Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2024 – 01:25 am BST

PDB ID	:	8OMV
Title	:	Crystal structure of the constitutively active S117E/S181E mutant of human IKK2
Authors	:	McEwen, A.G.; Li, C.; Moro, S.; Poussin-Courmontagne, P.; Zanier, K.
Deposited on	:	2023-03-31
Resolution	:	4.16 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

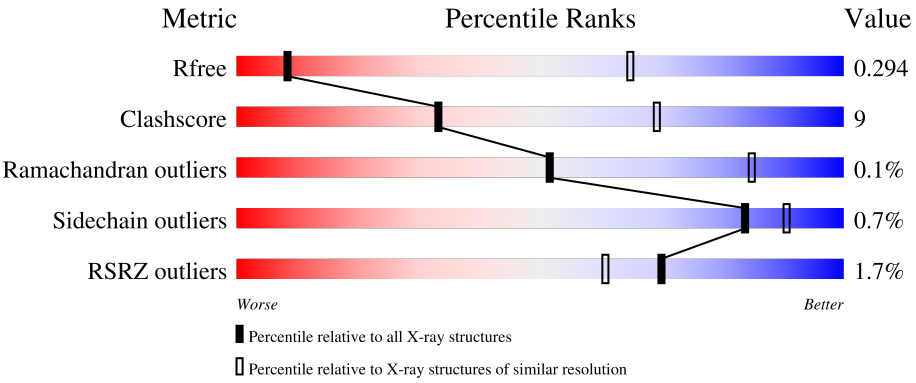
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.16 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	1020 (4.54-3.76)
Clashscore	141614	1028 (4.52-3.80)
Ramachandran outliers	138981	1005 (4.54-3.78)
Sidechain outliers	138945	1024 (4.54-3.76)
RSRZ outliers	127900	1055 (4.62-3.70)

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	671	% 72% 22% • 5%
1	B	671	74% 22% •
1	C	671	3% 75% 19% 6%
1	D	671	76% 18% • 5%
1	E	671	4% 66% 18% 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25125 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 Inhibitor of nuclear factor kappa-B kinase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	0	0
			5119	3219	902	965	33			
1	B	641	Total	C	N	O	S	0	0	0
			5183	3256	917	976	34			
1	C	630	Total	C	N	O	S	0	0	0
			5099	3208	901	957	33			
1	D	638	Total	C	N	O	S	0	0	0
			5152	3242	908	969	33			
1	E	566	Total	C	N	O	S	0	0	0
			4572	2871	810	859	32			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O14920
A	0	HIS	-	expression tag	UNP O14920
A	177	GLU	SER	engineered mutation	UNP O14920
A	181	GLU	SER	engineered mutation	UNP O14920
B	-1	GLY	-	expression tag	UNP O14920
B	0	HIS	-	expression tag	UNP O14920
B	177	GLU	SER	engineered mutation	UNP O14920
B	181	GLU	SER	engineered mutation	UNP O14920
C	-1	GLY	-	expression tag	UNP O14920
C	0	HIS	-	expression tag	UNP O14920
C	177	GLU	SER	engineered mutation	UNP O14920
C	181	GLU	SER	engineered mutation	UNP O14920
D	-1	GLY	-	expression tag	UNP O14920
D	0	HIS	-	expression tag	UNP O14920
D	177	GLU	SER	engineered mutation	UNP O14920
D	181	GLU	SER	engineered mutation	UNP O14920
E	-1	GLY	-	expression tag	UNP O14920
E	0	HIS	-	expression tag	UNP O14920
E	177	GLU	SER	engineered mutation	UNP O14920

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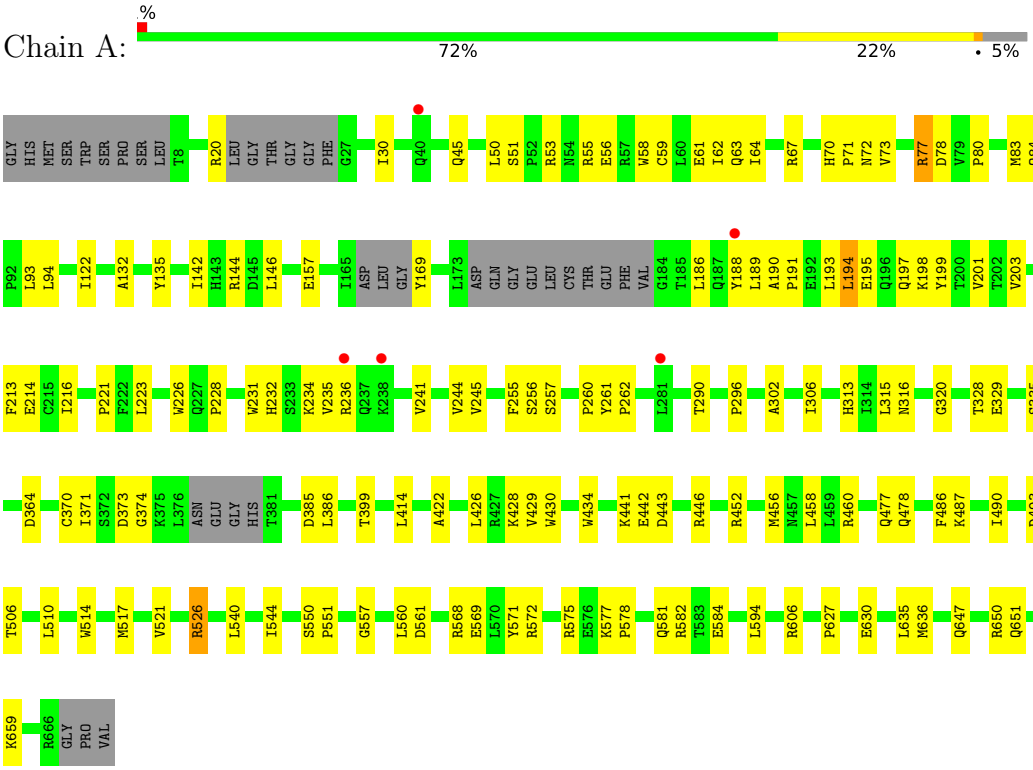
Chain	Residue	Modelled	Actual	Comment	Reference
E	181	GLU	SER	engineered mutation	UNP O14920

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.

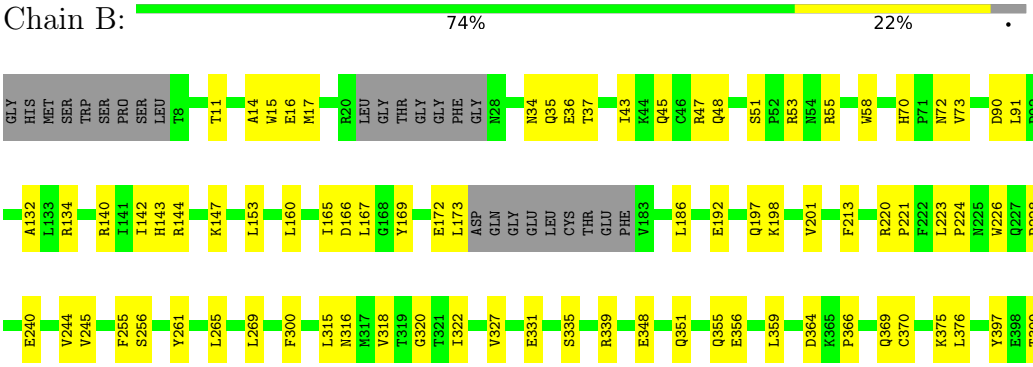
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

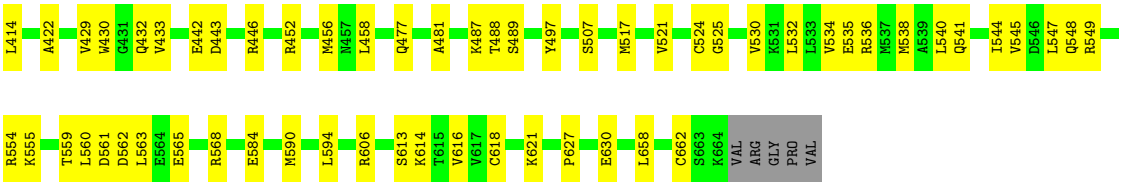
Chain A:



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

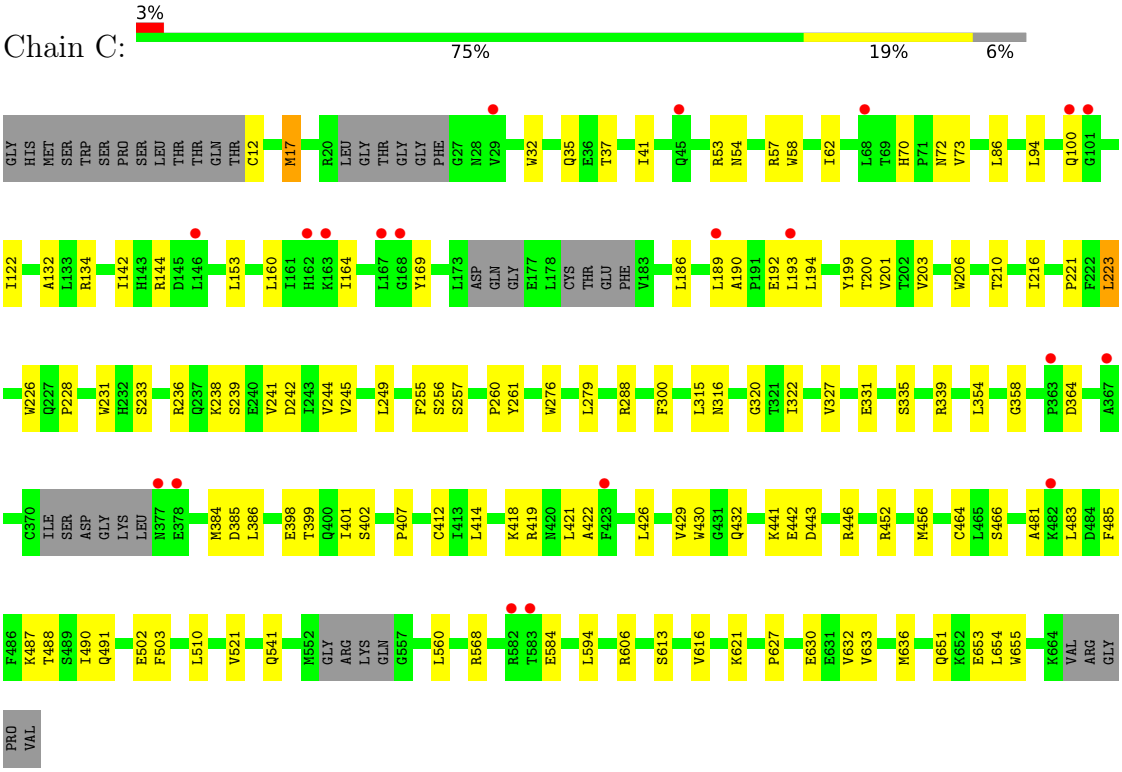
Chain B:





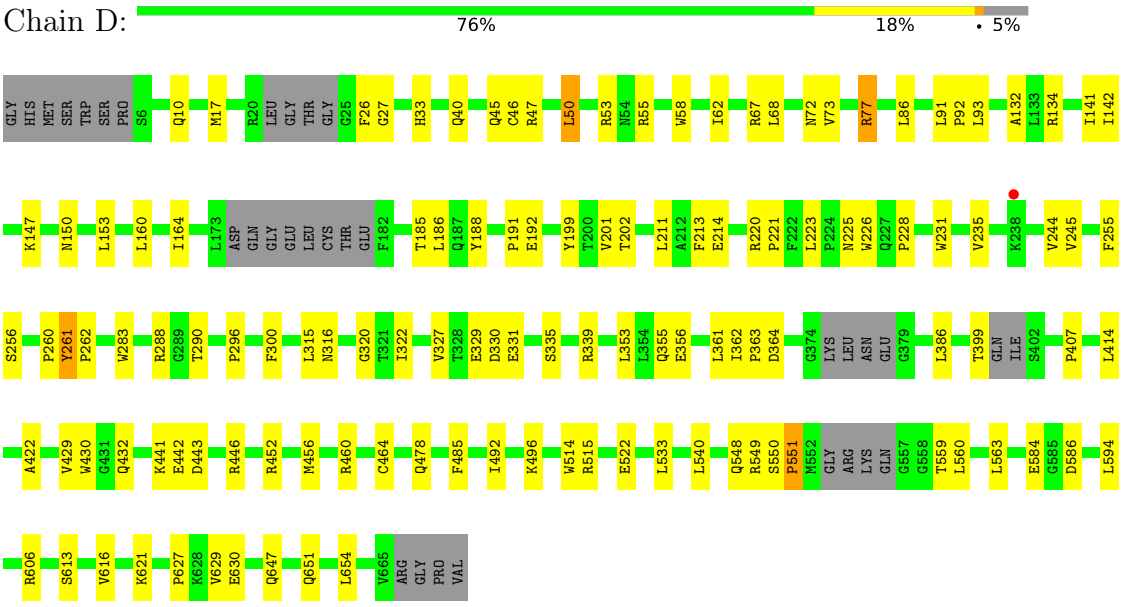
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain C:



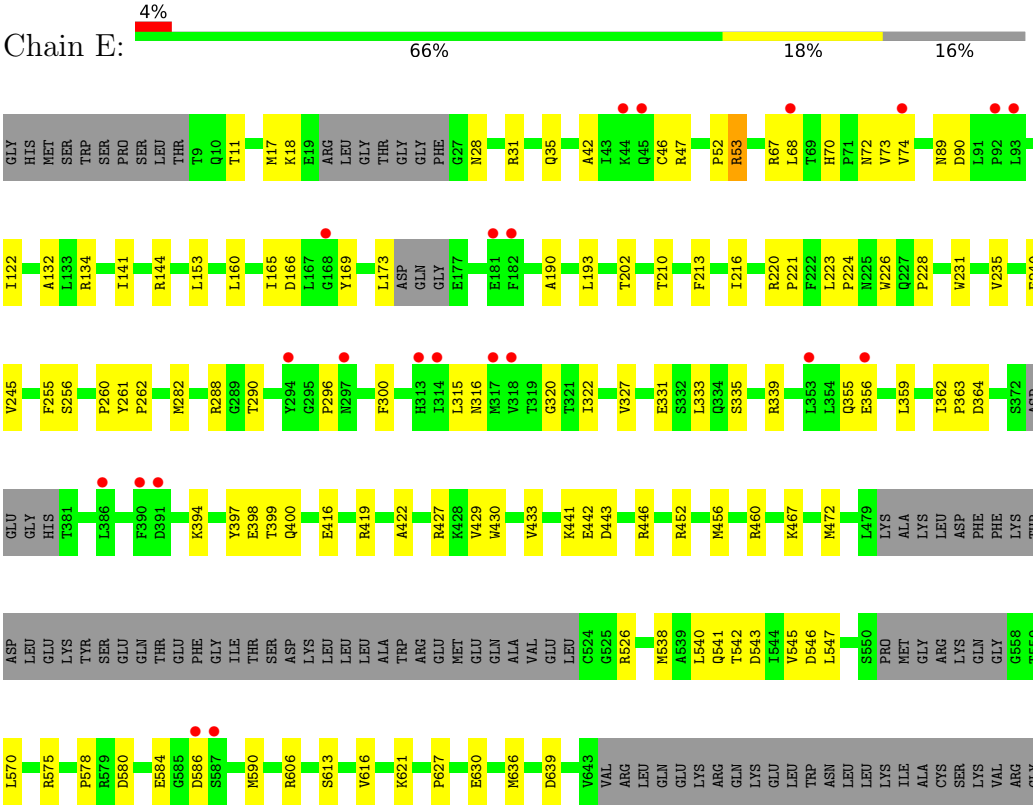
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain D:



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	226.29Å 136.80Å 204.36Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	63.25 – 4.16 63.25 – 4.16	Depositor EDS
% Data completeness (in resolution range)	43.5 (63.25-4.16) 43.5 (63.25-4.16)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.257 , 0.299 0.258 , 0.294	Depositor DCC
R_{free} test set	1018 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	155.1	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 309.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.036 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.032 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.036 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.037 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.047 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	25125	wwPDB-VP
Average B, all atoms (Å^2)	304.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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

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	0.25	0/5203	0.49	1/7028 (0.0%)
1	B	0.25	0/5270	0.49	0/7118
1	C	0.24	0/5183	0.49	0/6996
1	D	0.25	0/5238	0.48	1/7071 (0.0%)
1	E	0.24	0/4647	0.47	0/6278
All	All	0.25	0/25541	0.49	2/34491 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	50	LEU	C-N-CA	5.85	136.32	121.70
1	A	194	LEU	CA-CB-CG	5.15	127.15	115.30

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	5119	0	5131	117	0
1	B	5183	0	5212	91	0
1	C	5099	0	5127	87	0
1	D	5152	0	5172	81	0
1	E	4572	0	4595	76	0
All	All	25125	0	25237	434	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 9.

All (434) 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:A:55:ARG:HA	1:A:58:TRP:HD1	1.35	0.90
1:A:345:GLY:HA3	1:C:418:LYS:HG3	1.60	0.82
1:D:228:PRO:HA	1:D:231:TRP:HB3	1.65	0.78
1:B:140:ARG:HB3	1:B:173:LEU:HB2	1.67	0.77
1:B:366:PRO:O	1:B:369:GLN:NE2	2.16	0.77
1:A:63:GLN:HG2	1:A:67:ARG:HH12	1.50	0.76
1:A:557:GLY:HA2	1:A:560:LEU:HD13	1.66	0.76
1:D:26:PHE:HZ	1:D:47:ARG:HA	1.52	0.75
1:A:223:LEU:HB3	1:A:226:TRP:HB2	1.69	0.75
1:A:144:ARG:HH21	1:A:169:TYR:HB3	1.51	0.74
1:E:46:CYS:SG	1:E:89:ASN:ND2	2.61	0.73
1:C:62:ILE:HD12	1:C:94:LEU:HD23	1.70	0.73
1:A:55:ARG:HA	1:A:58:TRP:CD1	2.23	0.72
1:B:228:PRO:HA	1:B:231:TRP:HB3	1.71	0.72
1:E:441:LYS:HA	1:E:560:LEU:HD21	1.73	0.71
1:B:554:ARG:HH21	1:B:555:LYS:HB3	1.55	0.71
1:A:526:ARG:HH21	1:A:636:MET:HG3	1.54	0.70
1:C:419:ARG:HG2	1:C:421:LEU:HD13	1.74	0.70
1:C:228:PRO:HA	1:C:231:TRP:HB3	1.72	0.70
1:C:223:LEU:HB3	1:C:226:TRP:HB2	1.75	0.69
1:E:223:LEU:HB3	1:E:226:TRP:HB2	1.74	0.69
1:A:189:LEU:HD21	1:A:193:LEU:HD22	1.74	0.68
1:A:45:GLN:HA	1:A:93:LEU:HD13	1.74	0.68
1:C:189:LEU:HD23	1:C:194:LEU:HD23	1.75	0.68
1:A:144:ARG:HD2	1:A:199:TYR:HE2	1.58	0.67
1:A:188:TYR:OH	1:A:214:GLU:OE1	2.11	0.67
1:D:540:LEU:HD13	1:D:621:LYS:HE3	1.75	0.67
1:A:399:THR:HB	1:A:606:ARG:HG2	1.77	0.66
1:B:223:LEU:HB3	1:B:226:TRP:HB2	1.76	0.66
1:E:228:PRO:HA	1:E:231:TRP:HB3	1.78	0.66
1:E:429:VAL:HG23	1:E:430:TRP:HD1	1.60	0.66
1:B:524:CYS:SG	1:B:525:GLY:N	2.69	0.65
1:C:206:TRP:HB2	1:C:288:ARG:HD3	1.77	0.65
1:C:192:GLU:HB3	1:C:199:TYR:HB3	1.79	0.65
1:C:443:ASP:OD1	1:C:446:ARG:NH2	2.29	0.64
1:C:399:THR:HB	1:C:606:ARG:HG2	1.79	0.64
1:A:460:ARG:HH11	1:A:460:ARG:HB2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:TYR:HB3	1:D:407:PRO:HG3	1.81	0.63
1:E:540:LEU:HD13	1:E:621:LYS:HE3	1.79	0.63
1:D:429:VAL:HG23	1:D:430:TRP:HD1	1.63	0.62
1:B:458:LEU:HD21	1:B:544:ILE:HD12	1.81	0.62
1:A:70:HIS:HB3	1:A:73:VAL:HG12	1.80	0.62
1:D:185:THR:O	1:D:186:LEU:HD12	2.00	0.62
1:D:441:LYS:HA	1:D:560:LEU:HD21	1.80	0.62
1:E:223:LEU:HD12	1:E:231:TRP:HA	1.81	0.62
1:A:501:THR:HG22	1:A:506:THR:HG21	1.82	0.62
1:D:327:VAL:HG13	1:D:331:GLU:HB3	1.83	0.61
1:B:429:VAL:HG23	1:B:430:TRP:HD1	1.66	0.61
1:E:526:ARG:HE	1:E:636:MET:HG3	1.64	0.61
1:B:540:LEU:HD13	1:B:621:LYS:HE3	1.82	0.61
1:B:35:GLN:NE2	1:D:464:CYS:SG	2.74	0.61
1:D:27:GLY:O	1:D:45:GLN:NE2	2.34	0.61
1:A:477:GLN:OE1	1:B:477:GLN:NE2	2.33	0.61
1:B:549:ARG:O	1:B:549:ARG:NE	2.34	0.61
1:C:485:PHE:HE1	1:D:647:GLN:HG2	1.66	0.61
1:B:147:LYS:HD3	1:B:186:LEU:HD22	1.83	0.61
1:E:18:LYS:HB3	1:E:31:ARG:HE	1.66	0.61
1:C:488:THR:HA	1:C:491:GLN:HE21	1.66	0.60
1:C:186:LEU:HD11	1:C:228:PRO:HG3	1.83	0.60
1:C:327:VAL:HG13	1:C:331:GLU:HB3	1.83	0.60
1:A:429:VAL:HG23	1:A:430:TRP:HD1	1.67	0.60
1:C:429:VAL:HG23	1:C:430:TRP:HD1	1.66	0.60
1:B:355:GLN:HG3	1:B:356:GLU:H	1.67	0.60
1:E:67:ARG:HH12	1:E:141:ILE:HD11	1.66	0.60
1:E:327:VAL:HG13	1:E:331:GLU:HB3	1.82	0.60
1:E:11:THR:HG22	1:E:17:MET:H	1.67	0.59
1:A:647:GLN:OE1	1:A:650:ARG:NH2	2.36	0.59
1:E:134:ARG:HH21	1:E:300:PHE:HB3	1.67	0.59
1:B:134:ARG:HH21	1:B:300:PHE:HB3	1.68	0.58
1:B:327:VAL:HG13	1:B:331:GLU:HB3	1.84	0.58
1:C:502:GLU:HG2	1:C:503:PHE:CD2	2.37	0.58
1:D:548:GLN:HG2	1:D:549:ARG:HG2	1.84	0.58
1:E:190:ALA:HB3	1:E:193:LEU:HD12	1.84	0.58
1:E:538:MET:O	1:E:542:THR:HG23	2.04	0.58
1:C:53:ARG:HE	1:C:57:ARG:HH12	1.50	0.58
1:C:73:VAL:HG23	1:C:164:ILE:HB	1.85	0.58
1:E:261:TYR:HD1	1:E:262:PRO:HA	1.69	0.58
1:A:540:LEU:O	1:A:544:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLU:OE2	1:B:36:GLU:N	2.37	0.57
1:A:144:ARG:HD2	1:A:199:TYR:CE2	2.39	0.57
1:E:70:HIS:HB3	1:E:73:VAL:HG22	1.86	0.57
1:B:315:LEU:HD13	1:B:322:ILE:HG12	1.87	0.57
1:A:190:ALA:HB3	1:A:203:VAL:HG23	1.87	0.57
1:A:232:HIS:CE1	1:A:236:ARG:HD2	2.39	0.57
1:A:569:GLU:O	1:A:572:ARG:HG3	2.04	0.57
1:C:633:VAL:HA	1:C:636:MET:HG2	1.86	0.57
1:E:526:ARG:NH2	1:E:639:ASP:OD2	2.37	0.56
1:A:526:ARG:HH22	1:A:635:LEU:HB2	1.70	0.56
1:E:74:VAL:HG21	1:E:165:ILE:HG22	1.86	0.56
1:E:546:ASP:OD1	1:E:547:LEU:N	2.39	0.56
1:C:441:LYS:HA	1:C:560:LEU:HD21	1.85	0.56
1:D:231:TRP:CE2	1:D:235:VAL:HG21	2.40	0.56
1:E:399:THR:HB	1:E:606:ARG:HA	1.86	0.56
1:A:58:TRP:HZ2	1:A:91:LEU:HB2	1.70	0.56
1:A:193:LEU:HB2	1:A:203:VAL:HG21	1.88	0.56
1:E:210:THR:HA	1:E:221:PRO:HG3	1.87	0.56
1:C:483:LEU:HD22	1:C:521:VAL:HA	1.88	0.55
1:B:443:ASP:OD1	1:B:446:ARG:NH2	2.38	0.55
1:B:414:LEU:HD21	1:B:594:LEU:HD23	1.89	0.55
1:E:422:ALA:HA	1:E:584:GLU:HG2	1.88	0.55
1:A:651:GLN:NE2	1:B:489:SER:OG	2.34	0.55
1:D:33:HIS:CD2	1:D:40:GLN:HG3	2.41	0.55
1:D:261:TYR:CD1	1:D:262:PRO:HA	2.41	0.55
1:D:67:ARG:HH12	1:D:141:ILE:HD11	1.72	0.55
1:D:188:TYR:OH	1:D:214:GLU:OE1	2.19	0.54
1:E:443:ASP:OD1	1:E:446:ARG:NH2	2.38	0.54
1:C:422:ALA:HA	1:C:584:GLU:HG2	1.88	0.54
1:A:53:ARG:O	1:A:56:GLU:HG2	2.08	0.54
1:A:142:ILE:HD11	1:A:203:VAL:HG12	1.90	0.54
1:A:191:PRO:O	1:A:195:GLU:HG2	2.07	0.54
1:B:540:LEU:O	1:B:544:ILE:HG12	2.07	0.54
1:A:77:ARG:HD3	1:A:78:ASP:H	1.72	0.54
1:C:72:ASN:HB2	1:C:132:ALA:HB2	1.90	0.54
1:C:17:MET:SD	1:C:17:MET:N	2.75	0.54
1:C:144:ARG:HH21	1:C:169:TYR:HB3	1.72	0.54
1:E:153:LEU:HD12	1:E:160:LEU:HB3	1.90	0.54
1:C:316:ASN:O	1:C:320:GLY:N	2.41	0.54
1:A:62:ILE:HG23	1:A:94:LEU:HD22	1.90	0.53
1:C:134:ARG:HH21	1:C:300:PHE:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:CYS:SG	1:A:91:LEU:HD13	2.49	0.53
1:E:316:ASN:O	1:E:320:GLY:N	2.41	0.53
1:C:12:CYS:HB2	1:C:86:LEU:HB3	1.90	0.53
1:E:427:ARG:HH22	1:E:575:ARG:HH11	1.54	0.53
1:D:261:TYR:CG	1:D:262:PRO:HA	2.44	0.53
1:A:442:GLU:O	1:A:446:ARG:HG3	2.09	0.53
1:B:555:LYS:NZ	1:B:560:LEU:HB2	2.23	0.53
1:C:70:HIS:HB3	1:C:73:VAL:HG12	1.90	0.53
1:C:122:ILE:HD13	1:C:216:ILE:HG12	1.91	0.53
1:A:50:LEU:HD23	1:A:55:ARG:HG2	1.91	0.52
1:A:370:CYS:HA	1:A:385:ASP:HB2	1.90	0.52
1:C:354:LEU:HG	1:C:358:GLY:HA2	1.91	0.52
1:D:549:ARG:C	1:D:551:PRO:HD3	2.30	0.52
1:A:72:ASN:HB2	1:A:132:ALA:HB2	1.90	0.52
1:C:651:GLN:HE22	1:D:492:ILE:HD12	1.74	0.52
1:D:223:LEU:HB3	1:D:226:TRP:HB2	1.90	0.52
1:E:586:ASP:OD1	1:E:586:ASP:N	2.42	0.52
1:C:142:ILE:HD12	1:C:201:VAL:HA	1.91	0.52
1:D:50:LEU:HD21	1:D:55:ARG:HB2	1.92	0.52
1:D:452:ARG:O	1:D:456:MET:HG2	2.10	0.52
1:C:58:TRP:O	1:C:62:ILE:HG12	2.10	0.52
1:C:261:TYR:HB3	1:C:407:PRO:HG3	1.91	0.52
1:A:414:LEU:HD21	1:A:594:LEU:HD23	1.92	0.52
1:A:231:TRP:O	1:A:235:VAL:HG23	2.10	0.52
1:A:486:PHE:CE1	1:A:521:VAL:HG11	2.44	0.52
1:E:202:THR:HB	1:E:288:ARG:HD2	1.92	0.52
1:A:186:LEU:HB2	1:A:194:LEU:HD22	1.91	0.51
1:A:577:LYS:HE3	1:A:581:GLN:HB3	1.92	0.51
1:B:452:ARG:O	1:B:456:MET:HG2	2.10	0.51
1:B:72:ASN:HB2	1:B:132:ALA:HB2	1.90	0.51
1:D:153:LEU:HD12	1:D:160:LEU:HB3	1.91	0.51
1:D:443:ASP:OD1	1:D:446:ARG:NH2	2.38	0.51
1:E:122:ILE:HD13	1:E:216:ILE:HG12	1.91	0.51
1:E:627:PRO:HA	1:E:630:GLU:HB2	1.92	0.51
1:B:70:HIS:HB3	1:B:73:VAL:HG22	1.92	0.51
1:A:193:LEU:HG	1:A:199:TYR:CE1	2.45	0.51
1:D:91:LEU:HD23	1:D:92:PRO:HD2	1.93	0.51
1:A:244:VAL:HG11	1:A:260:PRO:HG3	1.92	0.51
1:A:443:ASP:OD1	1:A:446:ARG:NH1	2.44	0.51
1:B:318:VAL:HG22	1:B:397:TYR:HE1	1.76	0.51
1:A:571:TYR:OH	1:A:575:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:HD3	1:A:78:ASP:N	2.26	0.51
1:A:315:LEU:HD12	1:A:386:LEU:HD21	1.92	0.50
1:C:414:LEU:HD21	1:C:594:LEU:HD23	1.93	0.50
1:B:45:GLN:HA	1:B:93:LEU:HD22	1.92	0.50
1:A:84:GLN:OE1	1:A:84:GLN:N	2.43	0.50
1:D:72:ASN:HB2	1:D:132:ALA:HB2	1.94	0.50
1:D:522:GLU:OE1	1:D:522:GLU:N	2.44	0.50
1:E:355:GLN:NE2	1:E:359:LEU:O	2.45	0.50
1:B:375:LYS:C	1:B:376:LEU:HD23	2.32	0.50
1:C:242:ASP:HA	1:C:257:SER:HA	1.93	0.50
1:E:244:VAL:HG11	1:E:260:PRO:HG3	1.93	0.50
1:E:245:VAL:HG22	1:E:255:PHE:HD1	1.76	0.50
1:A:58:TRP:HA	1:A:61:GLU:HG2	1.92	0.49
1:C:276:TRP:O	1:C:279:LEU:HG	2.12	0.49
1:E:89:ASN:OD1	1:E:90:ASP:N	2.45	0.49
1:A:478:GLN:HG2	1:B:481:ALA:HB2	1.93	0.49
1:E:18:LYS:HD2	1:E:31:ARG:HH21	1.76	0.49
1:C:452:ARG:O	1:C:456:MET:HG2	2.11	0.49
1:C:464:CYS:SG	1:E:35:GLN:NE2	2.85	0.49
1:D:142:ILE:HD12	1:D:201:VAL:HA	1.93	0.49
1:A:245:VAL:HG22	1:A:255:PHE:HD1	1.78	0.49
1:C:153:LEU:HD12	1:C:160:LEU:HB3	1.94	0.49
1:C:315:LEU:HD13	1:C:322:ILE:HG12	1.95	0.49
1:E:416:GLU:OE2	1:E:419:ARG:NH1	2.37	0.49
1:A:345:GLY:HA3	1:C:418:LYS:CG	2.38	0.49
1:B:142:ILE:HD12	1:B:201:VAL:HA	1.94	0.49
1:D:223:LEU:HD12	1:D:231:TRP:HA	1.93	0.49
1:D:627:PRO:HA	1:D:630:GLU:HB2	1.95	0.49
1:A:197:GLN:HG2	1:A:198:LYS:N	2.28	0.49
1:B:545:VAL:HA	1:B:548:GLN:HB3	1.93	0.49
1:A:371:ILE:HG13	1:A:374:GLY:H	1.77	0.49
1:A:20:ARG:HA	1:A:30:ILE:HD13	1.95	0.49
1:D:244:VAL:CG1	1:D:256:SER:HB3	2.42	0.49
1:E:613:SER:HA	1:E:616:VAL:HG12	1.94	0.49
1:A:517:MET:O	1:A:521:VAL:HG22	2.13	0.49
1:B:58:TRP:CD1	1:B:91:LEU:HD13	2.48	0.49
1:B:192:GLU:N	1:B:192:GLU:OE1	2.44	0.49
1:C:613:SER:HA	1:C:616:VAL:HG22	1.95	0.48
1:B:561:ASP:OD1	1:B:562:ASP:N	2.46	0.48
1:E:144:ARG:HH21	1:E:169:TYR:HB3	1.77	0.48
1:C:245:VAL:HG22	1:C:255:PHE:HD1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:THR:O	1:C:203:VAL:HG22	2.13	0.48
1:D:134:ARG:HH21	1:D:300:PHE:HB3	1.77	0.48
1:B:245:VAL:HG22	1:B:255:PHE:HD1	1.79	0.48
1:A:434:TRP:CD1	1:A:568:ARG:HB3	2.49	0.48
1:B:348:GLU:HA	1:B:351:GLN:HE21	1.79	0.48
1:B:316:ASN:O	1:B:320:GLY:N	2.46	0.48
1:B:35:GLN:O	1:D:460:ARG:HD3	2.14	0.47
1:B:213:PHE:CG	1:B:221:PRO:HB3	2.49	0.47
1:B:554:ARG:HE	1:B:555:LYS:N	2.11	0.47
1:D:220:ARG:HD2	1:D:225:ASN:H	1.79	0.47
1:D:315:LEU:HB2	1:D:386:LEU:HD11	1.96	0.47
1:E:315:LEU:HD13	1:E:322:ILE:HG12	1.95	0.47
1:B:407:PRO:HG2	1:B:432:GLN:NE2	2.30	0.47
1:B:544:ILE:HD11	1:B:618:CYS:HB3	1.96	0.47
1:D:414:LEU:HD21	1:D:594:LEU:HD23	1.95	0.47
1:A:261:TYR:HD1	1:A:262:PRO:HA	1.78	0.47
1:B:223:LEU:HD12	1:B:231:TRP:HA	1.97	0.47
1:A:58:TRP:O	1:A:61:GLU:HG2	2.13	0.47
1:B:47:ARG:HG3	1:B:48:GLN:H	1.78	0.47
1:B:318:VAL:HG22	1:B:397:TYR:CE1	2.49	0.47
1:C:466:SER:HB2	1:C:541:GLN:NE2	2.29	0.47
1:A:190:ALA:HA	1:A:206:TRP:CD1	2.49	0.47
1:C:32:TRP:CZ3	1:C:86:LEU:HD13	2.50	0.47
1:A:58:TRP:CZ2	1:A:91:LEU:HB2	2.48	0.47
1:A:371:ILE:HD11	1:A:373:ASP:HB3	1.96	0.47
1:E:394:LYS:HB2	1:E:397:TYR:CZ	2.49	0.47
1:E:452:ARG:O	1:E:456:MET:HG2	2.14	0.47
1:B:397:TYR:HE2	1:B:616:VAL:HG11	1.80	0.47
1:E:18:LYS:HB2	1:E:31:ARG:HG3	1.97	0.47
1:C:144:ARG:HD2	1:C:199:TYR:CE1	2.50	0.47
1:B:355:GLN:HB3	1:B:359:LEU:HB2	1.97	0.46
1:D:290:THR:HA	1:D:296:PRO:HA	1.97	0.46
1:E:244:VAL:HG13	1:E:256:SER:HB3	1.96	0.46
1:E:356:GLU:CD	1:E:356:GLU:H	2.18	0.46
1:A:261:TYR:CD1	1:A:262:PRO:HA	2.50	0.46
1:A:316:ASN:O	1:A:320:GLY:N	2.48	0.46
1:C:315:LEU:HB2	1:C:386:LEU:HD11	1.98	0.46
1:A:190:ALA:HB2	1:A:206:TRP:HB3	1.97	0.46
1:D:192:GLU:HB3	1:D:199:TYR:HB3	1.97	0.46
1:C:58:TRP:CZ2	1:C:62:ILE:HD11	2.50	0.46
1:A:458:LEU:HD21	1:A:544:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HD12	1:B:160:LEU:HB3	1.97	0.46
1:D:47:ARG:H	1:D:47:ARG:HD2	1.81	0.46
1:E:335:SER:O	1:E:339:ARG:HG3	2.16	0.46
1:E:261:TYR:CD1	1:E:262:PRO:HA	2.50	0.46
1:A:244:VAL:CG1	1:A:256:SER:HB3	2.46	0.46
1:A:51:SER:O	1:A:55:ARG:HG3	2.15	0.46
1:A:186:LEU:HD13	1:A:228:PRO:HB3	1.98	0.46
1:D:46:CYS:H	1:D:93:LEU:HD22	1.81	0.46
1:D:68:LEU:HD21	1:D:141:ILE:HD12	1.98	0.46
1:A:460:ARG:HB2	1:A:460:ARG:NH1	2.31	0.45
1:C:655:TRP:CD1	1:D:496:LYS:HD3	2.51	0.45
1:D:77:ARG:NE	1:D:77:ARG:HA	2.32	0.45
1:A:493:ASP:HB3	1:A:514:TRP:HZ2	1.80	0.45
1:D:58:TRP:O	1:D:62:ILE:HG12	2.16	0.45
1:D:613:SER:HA	1:D:616:VAL:HG22	1.99	0.45
1:E:399:THR:HB	1:E:606:ARG:HG2	1.97	0.45
1:A:627:PRO:HA	1:A:630:GLU:HB2	1.98	0.45
1:B:627:PRO:HA	1:B:630:GLU:HB2	1.97	0.45
1:C:210:THR:HA	1:C:221:PRO:HG3	1.99	0.45
1:C:654:LEU:HD12	1:C:655:TRP:N	2.31	0.45
1:D:147:LYS:HG2	1:D:150:ASN:OD1	2.17	0.45
1:B:497:TYR:OH	1:B:507:SER:O	2.33	0.45
1:D:202:THR:HB	1:D:288:ARG:HD2	1.98	0.45
1:C:633:VAL:HA	1:C:636:MET:CG	2.47	0.45
1:D:355:GLN:HG3	1:D:356:GLU:H	1.81	0.45
1:A:142:ILE:HD12	1:A:201:VAL:HA	1.99	0.45
1:A:213:PHE:CG	1:A:221:PRO:HB3	2.52	0.45
1:A:452:ARG:O	1:A:456:MET:HG2	2.17	0.45
1:A:655:TRP:O	1:A:659:LYS:HG3	2.17	0.45
1:B:613:SER:HA	1:B:616:VAL:HG22	1.99	0.45
1:C:144:ARG:HD2	1:C:199:TYR:HE1	1.81	0.45
1:C:627:PRO:HA	1:C:630:GLU:HB2	1.97	0.45
1:D:244:VAL:HG11	1:D:260:PRO:HG3	1.99	0.45
1:D:586:ASP:OD1	1:D:586:ASP:N	2.45	0.45
1:E:42:ALA:O	1:E:96:MET:N	2.50	0.45
1:B:407:PRO:HG2	1:B:432:GLN:HE21	1.81	0.44
1:C:35:GLN:HE22	1:E:467:LYS:NZ	2.15	0.44
1:D:73:VAL:HG13	1:D:164:ILE:HG13	1.99	0.44
1:B:220:ARG:HD3	1:B:224:PRO:HA	1.98	0.44
1:C:442:GLU:O	1:C:446:ARG:HG3	2.18	0.44
1:D:514:TRP:HB2	1:D:515:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:LEU:HD13	1:D:629:VAL:HG22	1.99	0.44
1:A:422:ALA:HA	1:A:584:GLU:HG2	1.98	0.44
1:A:500:GLN:NE2	1:B:662:CYS:SG	2.91	0.44
1:A:146:LEU:O	1:A:188:TYR:HB3	2.18	0.44
1:A:190:ALA:HB3	1:A:203:VAL:CG2	2.48	0.44
1:B:244:VAL:HG13	1:B:256:SER:HB3	2.00	0.44
1:D:316:ASN:O	1:D:320:GLY:N	2.51	0.44
1:E:359:LEU:HD12	1:E:460:ARG:HH12	1.82	0.44
1:A:80:PRO:HD2	1:A:83:MET:SD	2.57	0.44
1:B:165:ILE:HG13	1:B:166:ASP:OD1	2.18	0.44
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.81	0.44
1:B:265:LEU:HD22	1:B:269:LEU:HD13	2.00	0.44
1:B:547:LEU:HD13	1:B:614:LYS:HB3	1.99	0.44
1:E:220:ARG:HB2	1:E:224:PRO:HA	2.00	0.44
1:B:55:ARG:NH2	1:B:90:ASP:OD1	2.51	0.44
1:B:335:SER:O	1:B:339:ARG:HG3	2.17	0.44
1:E:430:TRP:HZ3	1:E:570:LEU:HG	1.83	0.44
1:C:407:PRO:HG2	1:C:432:GLN:NE2	2.32	0.44
1:A:189:LEU:HD23	1:A:194:LEU:HB3	1.99	0.43
1:B:538:MET:O	1:B:541:GLN:HG2	2.17	0.43
1:C:192:GLU:OE1	1:C:288:ARG:NH2	2.49	0.43
1:C:335:SER:O	1:C:339:ARG:HG3	2.18	0.43
1:B:399:THR:HB	1:B:606:ARG:HG2	2.00	0.43
1:E:398:GLU:HG2	1:E:400:GLN:H	1.84	0.43
1:B:37:THR:HB	1:D:362:ILE:HG12	2.00	0.43
1:B:51:SER:OG	1:B:53:ARG:NH1	2.51	0.43
1:B:355:GLN:NE2	1:B:370:CYS:SG	2.73	0.43
1:C:54:ASN:HA	1:C:57:ARG:HE	1.82	0.43
1:C:238:LYS:HE3	1:C:238:LYS:HB3	1.83	0.43
1:C:249:LEU:HB3	1:C:421:LEU:HD21	2.00	0.43
1:E:244:VAL:CG1	1:E:256:SER:HB3	2.47	0.43
1:E:433:VAL:HG11	1:E:590:MET:HG2	2.00	0.43
1:C:244:VAL:HG13	1:C:256:SER:HB3	2.00	0.43
1:C:244:VAL:HG11	1:C:260:PRO:HG3	2.00	0.43
1:E:52:PRO:HD2	1:E:53:ARG:NH1	2.33	0.43
1:E:290:THR:HA	1:E:296:PRO:HA	2.01	0.43
1:C:86:LEU:HD12	1:C:86:LEU:O	2.18	0.43
1:C:244:VAL:CG1	1:C:256:SER:HB3	2.48	0.43
1:D:335:SER:O	1:D:339:ARG:HG3	2.18	0.43
1:D:363:PRO:HA	1:D:364:ASP:HA	1.74	0.43
1:E:173:LEU:HD23	1:E:173:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLU:OE1	1:B:172:GLU:N	2.42	0.43
1:C:654:LEU:HD13	1:D:654:LEU:HD21	2.00	0.43
1:D:73:VAL:HG22	1:D:164:ILE:HD11	2.01	0.43
1:A:199:TYR:HB2	1:A:203:VAL:HB	2.00	0.43
1:C:398:GLU:HB2	1:C:401:ILE:HD11	2.01	0.43
1:E:119:GLU:OE1	1:E:119:GLU:N	2.37	0.43
1:B:532:LEU:O	1:B:536:ARG:HG3	2.18	0.43
1:E:543:ASP:HA	1:E:546:ASP:OD2	2.19	0.43
1:B:15:TRP:CE3	1:B:34:ASN:HB2	2.54	0.43
1:E:72:ASN:HB2	1:E:132:ALA:HB2	2.00	0.43
1:A:568:ARG:HG3	1:A:569:GLU:OE1	2.19	0.43
1:C:190:ALA:HB3	1:C:193:LEU:HD13	2.00	0.43
1:A:70:HIS:CG	1:A:71:PRO:HD2	2.53	0.42
1:B:487:LYS:HE2	1:B:488:THR:N	2.34	0.42
1:D:315:LEU:HD13	1:D:322:ILE:HG12	2.00	0.42
1:E:68:LEU:HD21	1:E:141:ILE:HD12	2.01	0.42
1:A:658:LEU:HD13	1:B:658:LEU:HA	2.01	0.42
1:B:413:ILE:HD12	1:B:413:ILE:HA	1.90	0.42
1:B:422:ALA:HA	1:B:584:GLU:HG2	2.01	0.42
1:D:17:MET:H	1:D:17:MET:HG2	1.62	0.42
1:D:353:LEU:HD13	1:D:361:LEU:HD22	2.01	0.42
1:E:213:PHE:CG	1:E:221:PRO:HB3	2.54	0.42
1:B:517:MET:O	1:B:521:VAL:HG22	2.19	0.42
1:B:559:THR:O	1:B:563:LEU:HG	2.19	0.42
1:D:53:ARG:HD2	1:D:53:ARG:HA	1.85	0.42
1:E:442:GLU:O	1:E:446:ARG:HG3	2.20	0.42
1:A:122:ILE:HD13	1:A:216:ILE:HG12	2.02	0.42
1:A:241:VAL:HG22	1:A:257:SER:HB2	2.02	0.42
1:C:412:CYS:SG	1:C:419:ARG:NH1	2.92	0.42
1:C:426:LEU:HA	1:C:429:VAL:HG22	2.01	0.42
1:D:407:PRO:HG2	1:D:432:GLN:NE2	2.35	0.42
1:E:578:PRO:HB2	1:E:580:ASP:OD1	2.20	0.42
1:A:50:LEU:O	1:A:55:ARG:NH1	2.53	0.42
1:A:157:GLU:CD	1:A:157:GLU:H	2.23	0.42
1:A:210:THR:HA	1:A:221:PRO:HG3	2.02	0.42
1:A:335:SER:O	1:A:339:ARG:HG3	2.19	0.42
1:B:43:ILE:HA	1:B:94:LEU:O	2.20	0.42
1:D:442:GLU:O	1:D:446:ARG:HG3	2.20	0.42
1:A:434:TRP:NE1	1:A:568:ARG:HB3	2.34	0.42
1:B:197:GLN:HG3	1:B:198:LYS:H	1.85	0.42
1:B:244:VAL:CG1	1:B:256:SER:HB3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:PHE:CG	1:D:221:PRO:HB3	2.55	0.42
1:C:241:VAL:HG22	1:C:257:SER:HB2	2.01	0.42
1:B:14:ALA:HB1	1:B:36:GLU:OE2	2.20	0.42
1:B:565:GLU:O	1:B:568:ARG:HG3	2.20	0.42
1:C:233:SER:O	1:C:236:ARG:HG2	2.20	0.42
1:D:191:PRO:HB3	1:D:283:TRP:CZ3	2.55	0.42
1:D:231:TRP:O	1:D:235:VAL:HG23	2.20	0.42
1:D:514:TRP:HB2	1:D:515:ARG:NH1	2.35	0.42
1:A:223:LEU:HD22	1:A:226:TRP:CG	2.55	0.42
1:A:578:PRO:O	1:A:582:ARG:HG3	2.20	0.42
1:B:231:TRP:O	1:B:235:VAL:HG23	2.20	0.42
1:C:37:THR:HB	1:E:362:ILE:HG12	2.01	0.42
1:D:245:VAL:HG22	1:D:255:PHE:HD1	1.85	0.42
1:E:333:LEU:H	1:E:333:LEU:HD23	1.85	0.42
1:C:32:TRP:HZ3	1:C:86:LEU:HD13	1.85	0.42
1:A:62:ILE:HD12	1:A:94:LEU:HB2	2.01	0.41
1:C:238:LYS:HG2	1:C:239:SER:O	2.19	0.41
1:D:559:THR:O	1:D:563:LEU:HG	2.20	0.41
1:A:426:LEU:HA	1:A:429:VAL:HG22	2.01	0.41
1:B:144:ARG:NH2	1:B:169:TYR:HB2	2.35	0.41
1:B:532:LEU:HA	1:B:535:GLU:OE2	2.20	0.41
1:A:371:ILE:HG13	1:A:374:GLY:N	2.35	0.41
1:B:143:HIS:CE1	1:B:167:LEU:HA	2.56	0.41
1:A:510:LEU:HD12	1:A:657:LEU:HD21	2.02	0.41
1:D:10:GLN:HG3	1:D:86:LEU:HD13	2.02	0.41
1:A:290:THR:HA	1:A:296:PRO:HA	2.02	0.41
1:A:487:LYS:HA	1:A:490:ILE:HG22	2.03	0.41
1:C:481:ALA:HB2	1:D:478:GLN:HG2	2.02	0.41
1:E:316:ASN:O	1:E:320:GLY:CA	2.69	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.89	0.41
1:B:433:VAL:HG11	1:B:590:MET:HG2	2.02	0.41
1:C:316:ASN:O	1:C:320:GLY:CA	2.69	0.41
1:C:632:VAL:O	1:C:636:MET:HG2	2.20	0.41
1:E:28:ASN:ND2	1:E:166:ASP:OD2	2.53	0.41
1:B:442:GLU:O	1:B:446:ARG:HG3	2.21	0.41
1:B:559:THR:HA	1:B:562:ASP:OD2	2.21	0.41
1:D:422:ALA:HA	1:D:584:GLU:HG2	2.02	0.41
1:A:64:ILE:HA	1:A:67:ARG:HH11	1.85	0.41
1:A:193:LEU:HD23	1:A:193:LEU:O	2.21	0.41
1:A:302:ALA:O	1:A:306:ILE:HG13	2.21	0.41
1:A:441:LYS:HG3	1:A:561:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:THR:HG22	1:B:16:GLU:HA	2.03	0.41
1:C:510:LEU:HD12	1:C:653:GLU:HB3	2.03	0.41
1:D:647:GLN:O	1:D:651:GLN:HG2	2.20	0.41
1:E:231:TRP:O	1:E:235:VAL:HG23	2.21	0.41
1:A:58:TRP:O	1:A:62:ILE:HG12	2.21	0.41
1:A:328:THR:OG1	1:A:329:GLU:N	2.54	0.41
1:D:399:THR:HG23	1:D:606:ARG:HG2	2.01	0.41
1:A:83:MET:O	1:A:86:LEU:HD12	2.21	0.40
1:C:364:ASP:OD1	1:C:364:ASP:N	2.53	0.40
1:D:330:ASP:N	1:D:330:ASP:OD1	2.54	0.40
1:D:550:SER:N	1:D:551:PRO:HD3	2.36	0.40
1:E:240:GLU:OE1	1:E:282:MET:HA	2.21	0.40
1:A:223:LEU:HD11	1:A:234:LYS:HB2	2.03	0.40
1:A:656:ASN:HA	1:A:659:LYS:HE2	2.03	0.40
1:C:487:LYS:HA	1:C:490:ILE:HG22	2.03	0.40
1:E:363:PRO:HA	1:E:364:ASP:HA	1.73	0.40
1:A:313:HIS:O	1:A:386:LEU:HD12	2.22	0.40
1:C:276:TRP:CD1	1:C:279:LEU:HD21	2.56	0.40
1:D:134:ARG:HE	1:D:300:PHE:HB3	1.87	0.40
1:E:541:GLN:O	1:E:545:VAL:HG22	2.21	0.40
1:A:364:ASP:OD1	1:A:364:ASP:N	2.54	0.40
1:A:428:LYS:HB2	1:A:428:LYS:HE2	1.82	0.40
1:A:550:SER:HB2	1:A:551:PRO:HD3	2.04	0.40
1:B:240:GLU:CD	1:B:240:GLU:H	2.25	0.40
1:B:530:VAL:O	1:B:534:VAL:HG23	2.22	0.40
1:C:41:ILE:HD13	1:C:41:ILE:HA	1.85	0.40
1:D:329:GLU:OE1	1:D:329:GLU:N	2.42	0.40
1:E:223:LEU:HD23	1:E:223:LEU:HA	1.77	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	626/671 (93%)	600 (96%)	26 (4%)	0	100	100
1	B	635/671 (95%)	609 (96%)	25 (4%)	1 (0%)	47	80
1	C	618/671 (92%)	588 (95%)	28 (4%)	2 (0%)	41	76
1	D	626/671 (93%)	601 (96%)	25 (4%)	0	100	100
1	E	554/671 (83%)	527 (95%)	27 (5%)	0	100	100
All	All	3059/3355 (91%)	2925 (96%)	131 (4%)	3 (0%)	51	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	364	ASP
1	C	223	LEU
1	C	402	SER

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	568/605 (94%)	564 (99%)	4 (1%)	84	90
1	B	578/605 (96%)	575 (100%)	3 (0%)	88	93
1	C	568/605 (94%)	562 (99%)	6 (1%)	73	84
1	D	574/605 (95%)	569 (99%)	5 (1%)	78	88
1	E	513/605 (85%)	510 (99%)	3 (1%)	86	92
All	All	2801/3025 (93%)	2780 (99%)	21 (1%)	84	90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	86	LEU
1	A	135	TYR
1	A	526	ARG
1	B	17	MET

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Mol	Chain	Res	Type
1	B	107	TYR
1	B	261	TYR
1	C	17	MET
1	C	100	GLN
1	C	384	MET
1	C	385	ASP
1	C	568	ARG
1	C	621	LYS
1	D	77	ARG
1	D	211	LEU
1	D	261	TYR
1	D	485	PHE
1	D	551	PRO
1	E	47	ARG
1	E	53	ARG
1	E	472	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	109	ASN
1	A	432	GLN
1	A	448	GLN
1	A	500	GLN
1	A	651	GLN
1	B	33	HIS
1	B	35	GLN
1	B	89	ASN
1	B	109	ASN
1	B	313	HIS
1	B	351	GLN
1	B	477	GLN
1	B	478	GLN
1	C	109	ASN
1	C	448	GLN
1	C	491	GLN
1	D	33	HIS
1	D	35	GLN
1	D	70	HIS
1	D	109	ASN
1	D	369	GLN

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Mol	Chain	Res	Type
1	D	448	GLN
1	D	478	GLN
1	D	656	ASN
1	E	35	GLN
1	E	109	ASN
1	E	351	GLN
1	E	355	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	636/671 (94%)	-0.03	6 (0%) 84 77	118, 328, 413, 469	0
1	B	641/671 (95%)	-0.21	0 100 100	83, 216, 320, 393	0
1	C	630/671 (93%)	-0.06	20 (3%) 47 37	235, 335, 422, 482	0
1	D	638/671 (95%)	-0.20	1 (0%) 95 93	153, 264, 332, 413	0
1	E	566/671 (84%)	0.09	25 (4%) 34 28	290, 383, 445, 497	0
All	All	3111/3355 (92%)	-0.09	52 (1%) 70 61	83, 309, 419, 497	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	181	GLU	5.8
1	C	582	ARG	4.4
1	A	40	GLN	3.9
1	E	587	SER	3.8
1	E	45	GLN	3.8
1	E	356	GLU	3.6
1	C	146	LEU	3.5
1	E	182	PHE	3.3
1	C	189	LEU	3.2
1	E	586	ASP	3.1
1	A	238	LYS	3.1
1	C	29	VAL	3.0
1	E	168	GLY	3.0
1	C	583	THR	3.0
1	E	563	LEU	3.0
1	C	163	LYS	2.9
1	C	101	GLY	2.9
1	C	100	GLN	2.9
1	E	390	PHE	2.9
1	E	93	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	74	VAL	2.8
1	C	45	GLN	2.7
1	E	317	MET	2.7
1	E	313	HIS	2.7
1	E	386	LEU	2.7
1	E	68	LEU	2.7
1	C	378	GLU	2.6
1	E	294	TYR	2.6
1	C	482	LYS	2.6
1	E	44	LYS	2.6
1	E	297	ASN	2.5
1	E	391	ASP	2.5
1	A	188	TYR	2.5
1	C	68	LEU	2.5
1	E	243	ILE	2.5
1	C	363	PRO	2.4
1	C	367	ALA	2.4
1	C	168	GLY	2.4
1	C	423	PHE	2.3
1	A	206	TRP	2.3
1	C	162	HIS	2.2
1	E	92	PRO	2.1
1	A	281	LEU	2.1
1	A	236	ARG	2.1
1	C	193	LEU	2.1
1	D	238	LYS	2.1
1	C	377	ASN	2.1
1	E	314	ILE	2.1
1	E	353	LEU	2.1
1	E	318	VAL	2.1
1	C	167	LEU	2.0
1	E	242	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.