:A:289:PRO:HG2	2.35	0.41
1:A:316:HIS:CD2	1:A:338:LEU:HD12	2.56	0.41
1:A:360:PHE:O	1:A:364:MSE:HG2	2.20	0.41
1:B:71:GLU:CG	1:B:318:PRO:HG3	2.42	0.41
1:C:427:LEU:O	1:C:444:LYS:HE3	2.21	0.41
1:D:143:VAL:HG22	1:D:372:PHE:O	2.20	0.41
1:D:324:LYS:NZ	3:D:577:HOH:O	2.51	0.41
1:B:12:VAL:O	1:B:18:ALA:HA	2.20	0.41
1:B:92:PRO:HB3	1:B:123:LEU:O	2.20	0.41
1:D:92:PRO:HG2	1:D:93:LEU:H	1.86	0.41
1:D:274:ASP:OD1	1:D:277:GLN:HG3	2.21	0.41
1:D:278:PHE:CD1	1:D:285:ALA:HB3	2.56	0.41
1:C:434:ASP:OD1	1:C:436:GLU:N	2.48	0.41
1:D:133:ARG:NH1	1:D:133:ARG:CG	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:HB2	3:D:573:HOH:O	2.20	0.41
1:A:165:ASN:ND2	1:A:165:ASN:C	2.72	0.41
1:B:205:ARG:HH11	1:B:205:ARG:HG2	1.85	0.41
1:B:377:LYS:HG3	3:B:689:HOH:O	2.21	0.41
1:C:294:LEU:HD22	1:C:298:LYS:HD3	2.02	0.41
1:C:340:SER:O	1:C:344:VAL:HB	2.21	0.41
1:C:396:SER:HA	1:C:418:ILE:O	2.20	0.41
1:D:142:VAL:HG12	1:D:143:VAL:N	2.36	0.41
1:D:193:CYS:SG	1:D:219:THR:HG21	2.60	0.41
1:D:288:SER:O	1:D:290:PRO:N	2.54	0.41
1:B:124:GLY:O	1:B:145:PHE:HA	2.21	0.40
1:C:6:ILE:CG2	1:C:8:LYS:HD2	2.51	0.40
1:C:228:LEU:HD23	1:C:238:LEU:HD23	2.04	0.40
1:C:271:PHE:CE2	1:C:304:LEU:HG	2.56	0.40
1:D:101:ASP:HB2	1:D:136:GLU:OE1	2.21	0.40
1:D:102:ARG:NH2	1:D:139:GLU:OE1	2.54	0.40
1:A:241:CYS:O	1:A:242:HIS:C	2.60	0.40
1:C:375:GLN:NE2	1:C:450:LYS:NZ	2.69	0.40
1:D:62:ILE:HD11	1:D:88:MSE:SE	2.72	0.40
1:D:312:LEU:N	1:D:312:LEU:HD22	2.36	0.40
1:A:107:LEU:HD13	1:A:107:LEU:O	2.21	0.40
1:B:135:HIS:HD2	1:B:139:GLU:OE2	2.04	0.40
1:D:428:ARG:NH1	1:D:444:LYS:HE2	2.37	0.40
1:A:272:VAL:O	1:A:272:VAL:HG13	2.21	0.40
1:A:287:CYS:HB3	1:A:335:ILE:HG12	2.03	0.40
1:A:397:TYR:HB3	1:A:421:ARG:NH1	2.37	0.40
1:B:226:ARG:NE	1:C:226:ARG:HH21	2.19	0.40
1:C:73:TYR:OH	1:C:108:LYS:HE2	2.21	0.40
1:C:92:PRO:HG2	1:C:93:LEU:HG	2.04	0.40
1:C:377:LYS:HZ1	1:C:448:ILE:HD11	1.85	0.40
1:D:8:LYS:NZ	3:D:622:HOH:O	2.54	0.40
1:D:12:VAL:O	1:D:18:ALA:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	422/473 (89%)	405 (96%)	13 (3%)	4 (1%)	17 12
1	B	426/473 (90%)	410 (96%)	11 (3%)	5 (1%)	13 8
1	C	421/473 (89%)	405 (96%)	13 (3%)	3 (1%)	22 18
1	D	422/473 (89%)	402 (95%)	16 (4%)	4 (1%)	17 12
All	All	1691/1892 (89%)	1622 (96%)	53 (3%)	16 (1%)	17 12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	288	SER
1	B	288	SER
1	C	288	SER
1	D	96	LEU
1	D	288	SER
1	A	242	HIS
1	B	242	HIS
1	C	242	HIS
1	D	242	HIS
1	B	95	GLN
1	A	92	PRO
1	B	71	GLU
1	B	92	PRO
1	C	92	PRO
1	D	92	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	350/374 (94%)	309 (88%)	41 (12%)	5 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	354/374 (95%)	322 (91%)	32 (9%)	9 6
1	C	350/374 (94%)	318 (91%)	32 (9%)	9 6
1	D	350/374 (94%)	316 (90%)	34 (10%)	8 5
All	All	1404/1496 (94%)	1265 (90%)	139 (10%)	8 5

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	19	ARG
1	A	41	LYS
1	A	60	THR
1	A	75	THR
1	A	92	PRO
1	A	102	ARG
1	A	104	SER
1	A	106	GLU
1	A	108	LYS
1	A	131	ILE
1	A	133	ARG
1	A	142	VAL
1	A	143	VAL
1	A	162	ARG
1	A	165	ASN
1	A	201	LYS
1	A	202	ARG
1	A	205	ARG
1	A	207	THR
1	A	226	ARG
1	A	278	PHE
1	A	292	ARG
1	A	294	LEU
1	A	303	LYS
1	A	304	LEU
1	A	306	ASN
1	A	311	CYS
1	A	312	LEU
1	A	322	GLU
1	A	324	LYS
1	A	330	LYS
1	A	338	LEU

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Mol	Chain	Res	Type
1	A	362	LYS
1	A	375	GLN
1	A	377	LYS
1	A	384	LYS
1	A	409	LYS
1	A	428	ARG
1	A	444	LYS
1	A	450	LYS
1	B	19	ARG
1	B	70	TRP
1	B	71	GLU
1	B	77	THR
1	B	92	PRO
1	B	95	GLN
1	B	96	LEU
1	B	102	ARG
1	B	133	ARG
1	B	163	ASP
1	B	189	ASN
1	B	202	ARG
1	B	205	ARG
1	B	215	ARG
1	B	226	ARG
1	B	254	ARG
1	B	278	PHE
1	B	292	ARG
1	B	311	CYS
1	B	312	LEU
1	B	324	LYS
1	B	327	ASN
1	B	352	LYS
1	B	362	LYS
1	B	377	LYS
1	B	379	ARG
1	B	400	THR
1	B	407	ARG
1	B	409	LYS
1	B	428	ARG
1	B	444	LYS
1	B	450	LYS
1	C	5	LEU
1	C	78	ARG

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Mol	Chain	Res	Type
1	C	92	PRO
1	C	95	GLN
1	C	108	LYS
1	C	115	LYS
1	C	184	LEU
1	C	189	ASN
1	C	202	ARG
1	C	205	ARG
1	C	215	ARG
1	C	226	ARG
1	C	237	ARG
1	C	278	PHE
1	C	294	LEU
1	C	303	LYS
1	C	304	LEU
1	C	311	CYS
1	C	312	LEU
1	C	313	VAL
1	C	324	LYS
1	C	329	MSE
1	C	375	GLN
1	C	379	ARG
1	C	384	LYS
1	C	392	GLN
1	C	399	LEU
1	C	407	ARG
1	C	409	LYS
1	C	428	ARG
1	C	444	LYS
1	C	450	LYS
1	D	29	LYS
1	D	78	ARG
1	D	110	ASP
1	D	113	LYS
1	D	115	LYS
1	D	133	ARG
1	D	143	VAL
1	D	162	ARG
1	D	163	ASP
1	D	175	LYS
1	D	181	GLN
1	D	184	LEU

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Mol	Chain	Res	Type
1	D	189	ASN
1	D	191	LEU
1	D	202	ARG
1	D	205	ARG
1	D	215	ARG
1	D	222	GLU
1	D	226	ARG
1	D	272	VAL
1	D	278	PHE
1	D	292	ARG
1	D	298	LYS
1	D	304	LEU
1	D	311	CYS
1	D	324	LYS
1	D	329	MSE
1	D	330	LYS
1	D	377	LYS
1	D	384	LYS
1	D	392	GLN
1	D	424	LYS
1	D	428	ARG
1	D	450	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	174	GLN
1	A	209	HIS
1	A	239	HIS
1	A	269	HIS
1	A	277	GLN
1	A	296	ASN
1	A	306	ASN
1	A	339	GLN
1	A	375	GLN
1	A	408	HIS
1	B	94	ASN
1	B	95	GLN
1	B	135	HIS
1	B	181	GLN
1	B	189	ASN

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Mol	Chain	Res	Type
1	B	239	HIS
1	B	260	GLN
1	B	296	ASN
1	B	327	ASN
1	B	339	GLN
1	B	351	GLN
1	B	408	HIS
1	B	437	GLN
1	C	35	GLN
1	C	94	ASN
1	C	95	GLN
1	C	135	HIS
1	C	189	ASN
1	C	260	GLN
1	C	327	ASN
1	C	339	GLN
1	C	351	GLN
1	C	375	GLN
1	C	376	GLN
1	C	401	ASN
1	D	122	GLN
1	D	181	GLN
1	D	189	ASN
1	D	209	HIS
1	D	239	HIS
1	D	260	GLN
1	D	277	GLN
1	D	339	GLN
1	D	375	GLN
1	D	392	GLN
1	D	401	ASN
1	D	437	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	C	146	2,1	7,11,12	0.60	0	4,12,14	0.58	0
1	KCX	B	146	2,1	7,11,12	0.72	0	4,12,14	0.75	0
1	KCX	A	146	2,1	7,11,12	0.63	0	4,12,14	0.51	0
1	KCX	D	146	2,1	7,11,12	0.50	0	4,12,14	1.10	0

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
1	KCX	C	146	2,1	-	0/7/10/12	-
1	KCX	B	146	2,1	-	5/7/10/12	-
1	KCX	A	146	2,1	-	3/7/10/12	-
1	KCX	D	146	2,1	-	4/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	146	KCX	N-CA-CB-CG
1	A	146	KCX	C-CA-CB-CG
1	A	146	KCX	O-C-CA-CB
1	B	146	KCX	C-CA-CB-CG
1	B	146	KCX	O-C-CA-CB
1	D	146	KCX	N-CA-CB-CG
1	D	146	KCX	C-CA-CB-CG
1	D	146	KCX	O-C-CA-CB
1	D	146	KCX	CG-CD-CE-NZ
1	B	146	KCX	CE-CD-CG-CB
1	B	146	KCX	N-CA-CB-CG
1	B	146	KCX	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	146	KCX	1	0
1	A	146	KCX	1	0
1	D	146	KCX	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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)

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, 95^{th} 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	416/473 (87%)	0.20	13 (3%)	49	55	14, 27, 48, 63	0
1	B	420/473 (88%)	0.11	13 (3%)	49	55	14, 24, 45, 69	0
1	C	415/473 (87%)	0.08	14 (3%)	45	51	15, 26, 48, 59	0
1	D	416/473 (87%)	0.36	27 (6%)	18	23	18, 31, 54, 67	0
All	All	1667/1892 (88%)	0.19	67 (4%)	38	44	14, 27, 49, 69	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	LEU	5.9
1	B	96	LEU	5.4
1	D	94	ASN	5.1
1	A	288	SER	5.1
1	C	96	LEU	4.7
1	D	288	SER	4.6
1	B	70	TRP	4.2
1	D	205	ARG	4.1
1	A	96	LEU	4.0
1	A	205	ARG	3.9
1	C	205	ARG	3.9
1	C	204	GLY	3.8
1	B	288	SER	3.7
1	C	288	SER	3.7
1	D	202	ARG	3.5
1	D	2	SER	3.3
1	B	202	ARG	3.3
1	B	200	ALA	3.3
1	D	332	TRP	3.3
1	A	132	ASP	3.2
1	C	326	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	203	GLU	3.0
1	A	204	GLY	3.0
1	C	94	ASN	2.9
1	D	440	PRO	2.9
1	D	441	VAL	2.8
1	A	200	ALA	2.8
1	D	200	ALA	2.8
1	A	162	ARG	2.7
1	C	179	LEU	2.7
1	C	202	ARG	2.7
1	C	451	HIS	2.7
1	B	205	ARG	2.6
1	D	204	GLY	2.6
1	D	321	PRO	2.6
1	D	437	GLN	2.6
1	D	327	ASN	2.5
1	B	204	GLY	2.5
1	D	330	LYS	2.5
1	C	197	GLY	2.5
1	A	207	THR	2.4
1	A	94	ASN	2.4
1	A	202	ARG	2.4
1	B	94	ASN	2.4
1	D	197	GLY	2.4
1	C	203	GLU	2.3
1	B	326	GLY	2.3
1	D	325	ALA	2.3
1	C	97	PRO	2.2
1	D	311	CYS	2.2
1	D	201	LYS	2.2
1	D	394	ASN	2.2
1	D	298	LYS	2.2
1	D	320	PRO	2.2
1	D	322	GLU	2.1
1	B	69	HIS	2.1
1	D	213	ALA	2.1
1	B	207	THR	2.1
1	D	16	ASN	2.1
1	A	198	GLU	2.1
1	A	201	LYS	2.1
1	A	332	TRP	2.1
1	C	132	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	206	VAL	2.0
1	D	206	VAL	2.0
1	B	71	GLU	2.0
1	B	203	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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(Å^2)	Q<0.9
1	KCX	B	146	12/13	0.91	0.16	24,28,38,38	0
1	KCX	D	146	12/13	0.92	0.19	24,31,41,46	0
1	KCX	A	146	12/13	0.93	0.15	24,28,32,32	0
1	KCX	C	146	12/13	0.96	0.10	20,23,29,29	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	FE	D	455	1/1	0.94	0.16	44,44,44,44	0
2	FE	C	454	1/1	0.98	0.10	32,32,32,32	0
2	FE	C	455	1/1	0.98	0.10	36,36,36,36	0
2	FE	D	454	1/1	0.98	0.13	43,43,43,43	0
2	FE	B	455	1/1	0.98	0.12	35,35,35,35	0
2	FE	A	455	1/1	0.99	0.15	34,34,34,34	0
2	FE	A	454	1/1	0.99	0.09	35,35,35,35	0
2	FE	B	454	1/1	1.00	0.11	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.