



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:59 AM UTC

PDB ID : 8OMV / pdb_00008omv
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

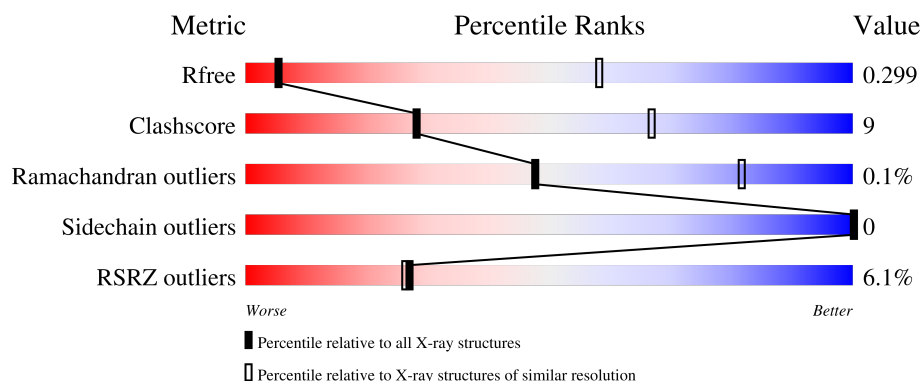
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1077 (4.50-3.82)
Clashscore	190562	1019 (4.48-3.84)
Ramachandran outliers	187476	1035 (4.50-3.82)
Sidechain outliers	187428	1022 (4.50-3.82)
RSRZ outliers	180081	1074 (4.50-3.82)

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

Mol	Chain	Length	Quality of chain
1	A	671	
1	B	671	
1	C	671	
1	D	671	
1	E	671	

2 Entry composition

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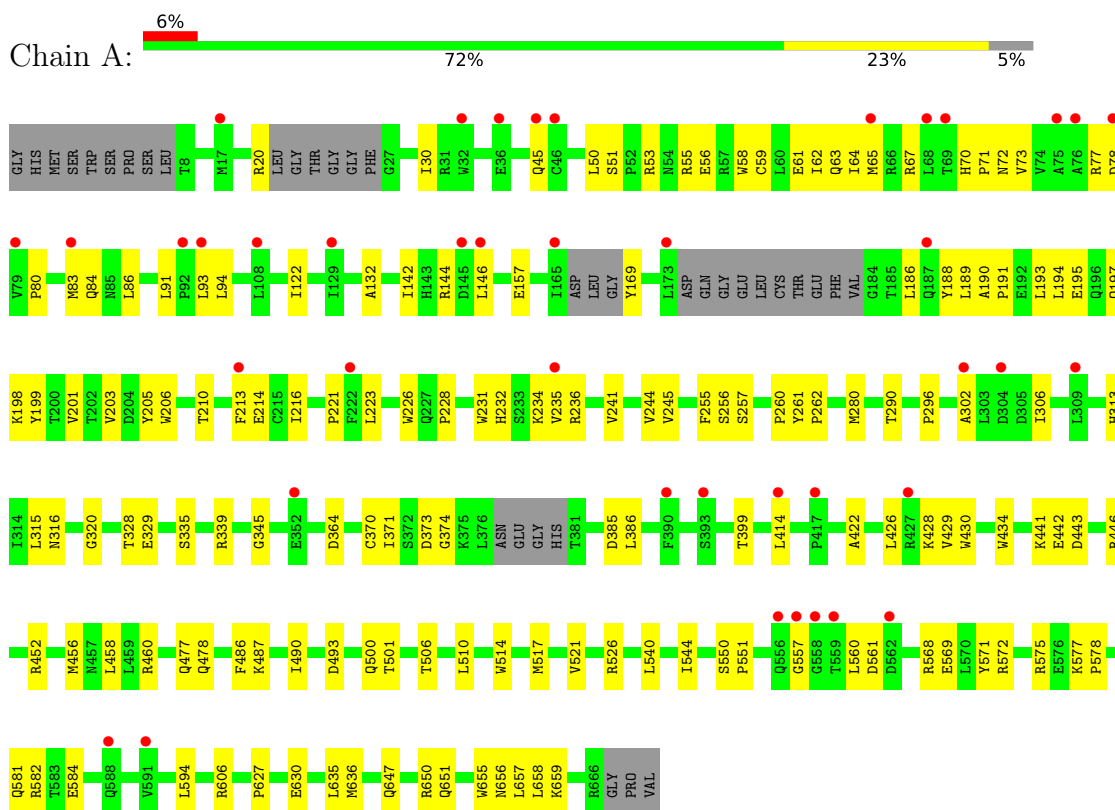
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Chain	Residue	Modelled	Actual	Comment	Reference
E	181	GLU	SER	engineered mutation	UNP O14920

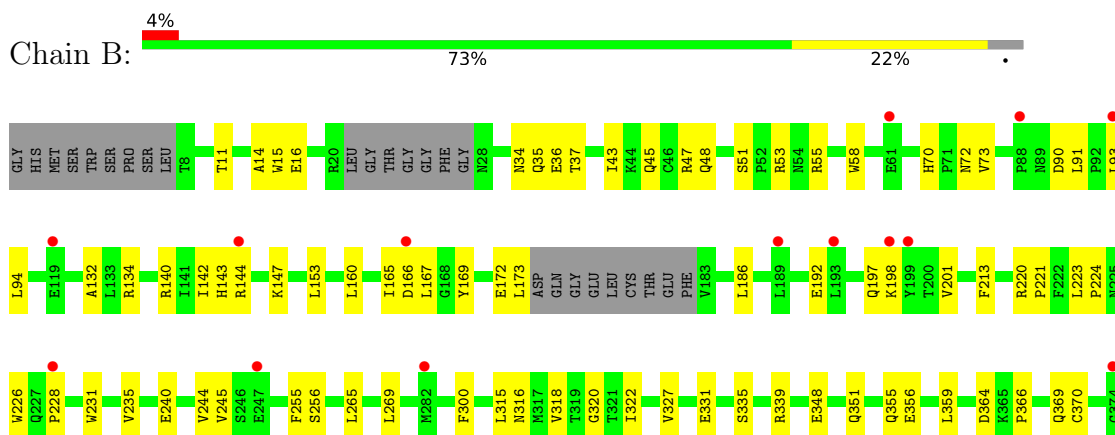
3 Residue-property plots

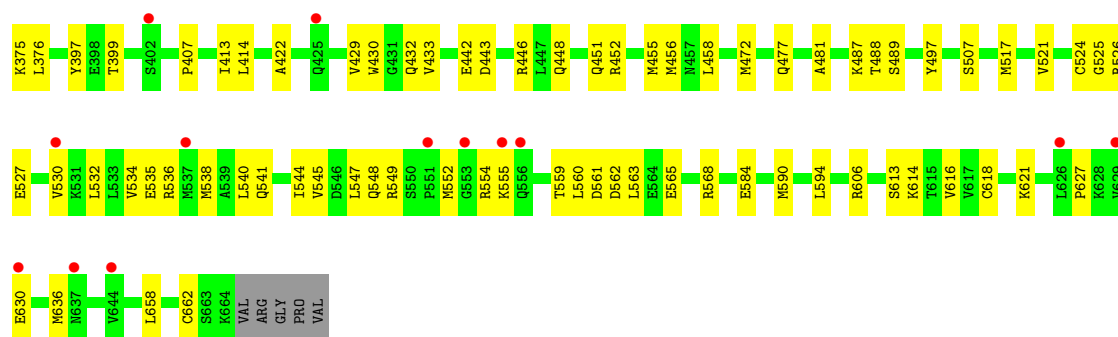
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

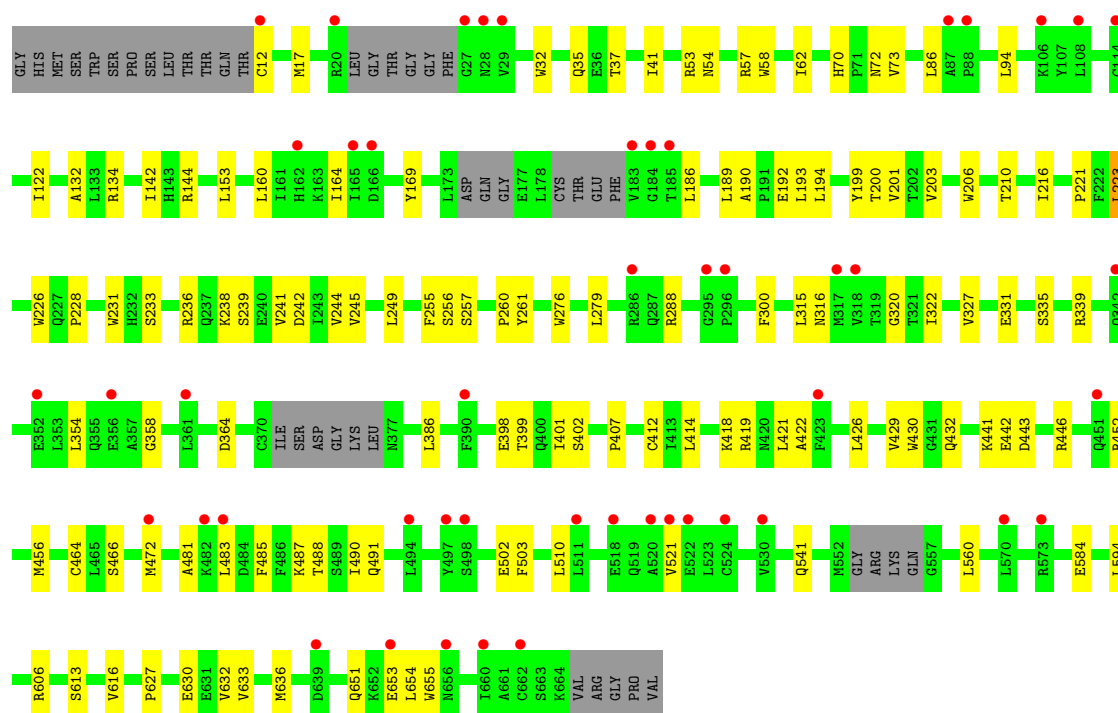
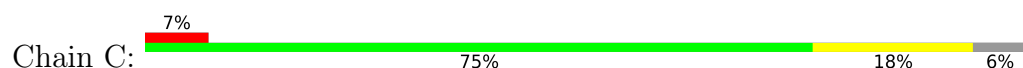


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

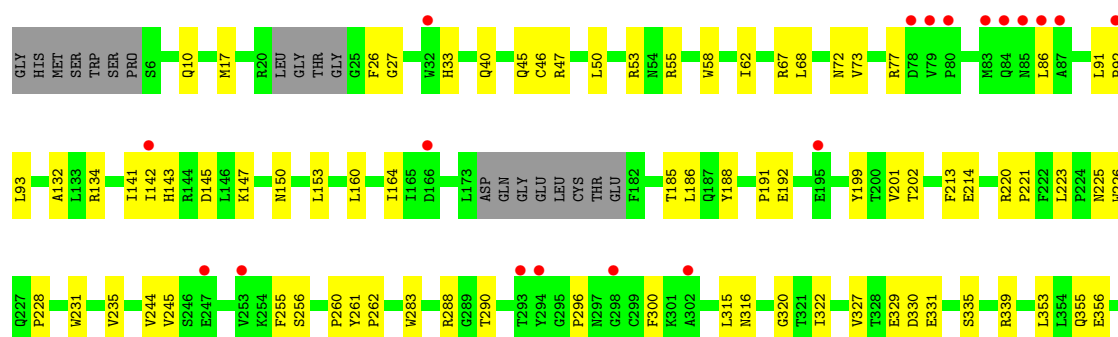
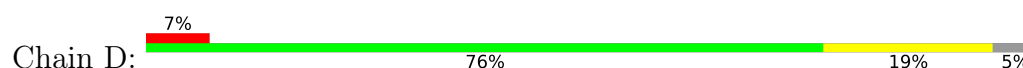


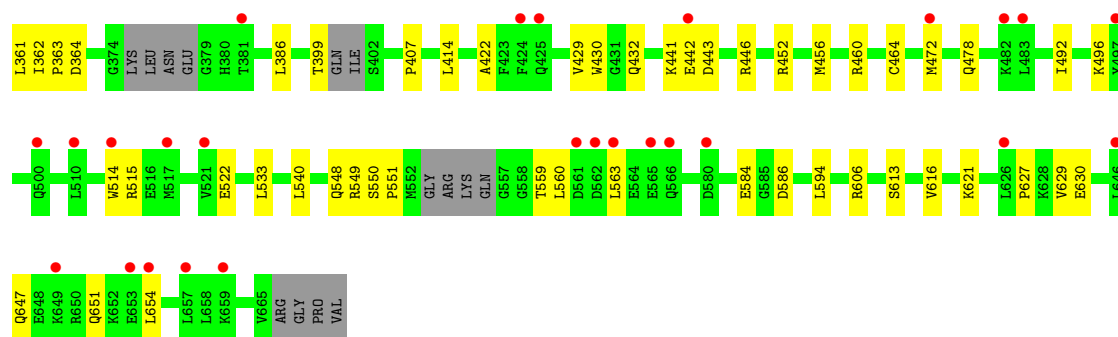


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

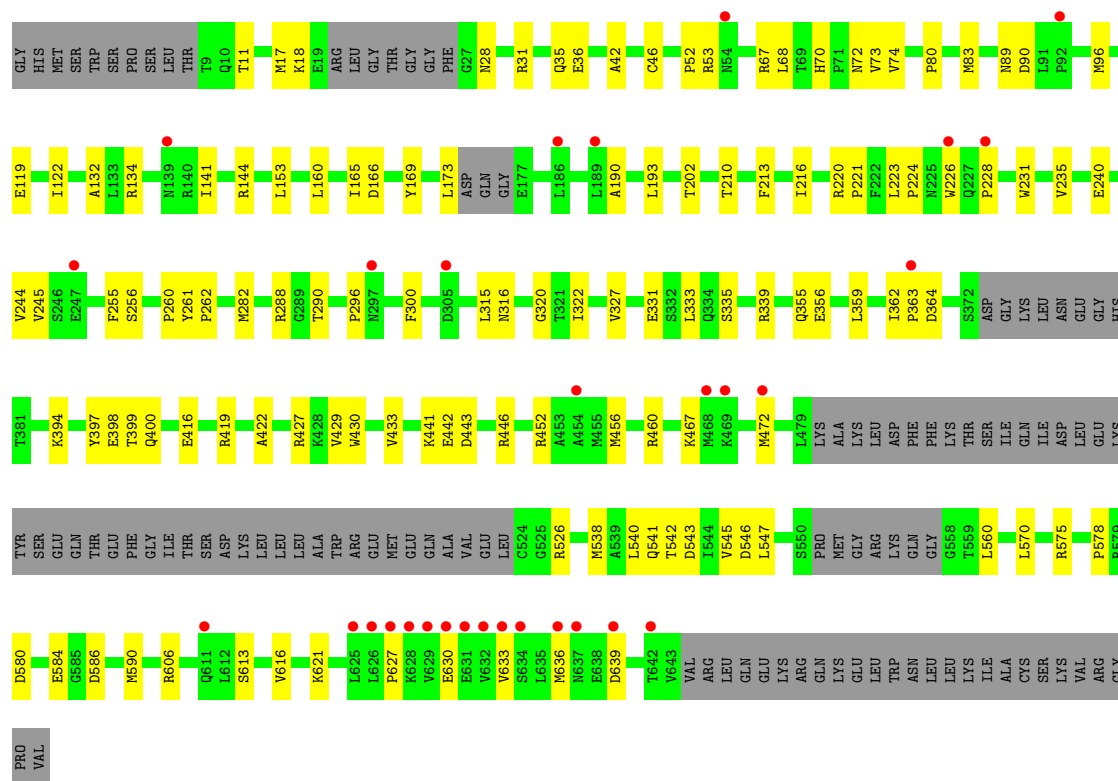


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta





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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.257 , 0.299 0.258 , 0.299	Depositor DCC
R_{free} test set	1018 reflections (2.16%)	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)	0.38 , 572.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	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	0.88	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/5203	0.34	0/7028
1	B	0.13	0/5270	0.33	0/7118
1	C	0.12	0/5183	0.32	0/6996
1	D	0.12	0/5238	0.31	0/7071
1	E	0.11	0/4647	0.30	0/6278
All	All	0.12	0/25541	0.32	0/34491

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5119	0	5131	119	0
1	B	5183	0	5212	97	0
1	C	5099	0	5127	89	0
1	D	5152	0	5172	83	0
1	E	4572	0	4595	79	0
All	All	25125	0	25237	449	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 (449) 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:B:526:ARG:HB2	1:B:636:MET:HE3	1.70	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:B:451:GLN:HB3	1:B:552:MET:HE1	1.75	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:E:472:MET:HE3	1:E:633:VAL:HG11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:448:GLN:HG3	1:B:552:MET:HE2	1.82	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
1:B:36:GLU:OE2	1:B:36:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:PRO:HG2	1:E:83:MET:HE2	1.86	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:D:549:ARG:C	1:D:551:PRO:HD3	2.30	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:B:375:LYS:C	1:B:376:LEU:HD23	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:356:GLU:CD	1:E:356:GLU:H	2.18	0.51
1:A:443:ASP:OD1	1:A:446:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:197:GLN:HG2	1:A:198:LYS:N	2.28	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:D:472:MET:HE3	1:D:472:MET:HB3	1.79	0.47
1:A:58:TRP:CZ2	1:A:91:LEU:HB2	2.48	0.47
1:A:205:TYR:HB3	1:A:280:MET:HE1	1.95	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:A:157:GLU:CD	1:A:157:GLU:H	2.23	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:A:65:MET:HE3	1:A:94:LEU:HD23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:240:GLU:H	1:B:240:GLU:CD	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:472:MET:HE3	1:B:472:MET:HB3	1.80	0.44
1:B:527:GLU:CD	1:B:527:GLU:H	2.25	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
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:C:472:MET:HE3	1:C:472:MET:HB3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:35:GLN:HG3	1:E:36:GLU:CD	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:O	1:A:55:ARG:NH1	2.53	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
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:C:636:MET:HE2	1:C:636:MET:HB3	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:B:451:GLN:HE22	1:B:455:MET:HE3	1.85	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:D:143:HIS:C	1:D:145:ASP:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	626/671 (93%)	600 (96%)	26 (4%)	0	100	100
1	B	635/671 (95%)	609 (96%)	25 (4%)	1 (0%)	43	76
1	C	618/671 (92%)	588 (95%)	28 (4%)	2 (0%)	36	70
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%)	48	82

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

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%)	568 (100%)	0	100	100
1	B	578/605 (96%)	578 (100%)	0	100	100
1	C	568/605 (94%)	568 (100%)	0	100	100
1	D	574/605 (95%)	574 (100%)	0	100	100
1	E	513/605 (85%)	513 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2801/3025 (93%)	2801 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	109	ASN
1	A	162	HIS
1	A	232	HIS
1	A	284	HIS
1	A	341	GLN
1	A	351	GLN
1	A	432	GLN
1	A	448	GLN
1	A	491	GLN
1	A	500	GLN
1	A	637	ASN
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	341	GLN
1	B	351	GLN
1	B	448	GLN
1	B	457	ASN
1	B	477	GLN
1	B	478	GLN
1	B	491	GLN
1	B	596	GLN
1	B	651	GLN
1	C	35	GLN
1	C	84	GLN
1	C	109	ASN
1	C	284	HIS
1	C	341	GLN
1	C	425	GLN
1	C	448	GLN
1	C	457	ASN

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Mol	Chain	Res	Type
1	C	491	GLN
1	C	637	ASN
1	C	656	ASN
1	D	35	GLN
1	D	70	HIS
1	D	72	ASN
1	D	85	ASN
1	D	89	ASN
1	D	109	ASN
1	D	287	GLN
1	D	341	GLN
1	D	369	GLN
1	D	392	ASN
1	D	448	GLN
1	D	478	GLN
1	D	500	GLN
1	D	588	GLN
1	D	611	GLN
1	E	35	GLN
1	E	109	ASN
1	E	113	ASN
1	E	341	GLN
1	E	351	GLN
1	E	355	GLN
1	E	448	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 oligosaccharides 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, 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	636/671 (94%)	0.45	41 (6%)	25	25	118, 328, 413, 469	0
1	B	641/671 (95%)	0.33	27 (4%)	40	34	83, 216, 320, 393	0
1	C	630/671 (93%)	0.55	48 (7%)	20	21	235, 335, 422, 482	0
1	D	638/671 (95%)	0.43	45 (7%)	22	22	153, 264, 332, 413	0
1	E	566/671 (84%)	0.45	30 (5%)	32	29	290, 383, 445, 497	0
All	All	3111/3355 (92%)	0.44	191 (6%)	27	26	83, 309, 419, 497	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	PRO	8.5
1	E	247	GLU	8.4
1	D	83	MET	7.2
1	D	195	GLU	7.0
1	E	629	VAL	6.6
1	B	556	GLN	6.2
1	D	79	VAL	6.1
1	D	84	GLN	6.0
1	A	93	LEU	5.5
1	E	632	VAL	5.5
1	D	562	ASP	5.4
1	C	660	ILE	5.4
1	D	561	ASP	5.4
1	B	374	GLY	5.3
1	C	88	PRO	5.2
1	D	653	GLU	5.0
1	A	427	ARG	4.9
1	C	521	VAL	4.8
1	D	86	LEU	4.8
1	C	524	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	12	CYS	4.5
1	E	611	GLN	4.2
1	E	628	LYS	4.1
1	C	390	PHE	4.0
1	E	633	VAL	4.0
1	B	425	GLN	3.8
1	C	520	ALA	3.8
1	E	634	SER	3.8
1	D	565	GLU	3.7
1	E	636	MET	3.7
1	C	522	GLU	3.7
1	D	483	LEU	3.6
1	D	566	GLN	3.5
1	A	108	LEU	3.5
1	B	199	TYR	3.5
1	D	580	ASP	3.5
1	E	639	ASP	3.5
1	E	468	MET	3.5
1	A	187	GLN	3.5
1	A	302	ALA	3.4
1	D	649	LYS	3.4
1	A	45	GLN	3.4
1	C	498	SER	3.4
1	C	29	VAL	3.4
1	C	166	ASP	3.3
1	D	92	PRO	3.3
1	A	390	PHE	3.3
1	B	144	ARG	3.3
1	D	500	GLN	3.3
1	A	79	VAL	3.3
1	B	551	PRO	3.2
1	C	295	GLY	3.2
1	A	352	GLU	3.2
1	D	563	LEU	3.2
1	E	189	LEU	3.2
1	E	631	GLU	3.1
1	B	637	ASN	3.1
1	C	662	CYS	3.1
1	C	511	LEU	3.1
1	A	46	CYS	3.1
1	A	393	SER	3.1
1	C	497	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	469	LYS	3.1
1	C	639	ASP	3.1
1	A	559	THR	3.1
1	D	514	TRP	3.0
1	D	424	PHE	3.0
1	A	83	MET	3.0
1	E	297	ASN	2.9
1	D	425	GLN	2.9
1	C	28	ASN	2.9
1	E	472	MET	2.9
1	A	75	ALA	2.9
1	D	654	LEU	2.9
1	A	17	MET	2.9
1	C	656	ASN	2.9
1	C	27	GLY	2.9
1	D	294	TYR	2.8
1	C	87	ALA	2.8
1	B	198	LYS	2.8
1	C	184	GLY	2.8
1	D	521	VAL	2.8
1	A	78	ASP	2.8
1	E	92	PRO	2.8
1	C	494	LEU	2.7
1	C	423	PHE	2.7
1	B	626	LEU	2.7
1	C	356	GLU	2.7
1	A	165	ILE	2.7
1	A	92	PRO	2.7
1	D	517	MET	2.7
1	A	417	PRO	2.7
1	C	518	GLU	2.6
1	C	286	ARG	2.6
1	C	317	MET	2.6
1	D	626	LEU	2.6
1	C	451	GLN	2.6
1	A	556	GLN	2.6
1	A	562	ASP	2.6
1	E	630	GLU	2.6
1	A	591	VAL	2.6
1	D	85	ASN	2.6
1	E	226	TRP	2.5
1	C	472	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	54	ASN	2.5
1	A	222	PHE	2.5
1	C	573	ARG	2.5
1	E	305	ASP	2.5
1	D	482	LYS	2.5
1	B	630	GLU	2.5
1	E	363	PRO	2.5
1	B	119	GLU	2.5
1	D	166	ASP	2.5
1	D	32	TRP	2.5
1	D	657	LEU	2.4
1	B	530	VAL	2.4
1	C	318	VAL	2.4
1	A	65	MET	2.4
1	B	193	LEU	2.4
1	C	162	HIS	2.4
1	A	309	LEU	2.4
1	C	20	ARG	2.4
1	C	108	LEU	2.4
1	E	139	ASN	2.4
1	B	537	MET	2.4
1	B	555	LYS	2.4
1	B	166	ASP	2.4
1	C	653	GLU	2.4
1	B	228	PRO	2.3
1	D	298	GLY	2.3
1	B	189	LEU	2.3
1	A	588	GLN	2.3
1	A	32	TRP	2.3
1	E	228	PRO	2.3
1	B	247	GLU	2.3
1	A	173	LEU	2.3
1	A	129	ILE	2.3
1	C	352	GLU	2.3
1	D	442	GLU	2.3
1	D	659	LYS	2.3
1	A	68	LEU	2.3
1	A	146	LEU	2.3
1	D	646	LEU	2.3
1	D	472	MET	2.3
1	D	381	THR	2.3
1	B	553	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	186	LEU	2.3
1	A	414	LEU	2.2
1	A	557	GLY	2.2
1	C	361	LEU	2.2
1	A	213	PHE	2.2
1	D	497	TYR	2.2
1	C	483	LEU	2.2
1	A	69	THR	2.2
1	D	510	LEU	2.2
1	C	530	VAL	2.2
1	A	76	ALA	2.2
1	C	342	GLN	2.2
1	A	235	VAL	2.2
1	B	282	MET	2.2
1	D	78	ASP	2.2
1	D	80	PRO	2.1
1	C	570	LEU	2.1
1	E	642	THR	2.1
1	B	644	VAL	2.1
1	A	558	GLY	2.1
1	E	627	PRO	2.1
1	A	145	ASP	2.1
1	A	304	ASP	2.1
1	E	454	ALA	2.1
1	C	114	CYS	2.1
1	C	185	THR	2.1
1	A	36	GLU	2.1
1	B	93	LEU	2.1
1	C	165	ILE	2.1
1	D	142	ILE	2.1
1	C	106	LYS	2.0
1	D	247	GLU	2.0
1	B	402	SER	2.0
1	B	629	VAL	2.0
1	C	183	VAL	2.0
1	E	625	LEU	2.0
1	B	88	PRO	2.0
1	E	637	ASN	2.0
1	B	61	GLU	2.0
1	C	482	LYS	2.0
1	D	87	ALA	2.0
1	D	302	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	253	VAL	2.0
1	D	293	THR	2.0
1	E	626	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.