



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 08:02 PM EST

PDB ID : 1F9E
Title : CASPASE-8 SPECIFICITY PROBED AT SUBSITE S4: CRYSTAL STRUCTURE OF THE CASPASE-8-Z-DEVD-CHO
Authors : Blanchard, H.; Donepudi, M.; Tschopp, M.; Kodandapani, L.; Wu, J.C.; Grutter, M.G.
Deposited on : 2000-07-10
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

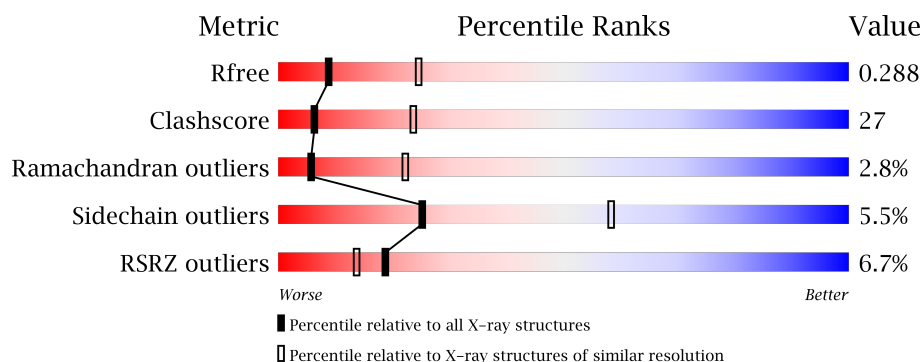
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	<div> <div>3%</div> <div>59%</div> <div>38%</div> <div>.</div> </div>
1	C	153	<div> <div>5%</div> <div>54%</div> <div>40%</div> <div>6%</div> </div>
1	E	153	<div> <div>5%</div> <div>54%</div> <div>41%</div> <div>5%</div> <div>.</div> </div>
1	G	153	<div> <div>0%</div> <div>63%</div> <div>35%</div> <div>.</div> </div>
1	I	153	<div> <div>9%</div> <div>57%</div> <div>37%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	153	
2	B	89	
2	D	89	
2	F	89	
2	H	89	
2	J	89	
2	L	89	
3	Q	5	
3	R	5	
3	S	5	
3	T	5	
3	U	5	
3	V	5	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11926 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 CASPASE-8 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	C	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	E	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	G	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	I	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	K	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			

- Molecule 2 is a protein called CASPASE-8 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			
2	D	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			
2	F	89	Total	C	N	O	S	0	0	0
			717	450	124	137	6			
2	H	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			
2	J	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			
2	L	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			

- Molecule 3 is a protein called (PHQ)DEV D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	R	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	S	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	T	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	U	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	V	5	Total	C	N	O	0	0	0
			42	26	4	12			

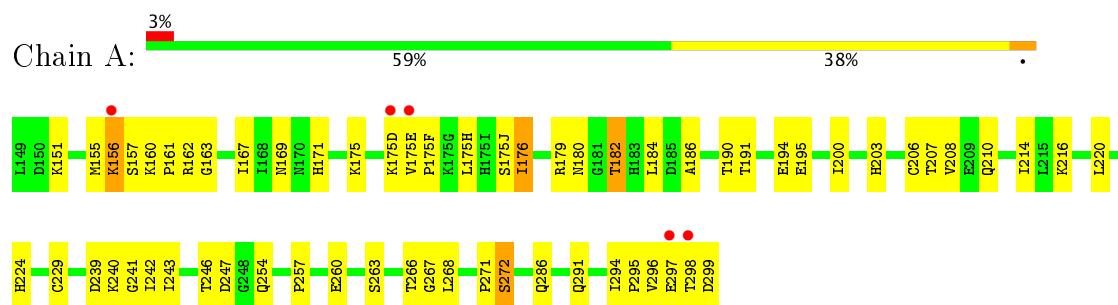
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	7	Total	O	0	0
			7	7		
4	Q	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		
4	D	4	Total	O	0	0
			4	4		
4	E	4	Total	O	0	0
			4	4		
4	F	3	Total	O	0	0
			3	3		
4	G	11	Total	O	0	0
			11	11		
4	H	1	Total	O	0	0
			1	1		
4	I	5	Total	O	0	0
			5	5		
4	K	2	Total	O	0	0
			2	2		
4	L	1	Total	O	0	0
			1	1		

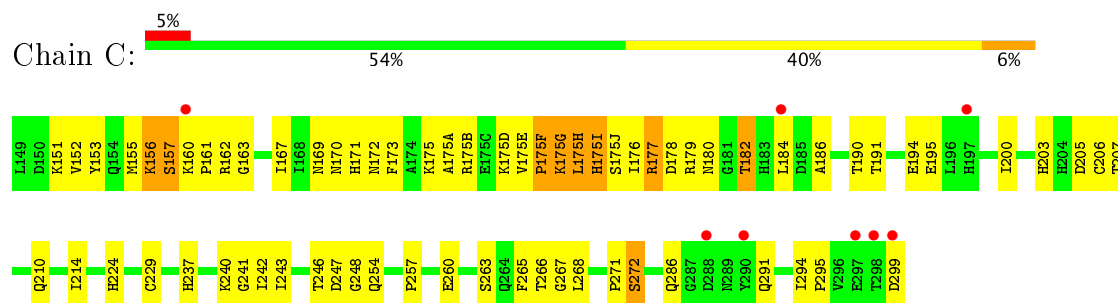
3 Residue-property plots

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

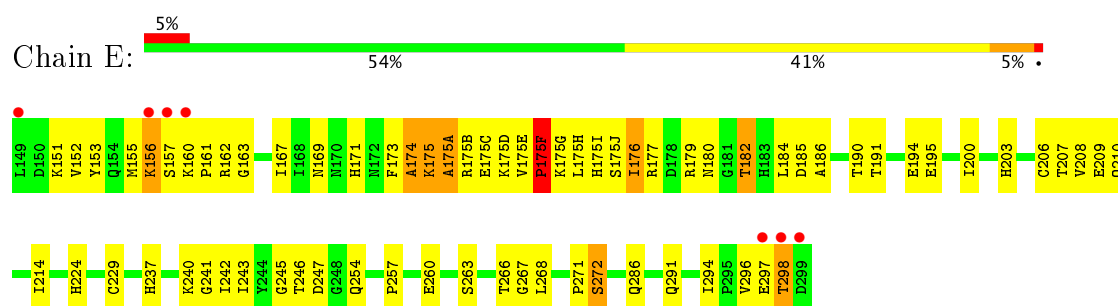
• Molecule 1: CASPASE-8 ALPHA CHAIN



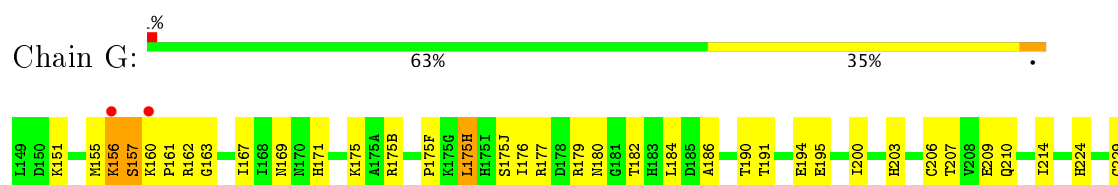
• Molecule 1: CASPASE-8 ALPHA CHAIN



• Molecule 1: CASPASE-8 ALPHA CHAIN

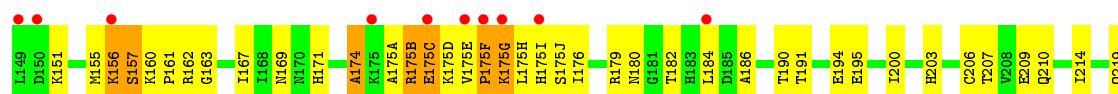


• Molecule 1: CASPASE-8 ALPHA CHAIN

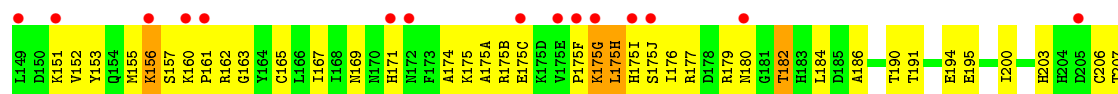




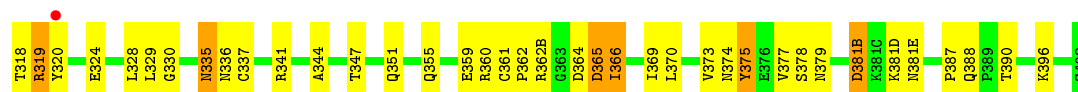
• Molecule 1: CASPASE-8 ALPHA CHAIN



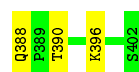
• Molecule 1: CASPASE-8 ALPHA CHAIN



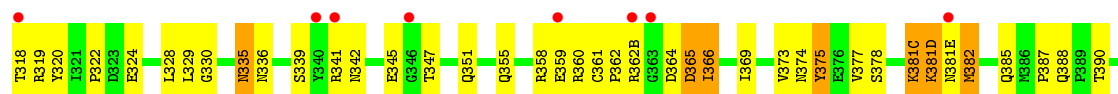
• Molecule 2: CASPASE-8 BETA CHAIN



• Molecule 2: CASPASE-8 BETA CHAIN



• Molecule 2: CASPASE-8 BETA CHAIN





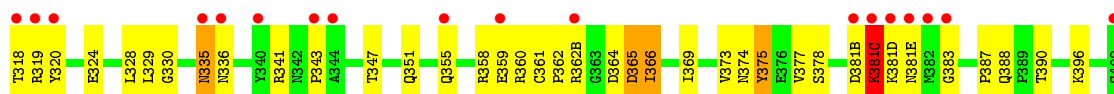
- Molecule 2: CASPASE-8 BETA CHAIN



- Molecule 2: CASPASE-8 BETA CHAIN



- Molecule 2: CASPASE-8 BETA CHAIN



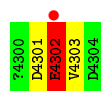
- Molecule 3: (PHQ)DEVD



- Molecule 3: (PHQ)DEVD



- Molecule 3: (PHQ)DEVD



- Molecule 3: (PHQ)DEVD

Chain T:  100%

24400
D4401
E4402
V4403
D4404

● Molecule 3: (PHQ)DEVD

Chain U:  40% 40% 20%

24500
D4501
E4502
V4503
D4504

● Molecule 3: (PHQ)DEVD

Chain V:  20% 40% 60%

24600
D4601
E4602
V4603
D4604

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.03Å 188.75Å 209.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.90 19.93 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-2.90) 99.5 (19.93-2.91)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.93Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.289 0.240 , 0.288	Depositor DCC
R_{free} test set	4318 reflections (10.07%)	DCC
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11926	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.54	0/1248	0.69	0/1682
1	C	0.52	0/1248	0.71	0/1682
1	E	0.50	0/1248	0.72	0/1682
1	G	0.55	0/1248	0.71	0/1682
1	I	0.49	0/1248	0.71	0/1682
1	K	0.48	0/1248	0.70	0/1682
2	B	0.51	0/732	0.74	0/989
2	D	0.48	0/732	0.71	0/989
2	F	0.54	0/731	0.74	0/989
2	H	0.53	0/732	0.71	0/989
2	J	0.46	0/732	0.69	0/989
2	L	0.49	0/732	0.71	0/989
3	Q	2.09	1/23 (4.3%)	1.84	0/30
3	R	2.35	0/23	1.96	0/30
3	S	2.16	1/23 (4.3%)	1.71	0/30
3	T	2.21	1/23 (4.3%)	2.06	1/30 (3.3%)
3	U	2.18	1/23 (4.3%)	1.68	0/30
3	V	2.16	0/23	1.89	0/30
All	All	0.56	4/12017 (0.0%)	0.73	1/16206 (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
3	Q	1	0
3	R	1	1
3	S	1	1
3	T	1	1
3	U	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	V	0	1
All	All	5	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	4102	GLU	CD-OE2	5.31	1.31	1.25
3	U	4502	GLU	CD-OE1	5.24	1.31	1.25
3	S	4302	GLU	CD-OE2	5.21	1.31	1.25
3	T	4402	GLU	CD-OE1	5.13	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	4401	ASP	N-CA-C	-5.57	95.95	111.00

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	Q	4101	ASP	CA
3	R	4201	ASP	CA
3	S	4301	ASP	CA
3	T	4401	ASP	CA
3	U	4501	ASP	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	R	4203	VAL	Mainchain
3	S	4303	VAL	Mainchain
3	T	4403	VAL	Mainchain
3	U	4503	VAL	Mainchain
3	V	4603	VAL	Mainchain

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	1220	0	1198	72	0
1	C	1220	0	1198	84	0
1	E	1220	0	1198	87	0
1	G	1220	0	1198	60	0
1	I	1220	0	1198	80	0
1	K	1220	0	1198	85	0
2	B	718	0	712	53	0
2	D	718	0	712	53	0
2	F	717	0	712	49	0
2	H	718	0	712	39	0
2	J	718	0	712	47	0
2	L	718	0	712	54	0
3	Q	42	0	28	2	0
3	R	42	0	28	2	0
3	S	42	0	28	3	0
3	T	42	0	28	2	0
3	U	42	0	28	2	0
3	V	42	0	28	3	0
4	A	6	0	0	2	0
4	B	7	0	0	2	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	3	0	0	0	0
4	G	11	0	0	4	0
4	H	1	0	0	0	0
4	I	5	0	0	1	0
4	K	2	0	0	0	0
4	L	1	0	0	0	0
4	Q	1	0	0	0	0
All	All	11926	0	11628	630	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 27.

All (630) 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:E:298:THR:HG23	2:H:319:ARG:HH21	1.15	1.10
2:B:319:ARG:HH22	1:C:299:ASP:HB2	1.13	1.09
1:A:160:LYS:HB2	1:A:161:PRO:HD3	1.35	1.08
1:K:160:LYS:HB2	1:K:161:PRO:HD3	1.38	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LYS:HB2	1:C:161:PRO:HD3	1.38	1.05
1:G:160:LYS:HB2	1:G:161:PRO:HD3	1.38	1.05
1:E:291:GLN:NE2	2:H:324:GLU:H	1.53	1.05
2:J:324:GLU:H	1:K:291:GLN:NE2	1.55	1.03
1:I:160:LYS:HB2	1:I:161:PRO:HD3	1.36	1.02
2:D:381(C):LYS:HD3	2:D:381(C):LYS:H	1.23	1.01
1:E:160:LYS:HB2	1:E:161:PRO:HD3	1.38	1.01
1:G:155:MET:HE3	1:G:162:ARG:HD2	1.42	1.01
1:I:155:MET:HE3	1:I:162:ARG:HD2	1.41	1.01
1:K:155:MET:HE3	1:K:162:ARG:HD2	1.41	1.00
1:A:155:MET:HE3	1:A:162:ARG:HD2	1.44	1.00
1:C:175(G):LYS:H	1:C:175(G):LYS:HD2	1.26	0.99
2:F:381(C):LYS:H	2:F:381(C):LYS:HD2	1.22	0.98
1:E:175(H):LEU:HB3	1:E:176:ILE:HD11	1.45	0.97
1:A:175:LYS:HZ3	1:A:175(D):LYS:HE3	1.29	0.96
1:C:155:MET:HE3	1:C:162:ARG:HD2	1.45	0.96
1:E:155:MET:HE3	1:E:162:ARG:HD2	1.45	0.95
2:B:324:GLU:H	1:C:291:GLN:NE2	1.64	0.94
1:I:175(G):LYS:HE3	1:I:175(H):LEU:HD21	1.48	0.93
1:E:298:THR:HG23	2:H:319:ARG:NH2	1.82	0.93
2:F:324:GLU:H	1:G:291:GLN:NE2	1.65	0.93
1:K:175(H):LEU:HG	1:K:176:ILE:HG13	1.49	0.91
1:K:174:ALA:HA	1:K:175(B):ARG:HH21	1.38	0.88
1:A:175:LYS:NZ	1:A:175(D):LYS:HE3	1.89	0.88
2:B:379:ASN:HD21	2:D:319:ARG:HH11	1.21	0.88
1:I:291:GLN:NE2	2:L:324:GLU:H	1.72	0.87
1:A:291:GLN:NE2	2:D:324:GLU:H	1.74	0.86
1:I:207:THR:HG23	1:I:210:GLN:NE2	1.92	0.84
2:F:381(C):LYS:CD	2:F:381(C):LYS:H	1.87	0.83
1:K:169:ASN:HD22	1:K:186:ALA:HB2	1.44	0.82
1:I:175(H):LEU:HB3	1:I:176:ILE:HD12	1.60	0.82
1:E:169:ASN:HD22	1:E:186:ALA:HB2	1.43	0.82
2:L:381(C):LYS:HG2	2:L:381(D):LYS:H	1.43	0.82
1:A:207:THR:HG23	1:A:210:GLN:NE2	1.95	0.82
1:C:190:THR:O	1:C:194:GLU:HB2	1.79	0.81
1:E:207:THR:HG23	1:E:210:GLN:NE2	1.95	0.81
1:K:207:THR:HG23	1:K:210:GLN:NE2	1.96	0.81
1:K:190:THR:O	1:K:194:GLU:HB2	1.81	0.81
1:C:169:ASN:HD22	1:C:186:ALA:HB2	1.45	0.81
1:G:169:ASN:HD22	1:G:186:ALA:HB2	1.46	0.80
1:C:207:THR:HG23	1:C:210:GLN:NE2	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:THR:O	1:E:194:GLU:HB2	1.82	0.80
1:A:190:THR:O	1:A:194:GLU:HB2	1.83	0.79
2:B:319:ARG:NH2	1:C:299:ASP:HB2	1.94	0.79
1:G:207:THR:HG23	1:G:210:GLN:NE2	1.97	0.79
1:I:296:VAL:O	2:L:318:THR:HA	1.81	0.79
2:J:324:GLU:HG3	1:K:291:GLN:HE22	1.45	0.79
2:L:381(C):LYS:HD3	2:L:381(C):LYS:N	1.97	0.79
1:I:267:GLY:HA3	1:K:294:ILE:HD13	1.63	0.79
1:I:190:THR:O	1:I:194:GLU:HB2	1.83	0.78
1:A:169:ASN:HD22	1:A:186:ALA:HB2	1.50	0.77
2:B:379:ASN:ND2	2:D:319:ARG:HH11	1.83	0.77
1:I:169:ASN:HD22	1:I:186:ALA:HB2	1.47	0.77
2:L:381(C):LYS:HD3	2:L:381(C):LYS:H	1.50	0.76
2:F:324:GLU:HG3	1:G:291:GLN:HE22	1.49	0.76
1:E:291:GLN:HE22	2:H:324:GLU:HG3	1.50	0.76
1:E:173:PHE:O	1:E:175(A):ALA:HB3	1.84	0.75
1:G:190:THR:O	1:G:194:GLU:HB2	1.86	0.74
1:E:291:GLN:HE22	2:H:324:GLU:H	1.31	0.74
2:J:324:GLU:H	1:K:291:GLN:HE21	1.33	0.74
1:E:291:GLN:HE21	2:H:324:GLU:H	1.35	0.74
1:I:291:GLN:HE22	2:L:324:GLU:HG3	1.53	0.74
2:J:324:GLU:H	1:K:291:GLN:HE22	1.36	0.73
1:I:207:THR:HG23	1:I:210:GLN:HE21	1.52	0.73
1:I:175(H):LEU:HD22	1:I:176:ILE:HD11	1.71	0.73
1:E:175(E):VAL:CB	1:E:175(H):LEU:HD12	2.19	0.73
2:B:324:GLU:H	1:C:291:GLN:HE22	1.37	0.73
1:A:291:GLN:HE22	2:D:324:GLU:HG3	1.52	0.73
1:E:176:ILE:HG22	1:E:237:HIS:CD2	2.24	0.73
1:C:175(H):LEU:O	1:C:176:ILE:HG12	1.89	0.72
1:E:267:GLY:HA3	1:G:294:ILE:HD13	1.70	0.72
2:F:388:GLN:HE21	2:H:390:THR:HG21	1.53	0.72
1:C:175(F):PRO:O	1:C:175(H):LEU:N	2.22	0.71
1:C:171:HIS:HE1	1:C:180:ASN:HD22	1.38	0.71
1:A:210:GLN:O	1:A:214:ILE:HG13	1.90	0.71
2:B:319:ARG:HH22	1:C:299:ASP:CB	1.99	0.71
1:C:175(E):VAL:HG21	1:C:248:GLY:HA3	1.71	0.71
1:G:241:GLY:H	1:G:286:GLN:NE2	1.88	0.71
1:E:291:GLN:NE2	2:H:324:GLU:N	2.36	0.71
1:E:175(H):LEU:O	1:E:176:ILE:HG13	1.91	0.71
1:C:177:ARG:HG3	1:C:177:ARG:HH11	1.54	0.71
1:I:175(H):LEU:HB3	1:I:176:ILE:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:175(H):LEU:C	1:K:176:ILE:HD11	2.10	0.71
1:G:210:GLN:O	1:G:214:ILE:HG13	1.91	0.70
2:J:388:GLN:HE21	2:L:390:THR:HG21	1.57	0.70
1:I:294:ILE:HD13	1:K:267:GLY:HA3	1.74	0.70
1:K:207:THR:HG23	1:K:210:GLN:HE21	1.56	0.70
1:A:207:THR:HG23	1:A:210:GLN:HE21	1.54	0.70
1:A:171:HIS:HE1	1:A:180:ASN:HD22	1.39	0.70
1:C:241:GLY:H	1:C:286:GLN:NE2	1.88	0.70
2:H:341:ARG:NH1	3:T:4404:ASA:OD1	2.24	0.69
1:E:171:HIS:HE1	1:E:180:ASN:HD22	1.40	0.69
1:E:241:GLY:H	1:E:286:GLN:NE2	1.89	0.69
1:E:294:ILE:HD13	1:G:267:GLY:HA3	1.74	0.69
2:J:324:GLU:N	1:K:291:GLN:NE2	2.38	0.69
1:C:175(I):HIS:O	1:C:176:ILE:N	2.25	0.69
2:D:381(C):LYS:CD	2:D:381(C):LYS:H	2.03	0.69
1:K:241:GLY:H	1:K:286:GLN:NE2	1.90	0.69
1:G:175(F):PRO:HG2	4:G:527:HOH:O	1.92	0.69
2:F:390:THR:HG21	2:H:388:GLN:HE21	1.57	0.69
1:A:241:GLY:H	1:A:286:GLN:NE2	1.89	0.69
1:C:207:THR:HG23	1:C:210:GLN:HE21	1.54	0.69
1:G:171:HIS:HE1	1:G:180:ASN:HD22	1.41	0.69
1:A:175:LYS:HZ3	1:A:175(D):LYS:CE	2.02	0.68
1:G:207:THR:HG23	1:G:210:GLN:HE21	1.57	0.68
1:I:241:GLY:H	1:I:286:GLN:NE2	1.91	0.68
1:K:177:ARG:HH11	1:K:177:ARG:HG3	1.57	0.68
2:B:341:ARG:NH1	3:Q:4104:ASA:OD1	2.27	0.68
1:A:294:ILE:HD13	1:C:267:GLY:HA3	1.76	0.68
1:C:175(F):PRO:HG2	1:C:175(G):LYS:HD2	1.74	0.68
1:C:240:LYS:HE2	2:D:336:ASN:ND2	2.08	0.68
1:K:171:HIS:HE1	1:K:180:ASN:ND2	1.93	0.67
1:C:191:THR:O	1:C:195:GLU:HG3	1.95	0.67
1:E:207:THR:HG23	1:E:210:GLN:HE21	1.56	0.67
1:A:191:THR:O	1:A:195:GLU:HG3	1.94	0.67
1:E:240:LYS:HE2	2:F:336:ASN:ND2	2.09	0.67
1:C:171:HIS:HE1	1:C:180:ASN:ND2	1.92	0.67
1:E:175(E):VAL:HB	1:E:175(H):LEU:HB2	1.76	0.67
1:E:191:THR:O	1:E:195:GLU:HG3	1.95	0.67
1:E:179:ARG:HH12	1:E:182:THR:HG23	1.60	0.67
1:K:171:HIS:HE1	1:K:180:ASN:HD22	1.40	0.67
2:J:396:LYS:NZ	1:K:299:ASP:HB3	2.09	0.67
1:A:175(H):LEU:HB3	1:A:176:ILE:CD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:HIS:HE1	1:A:180:ASN:ND2	1.93	0.67
2:B:319:ARG:HH11	2:D:379:ASN:HD21	1.42	0.67
2:F:396:LYS:CE	1:G:299:ASP:HB3	2.24	0.66
1:K:175(F):PRO:HG2	1:K:175(G):LYS:H	1.58	0.66
1:A:298:THR:HG23	2:D:319:ARG:HH21	1.60	0.66
1:I:171:HIS:HE1	1:I:180:ASN:HD22	1.42	0.66
2:F:388:GLN:HE21	2:H:390:THR:CG2	2.08	0.65
1:C:173:PHE:O	1:C:175(A):ALA:HB3	1.96	0.65
2:F:324:GLU:H	1:G:291:GLN:HE22	1.42	0.65
1:I:179:ARG:HH12	1:I:182:THR:HG23	1.61	0.65
2:B:319:ARG:NH1	2:D:379:ASN:HD21	1.93	0.65
1:E:210:GLN:O	1:E:214:ILE:HG13	1.96	0.65
1:K:175(H):LEU:HG	1:K:176:ILE:CG1	2.24	0.65
1:K:191:THR:O	1:K:195:GLU:HG3	1.95	0.65
1:C:210:GLN:O	1:C:214:ILE:HG13	1.96	0.65
1:K:210:GLN:O	1:K:214:ILE:HG13	1.97	0.65
1:A:267:GLY:HA3	1:C:294:ILE:HD13	1.78	0.65
1:K:179:ARG:HH12	1:K:182:THR:HG23	1.62	0.65
1:A:179:ARG:HH12	1:A:182:THR:HG23	1.61	0.65
1:E:171:HIS:HE1	1:E:180:ASN:ND2	1.94	0.65
1:I:191:THR:O	1:I:195:GLU:HG3	1.97	0.64
1:I:240:LYS:HE2	2:J:336:ASN:ND2	2.11	0.64
1:G:171:HIS:HE1	1:G:180:ASN:ND2	1.94	0.64
2:B:379:ASN:HD21	2:D:319:ARG:NH1	1.93	0.64
2:J:390:THR:HG21	2:L:388:GLN:HE21	1.62	0.64
2:B:324:GLU:HG3	1:C:291:GLN:HE22	1.61	0.64
1:E:175(H):LEU:HD22	1:E:176:ILE:CD1	2.27	0.64
1:C:179:ARG:HH12	1:C:182:THR:HG23	1.63	0.64
1:G:182:THR:HG23	4:G:501:HOH:O	1.97	0.64
1:A:160:LYS:HB2	1:A:161:PRO:CD	2.21	0.63
1:I:171:HIS:HE1	1:I:180:ASN:ND2	1.95	0.63
1:E:175(E):VAL:HB	1:E:175(H):LEU:HD12	1.80	0.63
1:E:176:ILE:CG2	1:E:237:HIS:CD2	2.81	0.63
1:G:191:THR:O	1:G:195:GLU:HG3	1.99	0.63
2:F:388:GLN:NE2	2:H:390:THR:HG21	2.12	0.63
2:F:324:GLU:H	1:G:291:GLN:HE21	1.45	0.63
1:K:247:ASP:OD2	1:K:254:GLN:HG2	1.99	0.63
1:C:175:LYS:HE3	1:C:175(D):LYS:HG3	1.80	0.62
1:E:291:GLN:HE22	2:H:324:GLU:N	1.95	0.62
2:J:374:ASN:OD1	2:J:387:PRO:HB2	1.99	0.62
2:L:374:ASN:OD1	2:L:387:PRO:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175(E):VAL:HB	1:C:175(H):LEU:HB3	1.81	0.62
1:I:182:THR:HG23	4:I:528:HOH:O	1.99	0.62
1:G:263:SER:O	1:G:266:THR:HG23	2.00	0.62
2:J:381(D):LYS:O	2:J:382:MET:N	2.33	0.62
2:F:374:ASN:OD1	2:F:387:PRO:HB2	2.00	0.62
1:A:175(H):LEU:HB3	1:A:176:ILE:HD11	1.80	0.61
1:C:160:LYS:HB2	1:C:161:PRO:CD	2.24	0.61
2:F:381(D):LYS:HG2	2:F:381(E):ASN:N	2.14	0.61
1:I:296:VAL:O	2:L:318:THR:CA	2.48	0.61
1:G:160:LYS:HB2	1:G:161:PRO:CD	2.24	0.61
1:G:240:LYS:HE2	2:H:336:ASN:ND2	2.15	0.61
2:J:388:GLN:HE21	2:L:390:THR:CG2	2.14	0.61
1:K:175:LYS:HD3	1:K:247:ASP:HB2	1.83	0.60
1:K:240:LYS:HE2	2:L:336:ASN:ND2	2.16	0.60
1:G:179:ARG:HH12	1:G:182:THR:HG23	1.65	0.60
2:H:374:ASN:OD1	2:H:387:PRO:HB2	2.01	0.60
1:I:210:GLN:O	1:I:214:ILE:HG13	2.00	0.60
2:B:318:THR:O	2:B:319:ARG:HB2	2.02	0.60
1:A:175:LYS:HZ3	1:A:175(D):LYS:HG3	1.67	0.60
1:I:247:ASP:OD2	1:I:254:GLN:HG2	2.02	0.60
1:C:160:LYS:CB	1:C:161:PRO:HD3	2.24	0.60
2:J:388:GLN:NE2	2:L:390:THR:HG21	2.16	0.60
1:C:263:SER:O	1:C:266:THR:HG23	2.01	0.60
2:L:381(C):LYS:NZ	3:V:4601:ASP:HB2	2.17	0.60
2:B:324:GLU:H	1:C:291:GLN:HE21	1.50	0.60
1:G:209:GLU:HB2	4:G:515:HOH:O	2.01	0.59
1:A:160:LYS:CB	1:A:161:PRO:HD3	2.21	0.59
1:E:176:ILE:HG22	1:E:237:HIS:NE2	2.17	0.59
2:F:390:THR:HG21	2:H:388:GLN:NE2	2.16	0.59
2:B:390:THR:HG21	2:D:388:GLN:HE21	1.67	0.59
1:A:299:ASP:HB3	2:D:396:LYS:NZ	2.17	0.59
1:E:247:ASP:OD2	1:E:254:GLN:HG2	2.02	0.59
2:B:388:GLN:OE1	4:B:511:HOH:O	2.17	0.59
2:F:390:THR:CG2	2:H:388:GLN:HE21	2.16	0.59
2:J:390:THR:HG21	2:L:388:GLN:NE2	2.18	0.59
2:D:329:LEU:HD12	2:D:330:GLY:N	2.18	0.59
2:J:390:THR:CG2	2:L:388:GLN:HE21	2.16	0.58
2:L:373:VAL:O	2:L:377:VAL:HG23	2.03	0.58
1:A:240:LYS:HE2	2:B:336:ASN:ND2	2.17	0.58
1:K:263:SER:O	1:K:266:THR:HG23	2.03	0.58
2:F:381(C):LYS:HD2	2:F:381(C):LYS:N	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:396:LYS:CE	1:K:299:ASP:HB3	2.34	0.58
2:F:369:ILE:O	2:F:373:VAL:HG23	2.04	0.58
1:C:175(G):LYS:O	1:C:175(H):LEU:HB2	2.02	0.58
1:G:247:ASP:OD2	1:G:254:GLN:HG2	2.04	0.58
1:A:247:ASP:OD2	1:A:254:GLN:HG2	2.03	0.58
1:E:160:LYS:HB2	1:E:161:PRO:CD	2.24	0.58
2:D:374:ASN:OD1	2:D:387:PRO:HB2	2.04	0.57
1:A:297:GLU:OE1	1:A:297:GLU:HA	2.03	0.57
1:I:291:GLN:HE21	2:L:324:GLU:H	1.50	0.57
1:A:175(H):LEU:HB3	1:A:176:ILE:HG12	1.87	0.57
1:A:291:GLN:HE22	2:D:324:GLU:H	1.47	0.57
1:E:169:ASN:ND2	1:E:186:ALA:HB2	2.18	0.57
1:I:263:SER:O	1:I:266:THR:HG23	2.04	0.57
1:I:175(F):PRO:O	1:I:175(H):LEU:N	2.36	0.57
1:I:160:LYS:HB2	1:I:161:PRO:CD	2.22	0.57
1:A:263:SER:O	1:A:266:THR:HG23	2.04	0.57
1:E:175(H):LEU:CB	1:E:176:ILE:HD11	2.30	0.57
1:C:247:ASP:OD2	1:C:254:GLN:HG2	2.05	0.56
1:G:241:GLY:H	1:G:286:GLN:HE22	1.52	0.56
2:J:324:GLU:N	1:K:291:GLN:HE22	2.01	0.56
2:F:373:VAL:O	2:F:377:VAL:HG23	2.06	0.56
2:F:375:TYR:CE2	1:G:151:LYS:HG3	2.39	0.56
1:I:291:GLN:HE22	2:L:324:GLU:H	1.48	0.56
1:A:175:LYS:CE	1:A:175(D):LYS:HE3	2.36	0.56
1:C:175(E):VAL:CG2	1:C:248:GLY:HA3	2.36	0.56
1:E:171:HIS:CE1	1:E:180:ASN:HD22	2.24	0.56
1:I:268:LEU:O	1:I:271:PRO:HD3	2.05	0.56
1:K:224:HIS:H	1:K:272:SER:CB	2.19	0.56
1:C:175(B):ARG:HA	1:C:175(I):HIS:HA	1.87	0.56
1:C:176:ILE:HG22	1:C:237:HIS:NE2	2.21	0.56
1:E:175(F):PRO:O	1:E:175(H):LEU:N	2.39	0.56
2:J:369:ILE:O	2:J:373:VAL:HG23	2.06	0.56
2:L:329:LEU:HD12	2:L:330:GLY:N	2.20	0.55
1:A:291:GLN:HE21	2:D:324:GLU:H	1.54	0.55
1:A:151:LYS:HG3	2:D:375:TYR:CE2	2.41	0.55
2:D:381(C):LYS:HD3	2:D:381(C):LYS:N	2.06	0.55
2:L:369:ILE:O	2:L:373:VAL:HG23	2.07	0.55
1:I:175(C):GLU:HG2	1:I:175(D):LYS:HG2	1.89	0.55
1:E:263:SER:O	1:E:266:THR:HG23	2.07	0.55
1:C:171:HIS:CE1	1:C:180:ASN:HD22	2.22	0.55
2:B:390:THR:HG21	2:D:388:GLN:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLY:H	1:C:286:GLN:HE22	1.52	0.55
2:B:344:ALA:HB2	3:Q:4100:PHQ:H71	1.89	0.55
1:E:175(H):LEU:HD22	1:E:176:ILE:HD11	1.87	0.55
1:E:241:GLY:H	1:E:286:GLN:HE22	1.54	0.55
2:B:374:ASN:OD1	2:B:387:PRO:HB2	2.07	0.54
4:A:509:HOH:O	2:D:319:ARG:HD2	2.06	0.54
2:D:342:ASN:HD21	3:R:4200:PHQ:H41	1.72	0.54
1:G:207:THR:CG2	1:G:210:GLN:HE21	2.20	0.54
1:I:207:THR:CG2	1:I:210:GLN:HE21	2.18	0.54
2:B:337:CYS:HB3	4:B:507:HOH:O	2.06	0.54
2:B:388:GLN:HE21	2:D:390:THR:HG21	1.72	0.54
1:A:171:HIS:CE1	1:A:180:ASN:HD22	2.23	0.54
1:A:224:HIS:H	1:A:272:SER:HB2	1.72	0.54
1:C:207:THR:CG2	1:C:210:GLN:HE21	2.20	0.54
1:G:224:HIS:H	1:G:272:SER:HB2	1.72	0.54
2:H:369:ILE:O	2:H:373:VAL:HG23	2.07	0.54
2:J:373:VAL:O	2:J:377:VAL:HG23	2.06	0.54
2:L:381(C):LYS:HG2	2:L:381(D):LYS:N	2.17	0.54
1:C:241:GLY:N	1:C:286:GLN:HE22	2.05	0.54
1:A:241:GLY:H	1:A:286:GLN:HE22	1.56	0.54
1:E:175(E):VAL:HG11	1:E:175(H):LEU:HD12	1.90	0.54
2:F:366:ILE:HD13	2:F:366:ILE:O	2.08	0.54
1:G:190:THR:HG23	1:G:200:ILE:HG21	1.90	0.54
1:K:169:ASN:ND2	1:K:186:ALA:HB2	2.19	0.54
1:K:224:HIS:H	1:K:272:SER:HB2	1.72	0.54
2:L:381(E):ASN:C	2:L:383:GLY:H	2.11	0.54
1:A:175:LYS:NZ	1:A:175(D):LYS:HG3	2.22	0.54
1:I:156:LYS:HB3	1:I:156:LYS:NZ	2.23	0.54
1:I:171:HIS:CE1	1:I:180:ASN:HD22	2.25	0.54
1:A:175(H):LEU:HB3	1:A:176:ILE:CG1	2.38	0.53
1:I:224:HIS:H	1:I:272:SER:CB	2.21	0.53
2:F:381(C):LYS:HE2	3:S:4301:ASP:OD2	2.07	0.53
2:F:329:LEU:HD12	2:F:330:GLY:N	2.23	0.53
1:A:207:THR:CG2	1:A:210:GLN:HE21	2.19	0.53
1:E:241:GLY:N	1:E:286:GLN:HE22	2.07	0.53
2:D:381(B):ASP:OD2	2:D:381(E):ASN:HB2	2.08	0.53
1:K:241:GLY:H	1:K:286:GLN:HE22	1.54	0.53
2:L:343:PRO:HG3	3:V:4602:GLU:OE1	2.08	0.53
1:K:241:GLY:N	1:K:286:GLN:HE22	2.07	0.53
1:I:295:PRO:HB3	2:L:320:TYR:CE1	2.44	0.53
1:A:190:THR:HG23	1:A:200:ILE:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:C	1:A:242:ILE:HD12	2.29	0.53
1:K:177:ARG:HH11	1:K:177:ARG:CG	2.22	0.53
1:C:240:LYS:HE2	2:D:336:ASN:HD22	1.74	0.53
1:E:207:THR:CG2	1:E:210:GLN:HE21	2.21	0.53
1:E:224:HIS:H	1:E:272:SER:HB2	1.73	0.53
1:I:169:ASN:ND2	1:I:186:ALA:HB2	2.22	0.53
2:J:379:ASN:HD22	2:L:319:ARG:NH1	2.07	0.53
2:F:341:ARG:O	3:S:4302:GLU:HB2	2.09	0.53
1:K:207:THR:CG2	1:K:210:GLN:HE21	2.21	0.53
2:J:324:GLU:CG	1:K:291:GLN:HE22	2.16	0.53
1:I:224:HIS:H	1:I:272:SER:HB2	1.75	0.52
1:I:242:ILE:HD12	1:I:242:ILE:C	2.30	0.52
1:K:171:HIS:CE1	1:K:180:ASN:HD22	2.23	0.52
2:B:324:GLU:N	1:C:291:GLN:HE22	2.06	0.52
1:E:242:ILE:HD12	1:E:242:ILE:C	2.29	0.52
1:E:224:HIS:H	1:E:272:SER:CB	2.22	0.52
1:G:156:LYS:NZ	1:G:156:LYS:HB3	2.25	0.52
1:G:241:GLY:N	1:G:286:GLN:HE22	2.07	0.52
2:B:329:LEU:HD12	2:B:330:GLY:N	2.25	0.52
2:B:390:THR:CG2	2:D:388:GLN:HE21	2.22	0.52
2:B:373:VAL:O	2:B:377:VAL:HG23	2.10	0.52
1:E:156:LYS:NZ	1:E:156:LYS:HB3	2.25	0.52
1:E:175(E):VAL:HG21	1:E:175(H):LEU:HD12	1.91	0.52
1:E:175(E):VAL:CG1	1:E:175(H):LEU:HD12	2.40	0.52
1:G:224:HIS:H	1:G:272:SER:CB	2.22	0.52
2:H:329:LEU:HD12	2:H:330:GLY:N	2.25	0.52
2:F:381(E):ASN:C	2:F:382:MET:HG2	2.30	0.52
2:J:329:LEU:HD12	2:J:330:GLY:N	2.25	0.52
1:I:151:LYS:HG3	2:L:375:TYR:CE2	2.44	0.52
1:K:156:LYS:HB3	1:K:156:LYS:NZ	2.25	0.52
1:G:268:LEU:O	1:G:271:PRO:HD3	2.10	0.52
2:H:373:VAL:O	2:H:377:VAL:HG23	2.10	0.52
1:I:175(B):ARG:O	1:I:175(C):GLU:C	2.47	0.52
1:A:156:LYS:NZ	1:A:156:LYS:HB3	2.25	0.51
2:B:319:ARG:HG2	2:B:320:TYR:N	2.25	0.51
1:C:156:LYS:NZ	1:C:156:LYS:HB3	2.26	0.51
2:D:369:ILE:O	2:D:373:VAL:HG23	2.10	0.51
1:K:174:ALA:CA	1:K:175(B):ARG:HH21	2.18	0.51
1:A:268:LEU:O	1:A:271:PRO:HD3	2.09	0.51
1:A:224:HIS:H	1:A:272:SER:CB	2.23	0.51
1:E:291:GLN:HE22	2:H:324:GLU:CG	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLY:N	1:A:286:GLN:HE22	2.09	0.51
1:K:160:LYS:HB2	1:K:161:PRO:CD	2.24	0.51
1:C:175(I):HIS:O	1:C:176:ILE:HG12	2.11	0.50
1:E:175(E):VAL:CG2	1:E:175(H):LEU:HD12	2.41	0.50
1:I:190:THR:HG23	1:I:200:ILE:HG21	1.92	0.50
1:E:240:LYS:HE2	2:F:336:ASN:HD22	1.76	0.50
1:G:171:HIS:CE1	1:G:180:ASN:HD22	2.24	0.50
1:I:175(H):LEU:O	1:I:175(J):SER:N	2.45	0.50
1:C:224:HIS:H	1:C:272:SER:CB	2.24	0.50
1:E:298:THR:CG2	2:H:319:ARG:HH21	2.05	0.50
1:I:241:GLY:H	1:I:286:GLN:HE22	1.57	0.50
2:L:381(E):ASN:C	2:L:383:GLY:N	2.65	0.50
1:I:161:PRO:O	1:I:162:ARG:HB2	2.12	0.50
1:C:175(H):LEU:C	1:C:175(I):HIS:O	2.48	0.49
1:E:190:THR:HG23	1:E:200:ILE:HG21	1.94	0.49
1:I:257:PRO:HB2	1:I:260:GLU:HG2	1.93	0.49
1:A:175:LYS:HZ3	1:A:175(D):LYS:CG	2.25	0.49
2:D:351:GLN:O	2:D:355:GLN:HG3	2.12	0.49
2:D:366:ILE:O	2:D:366:ILE:HD13	2.12	0.49
1:I:240:LYS:HE2	2:J:336:ASN:HD22	1.75	0.49
1:C:190:THR:HG23	1:C:200:ILE:HG21	1.95	0.49
1:E:297:GLU:OE1	1:E:297:GLU:HA	2.11	0.49
2:B:388:GLN:NE2	2:D:390:THR:HG21	2.28	0.49
1:C:224:HIS:H	1:C:272:SER:HB2	1.77	0.49
2:B:361:CYS:HB2	2:B:362:PRO:HD3	1.95	0.49
2:L:359:GLU:O	2:L:362(B):ARG:HD3	2.13	0.49
1:C:242:ILE:HD12	1:C:242:ILE:C	2.33	0.49
2:D:373:VAL:O	2:D:377:VAL:HG23	2.12	0.49
1:E:175(H):LEU:O	1:E:175(J):SER:N	2.46	0.49
2:F:324:GLU:N	1:G:291:GLN:HE22	2.09	0.49
2:J:381(D):LYS:C	2:J:382:MET:H	2.15	0.49
1:K:257:PRO:HB2	1:K:260:GLU:HG2	1.94	0.49
1:C:176:ILE:HG22	1:C:237:HIS:CD2	2.48	0.49
2:F:361:CYS:HB2	2:F:362:PRO:HD3	1.95	0.49
2:B:366:ILE:O	2:B:366:ILE:HD13	2.12	0.49
2:B:388:GLN:HE21	2:D:390:THR:CG2	2.25	0.48
1:K:297:GLU:HG2	1:K:298:THR:H	1.78	0.48
1:E:175(H):LEU:HB3	1:E:176:ILE:CD1	2.32	0.48
1:G:175(H):LEU:O	1:G:176:ILE:HG12	2.12	0.48
1:G:242:ILE:C	1:G:242:ILE:HD12	2.34	0.48
2:F:351:GLN:O	2:F:355:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:241:GLY:N	1:I:286:GLN:HE22	2.10	0.48
1:K:190:THR:HG23	1:K:200:ILE:HG21	1.95	0.48
2:B:319:ARG:HH11	2:D:379:ASN:ND2	2.11	0.48
1:E:240:LYS:HA	2:F:335:ASN:HD21	1.78	0.48
1:E:257:PRO:HB2	1:E:260:GLU:HG2	1.94	0.48
1:A:295:PRO:HB3	2:D:320:TYR:CE1	2.49	0.48
2:F:324:GLU:CG	1:G:291:GLN:HE22	2.22	0.48
1:I:175(H):LEU:O	1:I:176:ILE:HG13	2.12	0.48
1:K:160:LYS:CB	1:K:161:PRO:HD3	2.24	0.48
1:A:257:PRO:HB2	1:A:260:GLU:HG2	1.95	0.48
1:G:203:HIS:HB3	1:G:206:CYS:SG	2.53	0.48
1:E:294:ILE:HG21	1:G:267:GLY:HA3	1.96	0.48
1:I:175(F):PRO:C	1:I:175(H):LEU:H	2.17	0.48
2:J:351:GLN:O	2:J:355:GLN:HG3	2.14	0.48
1:E:174:ALA:O	1:E:175(A):ALA:N	2.47	0.48
2:F:359:GLU:O	2:F:362(B):ARG:HD3	2.13	0.48
2:H:359:GLU:O	2:H:362(B):ARG:HD3	2.13	0.48
1:I:267:GLY:HA3	1:K:294:ILE:CD1	2.41	0.48
2:L:365:ASP:O	2:L:369:ILE:HG13	2.14	0.48
1:G:169:ASN:ND2	1:G:186:ALA:HB2	2.22	0.48
2:J:375:TYR:CE2	1:K:151:LYS:HG3	2.49	0.48
1:K:161:PRO:O	1:K:162:ARG:HB2	2.13	0.48
1:C:257:PRO:HB2	1:C:260:GLU:HG2	1.95	0.47
2:D:361:CYS:HB2	2:D:362:PRO:HD3	1.96	0.47
1:G:175(H):LEU:HG	1:G:176:ILE:HG13	1.96	0.47
2:J:341:ARG:NH1	3:U:4504:ASA:OD1	2.47	0.47
2:D:359:GLU:O	2:D:362(B):ARG:HD3	2.13	0.47
1:E:174:ALA:C	1:E:175(A):ALA:N	2.67	0.47
1:G:257:PRO:HB2	1:G:260:GLU:HG2	1.95	0.47
2:F:324:GLU:N	1:G:291:GLN:NE2	2.48	0.47
1:I:175(E):VAL:HG12	1:I:175(F):PRO:HD2	1.96	0.47
1:A:175(J):SER:O	1:A:176:ILE:C	2.49	0.47
1:C:161:PRO:O	1:C:162:ARG:HB2	2.14	0.47
2:H:361:CYS:HB2	2:H:362:PRO:HD3	1.96	0.47
2:H:343:PRO:HB2	3:T:4400:PHQ:C6	2.45	0.47
2:B:359:GLU:O	2:B:362(B):ARG:HD3	2.15	0.47
1:A:240:LYS:HA	2:B:335:ASN:HD21	1.80	0.47
1:G:240:LYS:HA	2:H:335:ASN:HD21	1.80	0.47
1:I:176:ILE:CG2	1:I:237:HIS:CD2	2.98	0.47
1:K:175(H):LEU:CA	1:K:176:ILE:HD11	2.45	0.47
1:K:240:LYS:HA	2:L:335:ASN:HD21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:PRO:O	1:E:162:ARG:HB2	2.15	0.47
2:J:359:GLU:O	2:J:362(B):ARG:HD3	2.15	0.47
2:F:320:TYR:CE1	1:G:295:PRO:HB3	2.50	0.47
1:I:163:GLY:HA3	1:I:229:CYS:O	2.15	0.47
1:E:175:LYS:HA	1:E:175(C):GLU:HB3	1.96	0.47
2:F:322:PRO:HD2	2:H:378:SER:HB3	1.97	0.47
1:I:267:GLY:HA3	1:K:294:ILE:HG21	1.96	0.47
2:L:381(C):LYS:CG	2:L:381(D):LYS:H	2.20	0.47
1:C:268:LEU:O	1:C:271:PRO:HD3	2.15	0.47
1:C:240:LYS:HA	2:D:335:ASN:HD21	1.79	0.47
2:L:343:PRO:CG	3:V:4602:GLU:OE1	2.63	0.47
2:B:351:GLN:O	2:B:355:GLN:HG3	2.15	0.46
1:I:174:ALA:HA	1:I:175(B):ARG:HH21	1.80	0.46
1:I:291:GLN:HE22	2:L:324:GLU:CG	2.25	0.46
1:K:179:ARG:HH12	1:K:182:THR:CG2	2.27	0.46
1:K:203:HIS:HB3	1:K:206:CYS:SG	2.55	0.46
2:B:369:ILE:O	2:B:373:VAL:HG23	2.15	0.46
1:C:177:ARG:HG3	1:C:177:ARG:NH1	2.27	0.46
1:G:207:THR:OG1	1:G:210:GLN:HG3	2.15	0.46
1:I:240:LYS:HA	2:J:335:ASN:HD21	1.81	0.46
2:J:381(C):LYS:N	2:J:381(C):LYS:HD2	2.29	0.46
1:C:169:ASN:ND2	1:C:186:ALA:HB2	2.22	0.46
2:J:361:CYS:HB2	2:J:362:PRO:HD3	1.97	0.46
1:G:161:PRO:O	1:G:162:ARG:HB2	2.14	0.46
1:I:175(F):PRO:HB2	1:I:175(G):LYS:H	1.50	0.46
1:E:175:LYS:O	1:E:175(D):LYS:N	2.41	0.46
1:K:242:ILE:C	1:K:242:ILE:HD12	2.36	0.46
1:C:175(I):HIS:C	1:C:176:ILE:H	2.17	0.46
2:F:381(C):LYS:CD	2:F:381(C):LYS:N	2.68	0.46
2:B:381(B):ASP:OD2	2:B:381(E):ASN:HB2	2.16	0.46
2:J:365:ASP:O	2:J:369:ILE:HG13	2.16	0.46
1:K:268:LEU:O	1:K:271:PRO:HD3	2.16	0.46
2:L:366:ILE:O	2:L:366:ILE:HD13	2.16	0.46
1:G:163:GLY:HA3	1:G:229:CYS:O	2.16	0.45
1:I:175(B):ARG:O	1:I:175(D):LYS:N	2.49	0.45
2:L:361:CYS:HB2	2:L:362:PRO:HD3	1.98	0.45
1:A:179:ARG:HH12	1:A:182:THR:CG2	2.28	0.45
1:A:169:ASN:ND2	1:A:186:ALA:HB2	2.26	0.45
2:B:375:TYR:CE2	1:C:151:LYS:HG3	2.51	0.45
1:E:268:LEU:O	1:E:271:PRO:HD3	2.16	0.45
2:F:328:LEU:HD12	2:F:329:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175(F):PRO:C	1:I:175(H):LEU:N	2.69	0.45
1:E:160:LYS:CB	1:E:161:PRO:HD3	2.24	0.45
2:B:318:THR:O	2:B:319:ARG:CB	2.64	0.45
1:C:207:THR:HB	1:C:247:ASP:OD1	2.16	0.45
2:L:351:GLN:O	2:L:355:GLN:HG3	2.17	0.45
1:A:175(E):VAL:CG1	1:A:175(H):LEU:HG	2.47	0.45
2:D:328:LEU:HD12	2:D:329:LEU:N	2.31	0.45
1:C:175(H):LEU:O	1:C:175(I):HIS:O	2.34	0.45
1:C:203:HIS:HB3	1:C:206:CYS:SG	2.57	0.45
1:K:175(F):PRO:O	1:K:175(H):LEU:N	2.45	0.45
1:A:203:HIS:HB3	1:A:206:CYS:SG	2.57	0.45
1:K:177:ARG:HB3	1:K:177:ARG:CZ	2.45	0.45
2:F:319:ARG:NH1	2:H:379:ASN:HD21	2.15	0.45
1:E:151:LYS:HG3	2:H:375:TYR:CE2	2.52	0.45
2:L:381(C):LYS:H	2:L:381(C):LYS:CD	2.26	0.45
1:K:297:GLU:HG2	1:K:298:THR:N	2.32	0.45
1:C:175(E):VAL:O	1:C:175(F):PRO:C	2.55	0.45
2:F:360:ARG:HD3	2:F:364:ASP:OD2	2.16	0.45
1:K:163:GLY:HA3	1:K:229:CYS:O	2.17	0.45
1:K:177:ARG:NH1	1:K:177:ARG:CG	2.81	0.44
1:E:203:HIS:HB3	1:E:206:CYS:SG	2.57	0.44
2:F:396:LYS:HE2	1:G:299:ASP:HB3	1.95	0.44
2:J:366:ILE:O	2:J:366:ILE:HD13	2.17	0.44
2:J:395:ARG:HB3	2:L:375:TYR:HA	1.99	0.44
2:J:328:LEU:HD12	2:J:329:LEU:N	2.33	0.44
1:A:175:LYS:HZ3	1:A:175(D):LYS:CD	2.31	0.44
1:C:163:GLY:HA3	1:C:229:CYS:O	2.17	0.44
1:A:294:ILE:CD1	1:C:267:GLY:HA3	2.46	0.44
1:A:296:VAL:O	2:D:318:THR:HA	2.16	0.44
2:D:341:ARG:HA	2:D:347:THR:HA	2.00	0.44
1:I:207:THR:HB	1:I:247:ASP:OD1	2.18	0.44
1:E:209:GLU:OE1	1:E:209:GLU:HA	2.18	0.44
1:G:175(B):ARG:HD3	1:G:176:ILE:O	2.17	0.44
2:H:366:ILE:O	2:H:366:ILE:HD13	2.18	0.44
1:I:203:HIS:HB3	1:I:206:CYS:SG	2.58	0.44
1:K:171:HIS:CE1	1:K:180:ASN:ND2	2.81	0.44
1:A:161:PRO:O	1:A:162:ARG:HB2	2.17	0.44
2:D:360:ARG:HD3	2:D:364:ASP:OD2	2.17	0.44
2:F:365:ASP:O	2:F:369:ILE:HG13	2.17	0.44
1:G:179:ARG:HH12	1:G:182:THR:CG2	2.31	0.44
1:I:175(A):ALA:HB2	1:I:246:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175(H):LEU:CD2	1:I:176:ILE:HD11	2.46	0.44
2:J:358:ARG:O	2:J:362:PRO:HG2	2.18	0.44
2:J:396:LYS:HE2	1:K:299:ASP:HB3	1.98	0.44
2:L:360:ARG:HD3	2:L:364:ASP:OD2	2.16	0.44
2:B:396:LYS:HE3	1:C:299:ASP:OD2	2.18	0.44
2:H:328:LEU:HD12	2:H:329:LEU:N	2.33	0.44
1:I:291:GLN:HE22	2:L:324:GLU:N	2.15	0.44
1:K:175(I):HIS:O	1:K:176:ILE:HD13	2.17	0.44
2:D:343:PRO:HD2	3:R:4200:PHQ:C3	2.48	0.44
1:E:291:GLN:NE2	2:H:324:GLU:HG3	2.28	0.43
1:I:207:THR:HG22	1:I:246:THR:HG22	1.99	0.43
2:B:328:LEU:HD12	2:B:329:LEU:N	2.33	0.43
1:C:203:HIS:CG	1:C:214:ILE:HD13	2.53	0.43
2:D:339:SER:HA	2:D:385:GLN:OE1	2.18	0.43
2:F:358:ARG:O	2:F:362:PRO:HG2	2.18	0.43
1:K:240:LYS:HE2	2:L:336:ASN:HD22	1.82	0.43
1:K:243:ILE:HD11	1:K:282:ILE:CG2	2.48	0.43
1:E:175(E):VAL:O	1:E:175(F):PRO:O	2.36	0.43
1:A:175(E):VAL:HA	1:A:175(F):PRO:HD3	1.84	0.43
2:B:320:TYR:CE1	1:C:295:PRO:HB3	2.53	0.43
1:G:240:LYS:HE2	2:H:336:ASN:HD22	1.83	0.43
2:L:341:ARG:HA	2:L:347:THR:HA	2.01	0.43
1:C:179:ARG:HH12	1:C:182:THR:CG2	2.29	0.43
1:C:207:THR:HG22	1:C:246:THR:HG22	2.01	0.43
2:D:375:TYR:O	2:D:378:SER:HB2	2.19	0.43
1:E:207:THR:HG22	1:E:246:THR:HG22	2.00	0.43
2:F:375:TYR:O	2:F:378:SER:HB2	2.19	0.43
2:H:335:ASN:O	2:H:336:ASN:HB2	2.19	0.43
1:I:219:GLN:O	1:I:219:GLN:HG2	2.19	0.43
1:C:175(B):ARG:HH12	1:C:178:ASP:CG	2.22	0.43
1:E:179:ARG:HH12	1:E:182:THR:CG2	2.28	0.43
2:J:360:ARG:HD3	2:J:364:ASP:OD2	2.19	0.43
2:J:339:SER:HA	2:J:385:GLN:OE1	2.19	0.43
1:E:163:GLY:HA3	1:E:229:CYS:O	2.18	0.43
1:E:175(B):ARG:HD3	1:E:176:ILE:O	2.18	0.43
2:L:358:ARG:O	2:L:362:PRO:HG2	2.18	0.43
2:B:319:ARG:NH2	1:C:299:ASP:H	2.17	0.43
1:I:299:ASP:HB3	2:L:396:LYS:HE2	2.01	0.43
2:H:360:ARG:HD3	2:H:364:ASP:OD2	2.18	0.43
1:K:175:LYS:O	1:K:175(A):ALA:C	2.57	0.43
1:I:294:ILE:CD1	1:K:267:GLY:HA3	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:324:GLU:CB	1:K:291:GLN:HE22	2.32	0.42
2:D:381(B):ASP:O	2:D:382:MET:N	2.51	0.42
2:F:341:ARG:HA	2:F:347:THR:HA	2.00	0.42
2:J:338:VAL:HB	3:U:4503:VAL:HB	2.01	0.42
1:E:176:ILE:HG21	1:E:237:HIS:CD2	2.55	0.42
1:I:265:PHE:CD1	1:I:265:PHE:N	2.88	0.42
2:J:324:GLU:HG3	1:K:291:GLN:NE2	2.24	0.42
2:B:341:ARG:HA	2:B:347:THR:HA	2.01	0.42
2:D:342:ASN:OD1	2:D:345:GLU:HG2	2.20	0.42
1:E:175:LYS:HG2	1:E:175(C):GLU:OE2	2.18	0.42
1:K:175(F):PRO:CG	1:K:175(G):LYS:H	2.26	0.42
1:G:156:LYS:HG2	1:G:157:SER:H	1.85	0.42
1:I:299:ASP:HB3	2:L:396:LYS:CE	2.49	0.42
2:B:361:CYS:N	2:B:362:PRO:CD	2.83	0.42
1:K:175(H):LEU:O	1:K:176:ILE:HD11	2.19	0.42
1:K:207:THR:HG22	1:K:246:THR:HG22	2.02	0.42
2:F:375:TYR:C	2:F:375:TYR:CD1	2.93	0.42
2:H:351:GLN:O	2:H:355:GLN:HG3	2.20	0.42
1:I:179:ARG:HH12	1:I:182:THR:CG2	2.29	0.42
1:A:207:THR:OG1	1:A:210:GLN:HG3	2.20	0.42
1:E:208:VAL:HG23	1:E:245:GLY:HA3	2.02	0.42
2:J:396:LYS:HZ3	1:K:299:ASP:HB3	1.83	0.42
1:A:299:ASP:HB3	2:D:396:LYS:HZ3	1.83	0.41
2:B:319:ARG:NH2	1:C:299:ASP:CB	2.71	0.41
2:D:370:LEU:HA	2:D:370:LEU:HD23	1.89	0.41
1:G:296:VAL:HB	4:G:541:HOH:O	2.20	0.41
2:H:341:ARG:HA	2:H:347:THR:HA	2.01	0.41
2:J:322:PRO:HD2	2:L:378:SER:HB3	2.02	0.41
2:L:381(E):ASN:O	2:L:383:GLY:N	2.53	0.41
1:C:200:ILE:HD13	1:C:200:ILE:N	2.35	0.41
1:K:165:CYS:HA	1:K:231:ILE:O	2.20	0.41
1:K:265:PHE:CD1	1:K:265:PHE:N	2.88	0.41
1:K:297:GLU:CG	1:K:298:THR:H	2.32	0.41
1:A:175(H):LEU:O	1:A:175(J):SER:N	2.54	0.41
2:B:335:ASN:O	2:B:336:ASN:HB2	2.19	0.41
2:B:360:ARG:HD3	2:B:364:ASP:OD2	2.19	0.41
1:E:152:VAL:HG12	1:E:153:TYR:N	2.35	0.41
1:A:207:THR:HG22	1:A:246:THR:HG22	2.03	0.41
1:C:152:VAL:HG12	1:C:153:TYR:N	2.35	0.41
1:E:203:HIS:CG	1:E:214:ILE:HD13	2.56	0.41
1:A:208:VAL:CG2	1:A:254:GLN:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:370:LEU:HA	2:J:370:LEU:HD23	1.89	0.41
1:K:203:HIS:CG	1:K:214:ILE:HD13	2.55	0.41
2:B:365:ASP:O	2:B:369:ILE:HG13	2.21	0.41
2:F:339:SER:HA	2:F:385:GLN:OE1	2.21	0.41
2:H:342:ASN:OD1	2:H:345:GLU:HG2	2.20	0.41
1:A:266:THR:HG21	4:A:518:HOH:O	2.21	0.41
2:F:381(E):ASN:O	2:F:382:MET:HG2	2.21	0.41
1:I:171:HIS:CE1	1:I:180:ASN:ND2	2.82	0.41
1:I:297:GLU:OE1	1:I:297:GLU:HA	2.21	0.41
2:L:361:CYS:N	2:L:362:PRO:CD	2.84	0.41
1:C:176:ILE:CG2	1:C:237:HIS:CD2	3.04	0.41
1:C:241:GLY:CA	1:C:286:GLN:HE22	2.34	0.41
2:D:329:LEU:HD12	2:D:330:GLY:H	1.85	0.41
2:D:381(E):ASN:O	2:D:382:MET:HB2	2.20	0.41
1:E:177:ARG:NE	3:S:4302:GLU:HG2	2.36	0.41
1:G:160:LYS:CB	1:G:161:PRO:HD3	2.25	0.41
1:I:175(A):ALA:O	1:I:175(E):VAL:HG23	2.20	0.41
2:B:370:LEU:HA	2:B:370:LEU:HD23	1.90	0.41
1:I:203:HIS:CG	1:I:214:ILE:HD13	2.56	0.41
1:A:163:GLY:HA3	1:A:229:CYS:O	2.21	0.41
2:B:379:ASN:ND2	2:D:319:ARG:NH1	2.56	0.41
2:F:361:CYS:N	2:F:362:PRO:CD	2.84	0.41
2:L:335:ASN:O	2:L:336:ASN:HB2	2.21	0.41
1:A:216:LYS:HE3	1:A:220:LEU:HD11	2.03	0.41
1:A:239:ASP:OD1	1:A:240:LYS:N	2.51	0.41
2:B:319:ARG:O	2:B:320:TYR:HD1	2.04	0.41
2:F:342:ASN:OD1	2:F:345:GLU:HG2	2.21	0.41
2:H:361:CYS:N	2:H:362:PRO:CD	2.84	0.41
2:J:379:ASN:ND2	2:L:319:ARG:NH1	2.68	0.41
2:B:378:SER:HB3	2:D:322:PRO:HD2	2.03	0.40
1:G:207:THR:HG22	1:G:246:THR:HG22	2.02	0.40
1:I:209:GLU:OE1	1:I:209:GLU:HA	2.21	0.40
1:K:175(F):PRO:HG2	1:K:175(G):LYS:HG2	2.02	0.40
1:C:156:LYS:HG2	1:C:157:SER:H	1.86	0.40
1:E:182:THR:O	1:E:185:ASP:N	2.54	0.40
1:E:298:THR:O	1:E:298:THR:HG22	2.21	0.40
1:I:156:LYS:HG2	1:I:157:SER:H	1.86	0.40
1:K:200:ILE:HD13	1:K:200:ILE:N	2.36	0.40
2:L:329:LEU:HD12	2:L:330:GLY:H	1.86	0.40
1:A:175(E):VAL:HG11	1:A:175(H):LEU:HG	2.03	0.40
1:C:265:PHE:N	1:C:265:PHE:CD1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:CYS:N	2:D:362:PRO:CD	2.84	0.40
1:K:191:THR:HG22	1:K:195:GLU:OE2	2.22	0.40
1:K:207:THR:HB	1:K:247:ASP:OD1	2.21	0.40
2:L:328:LEU:HD12	2:L:329:LEU:N	2.36	0.40
1:A:207:THR:HB	1:A:247:ASP:OD1	2.21	0.40
1:C:170:ASN:HB3	1:C:173:PHE:CZ	2.56	0.40
1:C:172:ASN:N	1:C:205:ASP:OD1	2.49	0.40
1:E:267:GLY:HA3	1:G:294:ILE:CD1	2.45	0.40
2:J:360:ARG:NH2	2:J:372:GLU:OE2	2.42	0.40
1:K:152:VAL:HG12	1:K:153:TYR:N	2.37	0.40
2:L:375:TYR:C	2:L:375:TYR:CD1	2.95	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	151/153 (99%)	134 (89%)	15 (10%)	2 (1%)	14	43
1	C	151/153 (99%)	125 (83%)	19 (13%)	7 (5%)	3	11
1	E	151/153 (99%)	128 (85%)	13 (9%)	10 (7%)	1	4
1	G	151/153 (99%)	132 (87%)	17 (11%)	2 (1%)	14	43
1	I	151/153 (99%)	126 (83%)	16 (11%)	9 (6%)	2	5
1	K	151/153 (99%)	131 (87%)	15 (10%)	5 (3%)	4	18
2	B	87/89 (98%)	78 (90%)	7 (8%)	2 (2%)	7	27
2	D	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
2	F	87/89 (98%)	78 (90%)	8 (9%)	1 (1%)	17	48
2	H	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
2	J	87/89 (98%)	80 (92%)	5 (6%)	2 (2%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	87/89 (98%)	79 (91%)	7 (8%)	1 (1%)	17	48
3	Q	2/5 (40%)	2 (100%)	0	0	100	100
3	R	2/5 (40%)	2 (100%)	0	0	100	100
3	S	2/5 (40%)	2 (100%)	0	0	100	100
3	T	2/5 (40%)	2 (100%)	0	0	100	100
3	U	2/5 (40%)	2 (100%)	0	0	100	100
3	V	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1440/1482 (97%)	1264 (88%)	135 (9%)	41 (3%)	6	22

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	319	ARG
1	C	175(F)	PRO
1	C	175(G)	LYS
1	C	175(H)	LEU
1	C	175(J)	SER
1	E	174	ALA
1	E	175(F)	PRO
1	E	175(I)	HIS
1	I	175(B)	ARG
1	I	175(C)	GLU
1	I	175(G)	LYS
1	I	175(I)	HIS
2	J	381(D)	LYS
2	J	381(E)	ASN
1	K	175(H)	LEU
1	A	157	SER
1	C	157	SER
1	C	175(I)	HIS
1	E	157	SER
1	E	175(G)	LYS
2	F	381(D)	LYS
1	G	157	SER
1	I	157	SER
1	I	175(F)	PRO
1	K	157	SER
1	K	175(C)	GLU
1	K	175(G)	LYS
2	B	381(D)	LYS

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Mol	Chain	Res	Type
1	E	298	THR
1	I	174	ALA
2	L	381(C)	LYS
1	E	167	ILE
1	E	175(A)	ALA
1	I	266	THR
1	C	167	ILE
1	E	175	LYS
1	K	167	ILE
1	I	167	ILE
1	A	167	ILE
1	G	167	ILE
1	E	296	VAL

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	135/135 (100%)	129 (96%)	6 (4%)	33	67
1	C	135/135 (100%)	129 (96%)	6 (4%)	33	67
1	E	135/135 (100%)	128 (95%)	7 (5%)	27	61
1	G	135/135 (100%)	127 (94%)	8 (6%)	23	55
1	I	135/135 (100%)	131 (97%)	4 (3%)	46	80
1	K	135/135 (100%)	129 (96%)	6 (4%)	33	67
2	B	82/82 (100%)	77 (94%)	5 (6%)	22	53
2	D	82/82 (100%)	76 (93%)	6 (7%)	16	43
2	F	82/82 (100%)	75 (92%)	7 (8%)	12	35
2	H	82/82 (100%)	77 (94%)	5 (6%)	22	53
2	J	82/82 (100%)	77 (94%)	5 (6%)	22	53
2	L	82/82 (100%)	76 (93%)	6 (7%)	16	43
3	Q	3/3 (100%)	3 (100%)	0	100	100
3	R	3/3 (100%)	2 (67%)	1 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	3/3 (100%)	2 (67%)	1 (33%)	0	0
3	T	3/3 (100%)	3 (100%)	0	100	100
3	U	3/3 (100%)	3 (100%)	0	100	100
3	V	3/3 (100%)	3 (100%)	0	100	100
All	All	1320/1320 (100%)	1247 (94%)	73 (6%)	25	58

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	LYS
1	A	176	ILE
1	A	182	THR
1	A	184	LEU
1	A	243	ILE
1	A	272	SER
2	B	335	ASN
2	B	365	ASP
2	B	366	ILE
2	B	375	TYR
2	B	381(B)	ASP
1	C	156	LYS
1	C	177	ARG
1	C	182	THR
1	C	184	LEU
1	C	243	ILE
1	C	272	SER
2	D	318	THR
2	D	335	ASN
2	D	365	ASP
2	D	366	ILE
2	D	375	TYR
2	D	381(C)	LYS
3	R	4201	ASP
1	E	156	LYS
1	E	175(F)	PRO
1	E	176	ILE
1	E	182	THR
1	E	184	LEU
1	E	243	ILE
1	E	272	SER
2	F	318	THR

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Mol	Chain	Res	Type
2	F	335	ASN
2	F	365	ASP
2	F	366	ILE
2	F	375	TYR
2	F	381(C)	LYS
2	F	382	MET
3	S	4302	GLU
1	G	156	LYS
1	G	175	LYS
1	G	175(H)	LEU
1	G	175(J)	SER
1	G	177	ARG
1	G	184	LEU
1	G	243	ILE
1	G	272	SER
2	H	318	THR
2	H	335	ASN
2	H	365	ASP
2	H	366	ILE
2	H	375	TYR
1	I	156	LYS
1	I	184	LEU
1	I	243	ILE
1	I	272	SER
2	J	335	ASN
2	J	365	ASP
2	J	366	ILE
2	J	375	TYR
2	J	381(D)	LYS
1	K	156	LYS
1	K	175(J)	SER
1	K	182	THR
1	K	184	LEU
1	K	243	ILE
1	K	272	SER
2	L	335	ASN
2	L	365	ASP
2	L	366	ILE
2	L	375	TYR
2	L	381(B)	ASP
2	L	381(C)	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	171	HIS
1	A	180	ASN
1	A	210	GLN
1	A	226	ASN
1	A	286	GLN
1	A	291	GLN
2	B	335	ASN
2	B	336	ASN
2	B	379	ASN
2	B	388	GLN
1	C	169	ASN
1	C	171	HIS
1	C	180	ASN
1	C	210	GLN
1	C	226	ASN
1	C	286	GLN
1	C	291	GLN
2	D	335	ASN
2	D	336	ASN
2	D	379	ASN
1	E	169	ASN
1	E	171	HIS
1	E	180	ASN
1	E	210	GLN
1	E	226	ASN
1	E	286	GLN
1	E	291	GLN
2	F	335	ASN
2	F	336	ASN
1	G	169	ASN
1	G	171	HIS
1	G	180	ASN
1	G	210	GLN
1	G	226	ASN
1	G	286	GLN
1	G	291	GLN
2	H	335	ASN
2	H	336	ASN
1	I	169	ASN
1	I	171	HIS
1	I	180	ASN

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Mol	Chain	Res	Type
1	I	210	GLN
1	I	226	ASN
1	I	286	GLN
1	I	291	GLN
2	J	335	ASN
2	J	336	ASN
2	J	379	ASN
1	K	169	ASN
1	K	171	HIS
1	K	180	ASN
1	K	210	GLN
1	K	226	ASN
1	K	286	GLN
1	K	291	GLN
2	L	335	ASN
2	L	336	ASN
2	L	381(E)	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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$
3	ASA	Q	4104	1,3	4,7,7	2.43	3 (75%)	3,8,8	0.96	0
3	ASA	R	4204	1,3	4,7,7	1.79	2 (50%)	3,8,8	2.98	1 (33%)
3	ASA	S	4304	1,3	4,7,7	2.41	2 (50%)	3,8,8	0.98	0
3	ASA	T	4404	1,3	4,7,7	2.14	2 (50%)	3,8,8	0.74	0
3	ASA	U	4504	1,3	4,7,7	1.94	2 (50%)	3,8,8	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ASA	V	4604	1	4,7,7	2.23	2 (50%)	3,8,8	1.01	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
3	ASA	Q	4104	1,3	-	0/2/6/6	0/0/0/0
3	ASA	R	4204	1,3	-	0/2/6/6	0/0/0/0
3	ASA	S	4304	1,3	-	0/2/6/6	0/0/0/0
3	ASA	T	4404	1,3	-	0/2/6/6	0/0/0/0
3	ASA	U	4504	1,3	-	0/2/6/6	0/0/0/0
3	ASA	V	4604	1	-	0/2/6/6	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	4104	ASA	CA-N	-2.16	1.40	1.47
3	R	4204	ASA	CA-C	2.46	1.53	1.50
3	Q	4104	ASA	O-C	2.55	1.30	1.19
3	R	4204	ASA	O-C	2.55	1.30	1.19
3	U	4504	ASA	CA-C	2.58	1.53	1.50
3	T	4404	ASA	O-C	2.62	1.31	1.19
3	V	4604	ASA	O-C	2.85	1.32	1.19
3	U	4504	ASA	O-C	2.86	1.32	1.19
3	S	4304	ASA	O-C	3.11	1.33	1.19
3	T	4404	ASA	CA-C	3.28	1.54	1.50
3	V	4604	ASA	CA-C	3.34	1.54	1.50
3	Q	4104	ASA	CA-C	3.51	1.54	1.50
3	S	4304	ASA	CA-C	3.59	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	4204	ASA	O-C-CA	-5.07	111.01	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	4104	ASA	1	0
3	T	4404	ASA	1	0
3	U	4504	ASA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	4603:VAL	C	4604:ASA	N	1.20

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	153/153 (100%)	-0.01	5 (3%) 47 40	26, 51, 79, 97	0
1	C	153/153 (100%)	0.14	8 (5%) 28 23	30, 60, 85, 100	0
1	E	153/153 (100%)	0.33	7 (4%) 33 28	34, 65, 94, 99	0
1	G	153/153 (100%)	-0.05	2 (1%) 77 76	23, 49, 81, 96	0
1	I	153/153 (100%)	0.34	14 (9%) 10 6	42, 64, 96, 100	0
1	K	153/153 (100%)	0.66	21 (13%) 3 2	45, 72, 99, 100	0
2	B	89/89 (100%)	-0.10	1 (1%) 80 79	26, 48, 84, 95	0
2	D	89/89 (100%)	0.15	4 (4%) 34 29	27, 57, 91, 98	0
2	F	89/89 (100%)	0.54	8 (8%) 10 7	28, 66, 97, 99	0
2	H	89/89 (100%)	-0.16	2 (2%) 62 59	31, 49, 85, 96	0
2	J	89/89 (100%)	0.34	6 (6%) 19 14	37, 66, 97, 100	0
2	L	89/89 (100%)	0.81	18 (20%) 1 1	39, 70, 97, 100	0
3	Q	3/5 (60%)	-0.62	0 100 100	30, 30, 39, 42	0
3	R	3/5 (60%)	0.15	0 100 100	70, 70, 76, 87	0
3	S	3/5 (60%)	1.36	1 (33%) 0 0	72, 72, 86, 93	0
3	T	3/5 (60%)	-0.72	0 100 100	33, 33, 35, 48	0
3	U	3/5 (60%)	0.99	0 100 100	92, 92, 97, 99	0
3	V	3/5 (60%)	1.20	1 (33%) 0 0	100, 100, 100, 100	0
All	All	1470/1482 (99%)	0.25	98 (6%) 19 14	23, 60, 95, 100	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	402	SER	5.2
2	J	320	TYR	4.5
1	E	298	THR	4.5

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Mol	Chain	Res	Type	RSRZ
2	F	359	GLU	4.1
1	K	288	ASP	4.1
2	L	335	ASN	4.0
1	I	298	THR	4.0
1	K	298	THR	4.0
1	C	298	THR	3.8
2	L	344	ALA	3.8
2	L	382	MET	3.8
2	L	318	THR	3.8
1	K	160	LYS	3.7
2	J	318	THR	3.7
2	L	381(E)	ASN	3.6
2	L	383	GLY	3.5
2	L	381(D)	LYS	3.4
2	L	336	ASN	3.4
1	I	299	ASP	3.4
1	E	299	ASP	3.3
1	I	156	LYS	3.2
1	K	172	ASN	3.2
1	K	161	PRO	3.2
1	E	156	LYS	3.2
2	F	346	GLY	3.2
2	L	343	PRO	3.1
1	K	175(E)	VAL	3.1
1	K	171	HIS	3.1
1	C	160	LYS	3.1
1	I	175(E)	VAL	3.1
1	K	180	ASN	3.0
2	D	318	THR	3.0
1	K	175(J)	SER	3.0
2	D	336	ASN	3.0
1	I	175(F)	PRO	3.0
2	L	319	ARG	3.0
2	F	341	ARG	2.9
1	E	149	LEU	2.9
2	L	381(B)	ASP	2.9
2	F	318	THR	2.8
2	F	340	TYR	2.8
1	C	184	LEU	2.8
1	K	175(C)	GLU	2.8
1	I	175(C)	GLU	2.8
2	D	362(B)	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	363	GLY	2.7
1	C	297	GLU	2.7
1	K	299	ASP	2.7
1	I	149	LEU	2.7
2	H	319	ARG	2.7
2	F	362(B)	ARG	2.7
2	B	320	TYR	2.7
1	A	156	LYS	2.7
2	J	381(C)	LYS	2.7
2	L	362(B)	ARG	2.6
1	E	160	LYS	2.6
1	I	175(I)	HIS	2.6
1	K	156	LYS	2.6
1	I	150	ASP	2.6
1	K	149	LEU	2.6
1	C	290	TYR	2.5
1	K	236	SER	2.5
1	K	205	ASP	2.4
1	K	240	LYS	2.4
1	K	287	GLY	2.4
1	A	298	THR	2.4
2	J	381(E)	ASN	2.4
2	L	340	TYR	2.3
2	J	381(D)	LYS	2.3
1	G	160	LYS	2.3
2	F	381(E)	ASN	2.3
1	C	299	ASP	2.3
3	S	4302	GLU	2.3
2	H	318	THR	2.3
1	C	197	HIS	2.3
1	C	288	ASP	2.3
1	I	175	LYS	2.3
2	L	320	TYR	2.3
1	G	156	LYS	2.3
2	J	336	ASN	2.2
1	K	175(G)	LYS	2.2
2	D	383	GLY	2.2
1	A	175(D)	LYS	2.2
1	A	175(E)	VAL	2.2
1	K	175(I)	HIS	2.2
1	I	175(G)	LYS	2.2
1	K	175(F)	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	381(C)	LYS	2.2
2	L	359	GLU	2.2
1	A	297	GLU	2.1
2	L	355	GLN	2.1
1	E	297	GLU	2.1
1	E	157	SER	2.1
1	K	151	LYS	2.1
1	I	297	GLU	2.1
3	V	4602	GLU	2.1
1	I	184	LEU	2.1
1	I	236	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ASA	U	4504	8/8	0.88	0.28	-	65,76,82,89	0
3	ASA	S	4304	8/8	0.78	0.33	-	68,89,96,100	0
3	ASA	Q	4104	8/8	0.97	0.19	-	41,42,45,48	0
3	ASA	V	4604	8/8	0.76	0.47	-	89,99,100,100	0
3	ASA	R	4204	8/8	0.94	0.17	-	60,65,72,80	0
3	ASA	T	4404	8/8	0.96	0.18	-	19,30,35,35	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.