



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:12 AM UTC

PDB ID : 3ZZ0 / pdb_00003zz0
Title : Crystal structure of ribosomal elongation factor (EF)-G from *Staphylococcus aureus* with a fusidic acid hyper-sensitivity mutation M16I
Authors : Koripella, R.K.; Chen, Y.; Selmer, M.; Sanyal, S.
Deposited on : 2011-08-30
Resolution : 2.80 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

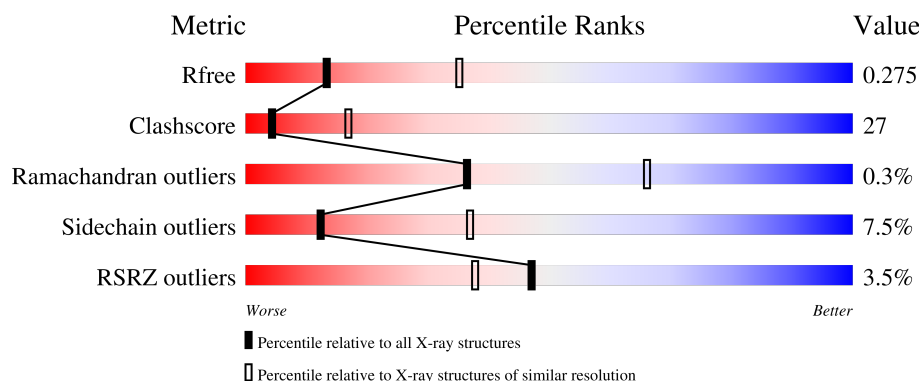
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	693	
1	B	693	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10068 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 Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	1
			5021	3154	841	1000	26			
1	B	649	Total	C	N	O	S	0	0	1
			5021	3154	841	1000	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ILE	MET	engineered mutation	UNP P68790
B	16	ILE	MET	engineered mutation	UNP P68790

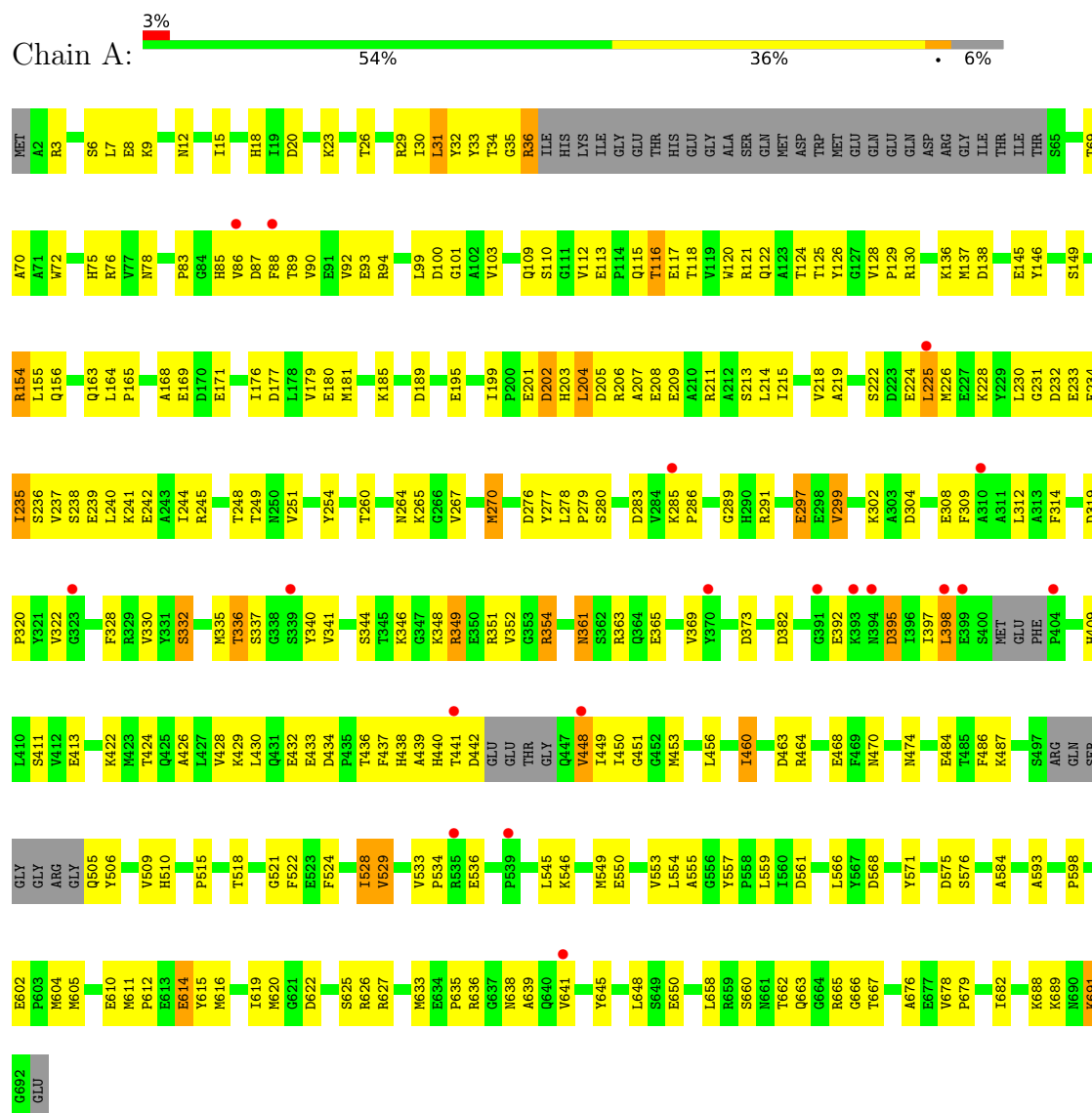
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	O	0	0
			11	11		
2	B	15	Total	O	0	0
			15	15		

3 Residue-property plots

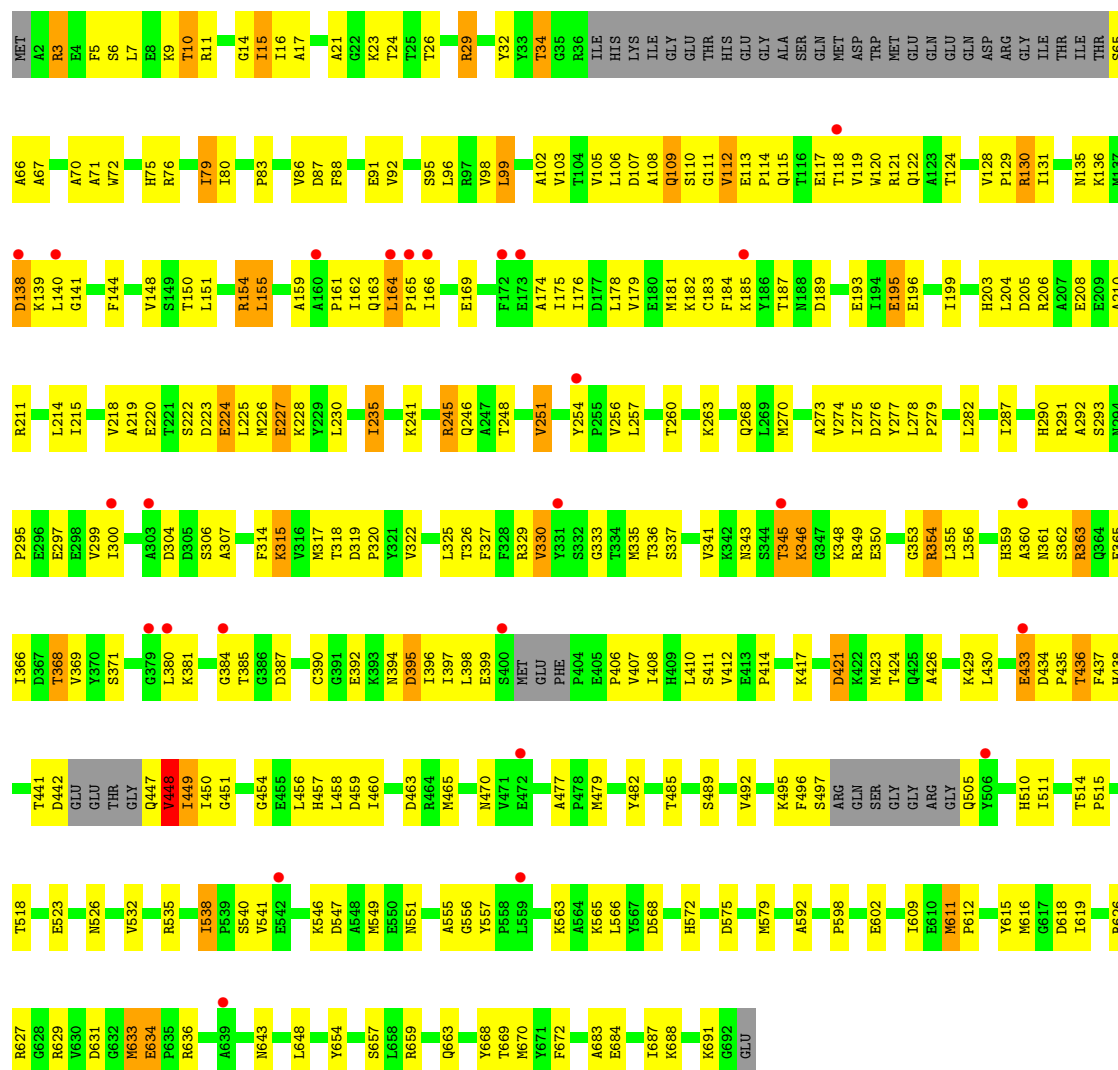
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Elongation factor G





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.94Å 125.46Å 106.27Å 90.00° 107.52° 90.00°	Depositor
Resolution (Å)	46.71 – 2.80 46.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (46.71-2.80) 91.2 (46.71-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.249 , 0.276 0.246 , 0.275	Depositor DCC
R_{free} test set	1739 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10068	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

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	0.35	1/5107 (0.0%)	0.79	4/6906 (0.1%)
1	B	0.36	1/5107 (0.0%)	0.86	9/6906 (0.1%)
All	All	0.35	2/10214 (0.0%)	0.82	13/13812 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	691	LYS	C-N	-6.91	1.23	1.33
1	B	691	LYS	C-N	-6.85	1.23	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	ILE	CA-C-N	-10.06	107.26	119.84
1	B	538	ILE	C-N-CA	-10.06	107.26	119.84
1	B	164	LEU	CA-C-N	9.26	131.42	119.84
1	B	164	LEU	C-N-CA	9.26	131.42	119.84
1	A	434	ASP	CA-C-N	6.55	126.18	119.56
1	A	434	ASP	C-N-CA	6.55	126.18	119.56
1	B	361	ASN	N-CA-C	6.19	120.97	113.17
1	B	448	VAL	N-CA-C	5.92	117.98	109.51
1	B	470	ASN	N-CA-C	5.84	117.75	110.91
1	B	540	SER	N-CA-C	-5.74	106.44	113.50
1	A	204	LEU	N-CA-C	5.73	117.39	111.03
1	A	395	ASP	N-CA-C	5.62	120.83	113.30
1	B	396	ILE	N-CA-C	5.44	117.46	109.63

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	5021	0	4934	253	1
1	B	5021	0	4934	282	2
2	A	11	0	0	2	0
2	B	15	0	0	1	0
All	All	10068	0	9868	534	2

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 (534) 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:B:109:GLN:N	1:B:109:GLN:OE1	1.80	1.12
1:A:615:TYR:OH	1:A:663:GLN:NE2	1.84	1.11
1:B:335:MET:HE1	1:B:341:VAL:HG11	1.31	1.09
1:B:195:GLU:CD	1:B:195:GLU:H	1.62	1.06
1:B:526:ASN:HD21	1:B:538:ILE:HD13	1.23	1.04
1:B:211:ARG:HH12	1:B:235:ILE:HD11	1.22	1.03
1:A:354:ARG:HG2	1:A:354:ARG:HH11	1.23	1.02
1:B:223:ASP:HA	1:B:226:MET:HG2	1.43	1.00
1:B:162:ILE:HD11	1:B:257:LEU:HG	1.45	0.99
1:B:11:ARG:NH2	1:B:275:ILE:O	1.98	0.96
1:A:302:LYS:HE2	1:A:304:ASP:HB2	1.48	0.94
1:A:614:GLU:N	1:A:614:GLU:OE1	2.03	0.92
1:B:109:GLN:O	1:B:110:SER:OG	1.88	0.91
1:A:29:ARG:HG3	1:A:267:VAL:HG11	1.51	0.91
1:A:441:THR:HA	1:A:448:VAL:HG23	1.52	0.91
1:A:208:GLU:N	1:A:208:GLU:OE1	2.04	0.90
1:A:222:SER:HB3	1:A:225:LEU:HD11	1.54	0.90
1:A:354:ARG:NH1	1:A:365:GLU:OE1	2.05	0.89
1:B:211:ARG:HH22	1:B:235:ILE:HD13	1.37	0.89
1:A:429:LYS:O	1:A:432:GLU:HG2	1.72	0.88
1:A:354:ARG:HH12	1:A:365:GLU:CD	1.82	0.88
1:B:224:GLU:N	1:B:224:GLU:OE1	2.07	0.87
1:A:688:LYS:HD2	1:A:691:LYS:HD3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:MET:HG3	1:B:619:ILE:HD11	1.54	0.86
1:A:117:GLU:OE2	1:A:636:ARG:NH2	2.08	0.85
1:A:348:LYS:HD3	1:A:349:ARG:H	1.43	0.84
1:A:441:THR:HA	1:A:448:VAL:CG2	2.08	0.84
1:A:348:LYS:CD	1:A:349:ARG:H	1.91	0.84
1:A:612:PRO:HG2	1:A:615:TYR:HE1	1.42	0.83
1:A:236:SER:N	1:A:239:GLU:OE2	2.11	0.83
1:B:136:LYS:HD3	1:B:139:LYS:HE2	1.59	0.82
1:B:17:ALA:HB3	1:B:23:LYS:NZ	1.94	0.82
1:B:410:LEU:HD12	1:B:450:ILE:HD11	1.62	0.81
1:B:572:HIS:CD2	1:B:575:ASP:HB2	2.15	0.81
1:B:349:ARG:NH1	1:B:392:GLU:OE2	2.15	0.80
1:A:12:ASN:HD22	1:A:78:ASN:HB2	1.46	0.80
1:B:163:GLN:O	1:B:164:LEU:HG	1.83	0.79
1:B:526:ASN:ND2	1:B:538:ILE:HD13	1.97	0.78
1:B:572:HIS:HD2	1:B:575:ASP:H	1.29	0.78
1:B:179:VAL:HG11	1:B:241:LYS:HG3	1.66	0.78
1:B:17:ALA:HB3	1:B:23:LYS:HZ2	1.48	0.78
1:B:335:MET:CE	1:B:341:VAL:HG11	2.14	0.77
1:B:523:GLU:OE1	1:B:563:LYS:NZ	2.17	0.77
1:B:611:MET:HG3	1:B:619:ILE:CD1	2.13	0.77
1:A:437:PHE:HE1	1:A:439:ALA:HB2	1.50	0.77
1:B:211:ARG:HH22	1:B:235:ILE:CD1	1.97	0.77
1:B:34:THR:HG22	1:B:71:ALA:O	1.84	0.76
1:A:3:ARG:HH12	1:A:7:LEU:H	1.32	0.76
1:A:201:GLU:HA	1:A:204:LEU:HD13	1.68	0.76
1:A:346:LYS:NZ	1:A:382:ASP:HB3	2.01	0.76
1:B:3:ARG:NE	1:B:5:PHE:O	2.13	0.76
1:B:15:ILE:HG23	1:B:103:VAL:O	1.86	0.76
1:B:335:MET:HE1	1:B:341:VAL:CG1	2.15	0.76
1:B:109:GLN:HE21	1:B:139:LYS:HE3	1.50	0.75
1:B:65:SER:OG	1:B:66:ALA:N	2.08	0.75
1:B:164:LEU:HD12	1:B:178:LEU:HD21	1.68	0.75
1:B:66:ALA:HB1	1:B:315:LYS:HE3	1.69	0.74
1:B:611:MET:HE3	1:B:619:ILE:HD12	1.68	0.73
1:A:658:LEU:O	1:A:662:THR:HG22	1.89	0.73
1:B:181:MET:SD	1:B:211:ARG:HD2	2.28	0.73
1:A:612:PRO:HG2	1:A:615:TYR:CE1	2.22	0.73
1:B:634:GLU:N	1:B:634:GLU:OE1	2.22	0.73
1:A:309:PHE:CZ	1:A:335:MET:HE3	2.22	0.73
1:A:349:ARG:NH1	1:A:392:GLU:OE1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ARG:NH1	1:B:235:ILE:HD11	2.00	0.73
1:A:199:ILE:HD12	1:A:199:ILE:H	1.54	0.72
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.53	0.72
1:B:182:LYS:HE2	1:B:196:GLU:CD	2.14	0.72
1:A:90:VAL:HG21	1:A:453:MET:HE1	1.73	0.71
1:A:204:LEU:O	1:A:208:GLU:OE1	2.09	0.71
1:A:312:LEU:HB2	1:A:398:LEU:HD13	1.73	0.71
1:B:345:THR:HG21	1:B:387:ASP:OD1	1.90	0.71
1:B:426:ALA:O	1:B:430:LEU:HG	1.92	0.70
1:B:129:PRO:HB3	1:B:248:THR:O	1.91	0.70
1:B:144:PHE:O	1:B:148:VAL:HG23	1.92	0.70
1:A:308:GLU:O	1:A:332:SER:OG	2.09	0.69
1:B:274:VAL:HG13	1:B:278:LEU:HD12	1.73	0.69
1:A:354:ARG:NH1	1:A:365:GLU:CD	2.48	0.69
1:A:244:ILE:O	1:A:248:THR:HG22	1.93	0.69
1:B:195:GLU:CD	1:B:195:GLU:N	2.39	0.69
1:A:154:ARG:HH22	1:A:610:GLU:CD	2.01	0.68
1:A:354:ARG:HG2	1:A:354:ARG:NH1	1.97	0.68
1:B:290:HIS:CD2	1:B:295:PRO:HA	2.28	0.68
1:B:631:ASP:O	1:B:643:ASN:HB3	1.93	0.68
1:B:227:GLU:HA	1:B:230:LEU:HB2	1.75	0.68
1:B:80:ILE:HD13	1:B:98:VAL:HG12	1.76	0.68
1:B:611:MET:HB2	1:B:612:PRO:HD2	1.76	0.68
1:A:12:ASN:ND2	1:A:78:ASN:HB2	2.09	0.67
1:B:354:ARG:HH11	1:B:354:ARG:CG	2.05	0.67
1:A:297:GLU:N	1:A:297:GLU:CD	2.53	0.67
1:A:110:SER:HB3	1:A:113:GLU:OE2	1.95	0.66
1:A:662:THR:HG21	1:A:666:GLY:N	2.09	0.66
1:B:109:GLN:HE21	1:B:139:LYS:CE	2.08	0.66
1:A:219:ALA:HB1	1:A:226:MET:HB2	1.78	0.66
1:B:395:ASP:OD1	1:B:395:ASP:N	2.28	0.66
1:A:214:LEU:O	1:A:218:VAL:HG23	1.96	0.66
1:B:203:HIS:CE1	1:B:206:ARG:HH11	2.13	0.66
1:B:319:ASP:CG	1:B:320:PRO:HD2	2.21	0.65
1:B:408:ILE:HD11	1:B:454:GLY:C	2.21	0.65
1:A:30:ILE:O	1:A:34:THR:OG1	2.14	0.65
1:B:602:GLU:CD	1:B:627:ARG:HH22	2.06	0.64
1:A:464:ARG:O	1:A:468:GLU:HB3	1.97	0.64
1:A:553:VAL:HG11	1:A:593:ALA:HB2	1.79	0.64
1:A:120:TRP:HZ2	1:A:254:TYR:CD2	2.15	0.64
1:A:633:MET:HB3	1:B:633:MET:HB3	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:HIS:HD2	1:B:575:ASP:N	1.96	0.64
1:A:456:LEU:O	1:A:460:ILE:HD12	1.98	0.64
1:B:138:ASP:OD2	1:B:260:THR:HG21	1.98	0.64
1:B:408:ILE:CG2	1:B:648:LEU:HD21	2.27	0.64
1:A:29:ARG:HD2	1:A:264:ASN:OD1	1.98	0.63
1:A:346:LYS:HZ1	1:A:382:ASP:HB3	1.62	0.63
1:B:227:GLU:OE1	1:B:227:GLU:N	2.30	0.63
1:B:343:ASN:OD1	1:B:345:THR:HG22	1.98	0.63
1:A:622:ASP:O	1:A:625:SER:OG	2.15	0.62
1:A:554:LEU:HD11	1:A:598:PRO:HB2	1.79	0.62
1:B:257:LEU:HD22	1:B:270:MET:HA	1.81	0.62
1:A:34:THR:HB	1:A:70:ALA:HB1	1.81	0.62
1:A:304:ASP:OD1	2:A:2005:HOH:O	2.16	0.62
1:A:154:ARG:NH2	1:A:610:GLU:OE1	2.27	0.61
1:A:204:LEU:O	1:A:207:ALA:N	2.31	0.61
1:A:211:ARG:O	1:A:215:ILE:HG13	2.00	0.61
1:A:248:THR:HG21	1:A:277:TYR:HB3	1.82	0.61
1:A:90:VAL:CG2	1:A:453:MET:HE1	2.29	0.61
1:A:411:SER:HA	1:A:449:ILE:HD13	1.81	0.61
1:B:304:ASP:OD1	1:B:306:SER:N	2.33	0.61
1:A:20:ASP:O	1:A:136:LYS:NZ	2.28	0.61
1:A:129:PRO:HG2	1:A:279:PRO:HG3	1.80	0.61
1:A:237:VAL:HG23	1:A:238:SER:H	1.65	0.61
1:A:297:GLU:N	1:A:297:GLU:OE1	2.33	0.61
1:A:302:LYS:HE2	1:A:304:ASP:CB	2.25	0.61
1:A:3:ARG:HH12	1:A:7:LEU:N	1.98	0.61
1:A:189:ASP:OD1	1:A:265:LYS:NZ	2.34	0.61
1:B:87:ASP:HB3	1:B:456:LEU:CD2	2.30	0.60
1:B:315:LYS:HG2	1:B:327:PHE:HB2	1.82	0.60
1:A:115:GLN:OE1	1:A:115:GLN:N	2.31	0.60
1:A:344:SER:OG	1:A:397:ILE:HG12	2.02	0.60
1:B:163:GLN:HA	1:B:176:ILE:O	2.02	0.60
1:B:226:MET:O	1:B:230:LEU:HD13	2.01	0.60
1:B:336:THR:HG22	1:B:368:THR:HB	1.83	0.60
1:B:510:HIS:CD2	1:B:568:ASP:HB3	2.37	0.60
1:A:413:GLU:HB3	1:A:474:ASN:HB2	1.84	0.60
1:B:185:LYS:HB2	1:B:195:GLU:OE1	2.02	0.60
1:A:203:HIS:CE1	1:A:206:ARG:NH1	2.70	0.59
1:B:384:GLY:N	1:B:387:ASP:OD2	2.29	0.59
1:A:121:ARG:O	1:A:125:THR:HG23	2.02	0.59
1:A:510:HIS:HB2	1:A:568:ASP:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:PRO:HG2	1:B:615:TYR:HE2	1.67	0.59
1:A:29:ARG:CG	1:A:267:VAL:HG11	2.30	0.59
1:B:66:ALA:HB1	1:B:315:LYS:CE	2.33	0.59
1:B:450:ILE:HD12	1:B:450:ILE:O	2.02	0.59
1:A:291:ARG:HB3	1:A:395:ASP:OD2	2.02	0.59
1:B:366:ILE:HD11	1:B:369:VAL:HG22	1.85	0.59
1:A:319:ASP:OD1	1:A:320:PRO:HD2	2.03	0.59
1:A:340:TYR:OH	1:A:351:ARG:NH1	2.36	0.59
1:B:224:GLU:O	1:B:228:LYS:NZ	2.32	0.59
1:B:346:LYS:HZ2	1:B:346:LYS:HB3	1.68	0.59
1:B:112:VAL:HG21	1:B:155:LEU:CD1	2.33	0.59
1:B:245:ARG:HG3	1:B:276:ASP:O	2.04	0.58
1:B:612:PRO:HG2	1:B:615:TYR:CE2	2.38	0.58
1:A:688:LYS:O	1:A:691:LYS:HG3	2.04	0.58
1:B:317:MET:HG2	1:B:318:THR:N	2.18	0.58
1:B:421:ASP:OD1	1:B:421:ASP:N	2.26	0.58
1:B:109:GLN:NE2	1:B:139:LYS:CE	2.66	0.58
1:B:203:HIS:CE1	1:B:206:ARG:NH1	2.72	0.58
1:A:619:ILE:O	1:A:622:ASP:HB3	2.04	0.58
1:A:69:THR:HG22	1:A:76:ARG:NH1	2.19	0.58
1:A:285:LYS:HD2	1:A:286:PRO:HD2	1.85	0.58
1:B:7:LEU:O	1:B:10:THR:OG1	2.22	0.58
1:B:17:ALA:HB2	1:B:105:VAL:HB	1.86	0.58
1:B:109:GLN:NE2	1:B:139:LYS:HE3	2.18	0.58
1:B:602:GLU:OE2	1:B:627:ARG:NH2	2.34	0.57
1:A:615:TYR:HH	1:A:663:GLN:HE22	1.50	0.57
1:A:29:ARG:HD2	1:A:33:TYR:CE2	2.39	0.57
1:A:103:VAL:HG11	1:A:270:MET:HE1	1.87	0.57
1:B:223:ASP:CA	1:B:226:MET:HG2	2.25	0.57
1:A:441:THR:O	1:A:442:ASP:C	2.48	0.57
1:A:626:ARG:NH1	1:A:650:GLU:O	2.36	0.57
1:B:572:HIS:CD2	1:B:575:ASP:H	2.17	0.57
1:A:312:LEU:HB2	1:A:398:LEU:CD1	2.34	0.57
1:A:361:ASN:OD1	1:A:361:ASN:N	2.37	0.56
1:B:124:THR:HA	1:B:130:ARG:HH22	1.69	0.56
1:A:433:GLU:OE1	1:A:464:ARG:NH2	2.30	0.56
1:A:662:THR:HG21	1:A:666:GLY:CA	2.35	0.56
1:B:394:ASN:OD1	1:B:395:ASP:N	2.38	0.56
1:A:208:GLU:N	1:A:208:GLU:CD	2.62	0.56
1:A:528:ILE:HG12	1:A:533:VAL:HB	1.87	0.56
1:B:359:HIS:HB2	1:B:362:SER:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:MET:O	1:A:199:ILE:HD11	2.04	0.56
1:B:164:LEU:HD11	1:B:210:ALA:CB	2.35	0.56
1:B:257:LEU:HD21	1:B:273:ALA:HB2	1.87	0.56
1:A:83:PRO:HG2	1:A:92:VAL:HB	1.87	0.56
1:B:95:SER:O	1:B:98:VAL:N	2.39	0.56
1:B:417:LYS:O	1:B:421:ASP:OD1	2.24	0.56
1:B:138:ASP:O	1:B:169:GLU:HA	2.05	0.56
1:B:354:ARG:HH12	1:B:365:GLU:CD	2.13	0.56
1:B:460:ILE:O	1:B:463:ASP:HB3	2.04	0.55
1:A:679:PRO:HG2	1:A:682:ILE:HD12	1.88	0.55
1:B:204:LEU:O	1:B:208:GLU:HG2	2.06	0.55
1:B:67:ALA:HB2	1:B:315:LYS:HZ1	1.70	0.55
1:B:510:HIS:HB2	1:B:568:ASP:HB3	1.89	0.55
1:A:122:GLN:O	1:A:126:TYR:HD1	1.89	0.55
1:A:146:TYR:O	1:A:149:SER:HB3	2.07	0.55
1:B:140:LEU:C	1:B:140:LEU:HD12	2.32	0.54
1:B:333:GLY:N	1:B:371:SER:OG	2.40	0.54
1:A:26:THR:O	1:A:30:ILE:HG13	2.07	0.54
1:B:109:GLN:O	1:B:110:SER:CB	2.56	0.54
1:A:120:TRP:CD1	1:A:155:LEU:HD13	2.43	0.54
1:A:202:ASP:OD1	1:A:202:ASP:N	2.29	0.54
1:B:668:TYR:CD1	1:B:669:THR:N	2.75	0.54
1:A:348:LYS:HD2	1:A:349:ARG:H	1.72	0.54
1:B:189:ASP:CG	1:B:263:LYS:HD3	2.33	0.54
1:A:662:THR:HG21	1:A:666:GLY:HA3	1.90	0.53
1:B:115:GLN:O	1:B:118:THR:OG1	2.12	0.53
1:A:9:LYS:HD2	1:A:75:HIS:NE2	2.22	0.53
1:A:203:HIS:CE1	1:A:206:ARG:HH11	2.25	0.53
1:A:438:HIS:NE2	1:A:440:HIS:CD2	2.76	0.53
1:B:356:LEU:HD23	1:B:365:GLU:HA	1.89	0.53
1:A:245:ARG:HD2	1:A:276:ASP:O	2.08	0.53
1:A:460:ILE:O	1:A:463:ASP:HB3	2.07	0.53
1:B:128:VAL:O	1:B:130:ARG:NE	2.32	0.53
1:B:211:ARG:O	1:B:214:LEU:HB3	2.09	0.53
1:B:226:MET:O	1:B:230:LEU:HB2	2.08	0.53
1:B:551:ASN:O	1:B:556:GLY:HA2	2.08	0.53
1:A:145:GLU:HA	1:A:145:GLU:OE1	2.08	0.53
1:A:222:SER:O	1:A:225:LEU:CD1	2.57	0.53
1:B:15:ILE:CG2	1:B:23:LYS:HE2	2.38	0.53
1:B:224:GLU:O	1:B:227:GLU:OE1	2.26	0.53
1:B:684:GLU:OE1	1:B:688:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ARG:HH11	1:A:627:ARG:HB3	1.73	0.53
1:B:345:THR:CG2	1:B:346:LYS:HG2	2.39	0.53
1:A:124:THR:HG23	1:A:130:ARG:HH12	1.74	0.53
1:A:230:LEU:HD12	1:A:231:GLY:N	2.24	0.53
1:B:32:TYR:CD1	1:B:32:TYR:C	2.87	0.53
1:A:222:SER:C	1:A:225:LEU:HD11	2.34	0.52
1:B:161:PRO:HA	1:B:256:VAL:HB	1.91	0.52
1:A:83:PRO:HG2	1:A:92:VAL:CA	2.40	0.52
1:A:155:LEU:O	1:A:156:GLN:HG2	2.10	0.52
1:B:211:ARG:O	1:B:215:ILE:HD12	2.09	0.52
1:B:423:MET:O	1:B:426:ALA:N	2.42	0.52
1:B:159:ALA:HB2	1:B:254:TYR:HB2	1.92	0.52
1:A:528:ILE:HD13	1:A:566:LEU:HG	1.92	0.52
1:B:489:SER:OG	1:B:515:PRO:HD3	2.10	0.52
1:A:32:TYR:CD1	1:A:32:TYR:C	2.88	0.52
1:A:100:ASP:O	1:A:128:VAL:HG13	2.09	0.52
1:B:112:VAL:HG21	1:B:155:LEU:HD11	1.92	0.52
1:A:36:ARG:O	1:A:36:ARG:HG3	2.09	0.52
1:A:240:LEU:O	1:A:244:ILE:HG13	2.10	0.52
1:A:340:TYR:CE2	1:A:351:ARG:HG2	2.45	0.52
1:A:636:ARG:HD3	1:A:641:VAL:HG23	1.92	0.52
1:A:34:THR:HG22	1:A:72:TRP:HB2	1.92	0.51
1:A:335:MET:HE2	1:A:341:VAL:HG11	1.92	0.51
1:B:34:THR:HB	1:B:70:ALA:HB1	1.92	0.51
1:A:611:MET:SD	1:A:619:ILE:HG12	2.50	0.51
1:A:554:LEU:HD21	1:A:598:PRO:HG2	1.92	0.51
1:A:177:ASP:OD2	1:A:180:GLU:HB2	2.10	0.51
1:A:636:ARG:O	1:A:639:ALA:O	2.28	0.51
1:B:317:MET:HG2	1:B:318:THR:H	1.75	0.51
1:B:346:LYS:HB3	1:B:346:LYS:NZ	2.25	0.51
1:A:614:GLU:H	1:A:614:GLU:CD	2.10	0.51
1:B:6:SER:H	1:B:9:LYS:CE	2.24	0.51
1:A:616:MET:SD	1:A:633:MET:HE1	2.51	0.51
1:A:241:LYS:HG3	1:A:277:TYR:HE1	1.76	0.51
1:A:546:LYS:O	1:A:550:GLU:HG2	2.11	0.51
1:B:117:GLU:OE2	1:B:121:ARG:NH2	2.44	0.51
1:B:345:THR:HG22	1:B:346:LYS:HG2	1.93	0.51
1:B:108:ALA:HB2	1:B:135:ASN:O	2.11	0.50
1:B:319:ASP:HB3	1:B:322:VAL:HG22	1.93	0.50
1:A:289:GLY:C	1:A:299:VAL:HG23	2.36	0.50
1:A:413:GLU:OE1	1:A:474:ASN:ND2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:MET:SD	1:B:611:MET:N	2.84	0.50
1:B:683:ALA:O	1:B:687:ILE:HG13	2.11	0.50
1:B:72:TRP:O	1:B:75:HIS:HB2	2.11	0.50
1:B:260:THR:HG23	1:B:260:THR:O	2.11	0.50
1:A:86:VAL:C	1:A:88:PHE:H	2.20	0.50
1:B:354:ARG:CG	1:B:354:ARG:NH1	2.69	0.49
1:B:102:ALA:O	1:B:130:ARG:HA	2.12	0.49
1:B:185:LYS:HB2	1:B:195:GLU:CD	2.38	0.49
1:B:535:ARG:HA	1:B:538:ILE:HD12	1.94	0.49
1:B:109:GLN:NE2	1:B:139:LYS:HE2	2.28	0.49
1:A:437:PHE:CD1	1:A:438:HIS:N	2.81	0.49
1:B:541:VAL:HG11	1:B:566:LEU:HD22	1.94	0.49
1:B:115:GLN:O	1:B:119:VAL:HG23	2.12	0.49
1:A:346:LYS:HZ3	1:A:382:ASP:HB3	1.76	0.49
1:B:131:ILE:HG23	1:B:278:LEU:HD21	1.95	0.49
1:B:349:ARG:CZ	1:B:392:GLU:OE2	2.60	0.49
1:A:486:PHE:O	1:A:515:PRO:HB3	2.12	0.49
1:B:29:ARG:HE	1:B:29:ARG:HA	1.77	0.49
1:B:113:GLU:HB3	1:B:114:PRO:CD	2.42	0.49
1:A:138:ASP:HA	1:A:169:GLU:O	2.12	0.49
1:A:615:TYR:OH	1:A:665:ARG:NH1	2.44	0.49
1:A:204:LEU:O	1:A:205:ASP:C	2.53	0.49
1:A:534:PRO:HD3	1:A:571:TYR:CD1	2.48	0.48
1:B:9:LYS:HA	1:B:75:HIS:CE1	2.48	0.48
1:A:228:LYS:NZ	1:A:233:GLU:HB3	2.27	0.48
1:A:438:HIS:NE2	1:A:440:HIS:NE2	2.62	0.48
1:B:109:GLN:HB3	1:B:141:GLY:O	2.12	0.48
1:B:454:GLY:O	1:B:457:HIS:HB3	2.13	0.48
1:A:94:ARG:HD3	1:A:314:PHE:HA	1.94	0.48
1:A:237:VAL:HG23	1:A:238:SER:N	2.29	0.48
1:B:23:LYS:O	1:B:23:LYS:HD3	2.14	0.48
1:B:304:ASP:O	1:B:333:GLY:N	2.44	0.48
1:B:407:VAL:HG11	1:B:672:PHE:CD1	2.48	0.48
1:B:505:GLN:HA	1:B:575:ASP:O	2.14	0.48
1:B:612:PRO:CG	1:B:615:TYR:HE2	2.25	0.48
1:A:340:TYR:OH	1:A:351:ARG:CZ	2.62	0.48
1:A:8:GLU:N	1:A:8:GLU:CD	2.71	0.48
1:A:137:MET:HE2	1:A:165:PRO:HB2	1.96	0.48
1:A:225:LEU:N	1:A:225:LEU:HD12	2.28	0.48
1:B:118:THR:OG1	1:B:119:VAL:N	2.46	0.48
1:B:434:ASP:OD1	1:B:436:THR:OG1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:SER:O	1:A:242:GLU:HB3	2.13	0.48
1:B:406:PRO:HD3	1:B:438:HIS:HE1	1.79	0.48
1:B:219:ALA:O	1:B:222:SER:O	2.31	0.48
1:B:434:ASP:OD1	1:B:434:ASP:C	2.56	0.48
1:A:3:ARG:NH1	1:A:6:SER:HA	2.29	0.47
1:A:120:TRP:HZ2	1:A:254:TYR:CE2	2.32	0.47
1:A:224:GLU:HG2	1:A:225:LEU:N	2.28	0.47
1:A:688:LYS:O	1:A:691:LYS:NZ	2.30	0.47
1:B:121:ARG:CZ	1:B:636:ARG:HD3	2.44	0.47
1:A:163:GLN:O	1:A:164:LEU:HD23	2.15	0.47
1:B:114:PRO:O	1:B:118:THR:HG23	2.14	0.47
1:B:406:PRO:HD3	1:B:438:HIS:CE1	2.48	0.47
1:B:437:PHE:HB2	1:B:451:GLY:O	2.14	0.47
1:B:477:ALA:O	1:B:479:MET:HG3	2.13	0.47
1:A:8:GLU:CD	1:A:8:GLU:H	2.23	0.47
1:A:424:THR:O	1:A:428:VAL:HG23	2.14	0.47
1:B:322:VAL:CG2	1:B:325:LEU:HD21	2.45	0.47
1:B:88:PHE:O	1:B:92:VAL:HG23	2.14	0.47
1:B:138:ASP:C	1:B:169:GLU:HA	2.40	0.47
1:B:450:ILE:CD1	1:B:458:LEU:HD22	2.44	0.47
1:A:426:ALA:O	1:A:430:LEU:HG	2.15	0.47
1:A:635:PRO:O	1:A:636:ARG:HD2	2.14	0.46
1:B:235:ILE:HD12	1:B:235:ILE:O	2.15	0.46
1:A:605:MET:HG2	1:A:648:LEU:HB2	1.97	0.46
1:B:6:SER:OG	1:B:9:LYS:HE2	2.15	0.46
1:B:106:LEU:HD11	1:B:151:LEU:HD21	1.97	0.46
1:A:638:ASN:ND2	2:A:2011:HOH:O	2.43	0.46
1:B:287:ILE:HD13	1:B:398:LEU:HD23	1.96	0.46
1:B:314:PHE:C	1:B:385:THR:HG23	2.40	0.46
1:A:662:THR:HG21	1:A:666:GLY:H	1.81	0.46
1:B:6:SER:H	1:B:9:LYS:HE3	1.79	0.46
1:B:96:LEU:O	1:B:99:LEU:HD12	2.15	0.46
1:A:348:LYS:HD3	1:A:349:ARG:N	2.22	0.46
1:A:679:PRO:CG	1:A:682:ILE:HD12	2.45	0.46
1:B:211:ARG:NH2	1:B:235:ILE:CD1	2.74	0.46
1:B:437:PHE:C	1:B:438:HIS:CD2	2.94	0.46
1:A:120:TRP:CZ2	1:A:254:TYR:CD2	2.99	0.46
1:A:241:LYS:HG3	1:A:277:TYR:CE1	2.51	0.46
1:B:163:GLN:C	1:B:164:LEU:HG	2.39	0.46
1:A:85:HIS:O	1:A:88:PHE:HB2	2.16	0.46
1:A:163:GLN:HA	1:A:176:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LYS:HA	1:B:75:HIS:ND1	2.31	0.46
1:B:15:ILE:HG21	1:B:23:LYS:HE2	1.98	0.46
1:B:322:VAL:HG21	1:B:325:LEU:HD21	1.96	0.46
1:B:423:MET:HG3	1:B:465:MET:CE	2.46	0.46
1:B:23:LYS:HD3	1:B:23:LYS:C	2.41	0.46
1:B:181:MET:HE3	1:B:199:ILE:CD1	2.45	0.45
1:B:337:SER:HB2	1:B:353:GLY:O	2.17	0.45
1:B:429:LYS:NZ	1:B:433:GLU:OE2	2.42	0.45
1:A:260:THR:O	1:A:260:THR:HG23	2.16	0.45
1:A:506:TYR:O	1:A:576:SER:HA	2.16	0.45
1:B:408:ILE:HG23	1:B:648:LEU:HD21	1.97	0.45
1:A:230:LEU:HD12	1:A:230:LEU:C	2.42	0.45
1:B:304:ASP:OD1	1:B:304:ASP:C	2.58	0.45
1:B:304:ASP:OD1	1:B:307:ALA:N	2.49	0.45
1:A:112:VAL:HG13	1:A:116:THR:HB	1.98	0.45
1:B:79:ILE:C	1:B:79:ILE:HD12	2.41	0.45
1:A:168:ALA:O	1:A:171:GLU:N	2.49	0.45
1:A:222:SER:CB	1:A:225:LEU:HD11	2.36	0.45
1:A:260:THR:HG22	1:A:265:LYS:HB2	1.98	0.45
1:A:437:PHE:HD1	1:A:438:HIS:N	2.15	0.45
1:A:463:ASP:OD1	1:A:463:ASP:C	2.60	0.45
1:A:487:LYS:HD2	1:A:487:LYS:HA	1.75	0.45
1:A:522:PHE:CE1	1:A:524:PHE:HB2	2.51	0.45
1:B:485:THR:O	1:B:598:PRO:HA	2.17	0.45
1:B:128:VAL:HA	1:B:129:PRO:HD3	1.75	0.45
1:A:3:ARG:CZ	1:A:6:SER:HA	2.46	0.45
1:A:437:PHE:HB2	1:A:451:GLY:O	2.16	0.45
1:B:354:ARG:NH1	1:B:365:GLU:CD	2.75	0.45
1:B:626:ARG:O	1:B:627:ARG:HB3	2.17	0.45
1:A:248:THR:CG2	1:A:277:TYR:O	2.65	0.45
1:A:441:THR:CA	1:A:448:VAL:HG23	2.37	0.45
1:A:509:VAL:HG22	1:A:584:ALA:HB1	1.99	0.45
1:B:96:LEU:HD22	1:B:128:VAL:HG21	1.98	0.45
1:B:546:LYS:O	1:B:549:MET:N	2.50	0.45
1:A:204:LEU:O	1:A:206:ARG:N	2.50	0.45
1:A:211:ARG:NH2	1:A:235:ILE:O	2.51	0.44
1:A:521:GLY:O	1:A:561:ASP:HA	2.16	0.44
1:B:23:LYS:HG3	1:B:24:THR:N	2.32	0.44
1:B:162:ILE:HG13	1:B:256:VAL:O	2.17	0.44
1:B:497:SER:C	1:B:505:GLN:O	2.61	0.44
1:A:9:LYS:HD2	1:A:75:HIS:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LYS:C	1:A:691:LYS:NZ	2.75	0.44
1:A:593:ALA:O	1:A:598:PRO:HD3	2.18	0.44
1:B:345:THR:CG2	1:B:346:LYS:N	2.81	0.44
1:A:245:ARG:NH2	1:A:283:ASP:OD2	2.50	0.44
1:B:109:GLN:H	1:B:109:GLN:CD	2.05	0.44
1:B:329:ARG:HD2	1:B:330:VAL:N	2.32	0.44
1:B:659:ARG:O	1:B:663:GLN:N	2.50	0.44
1:B:292:ALA:H	1:B:395:ASP:HB2	1.83	0.44
1:B:546:LYS:HD3	2:B:2015:HOH:O	2.18	0.44
1:B:615:TYR:O	1:B:618:ASP:N	2.51	0.44
1:A:612:PRO:O	1:A:615:TYR:HD1	2.00	0.44
1:A:636:ARG:HD3	1:A:641:VAL:CG2	2.48	0.44
1:A:88:PHE:O	1:A:89:THR:C	2.61	0.44
1:A:602:GLU:HG2	1:A:678:VAL:HG22	1.98	0.44
1:B:10:THR:HG22	1:B:76:ARG:CG	2.48	0.44
1:B:21:ALA:HB1	1:B:105:VAL:HG12	2.00	0.44
1:B:546:LYS:HG3	1:B:547:ASP:N	2.33	0.44
1:B:23:LYS:O	1:B:26:THR:N	2.50	0.43
1:B:150:THR:O	1:B:154:ARG:HG2	2.18	0.43
1:B:112:VAL:HG21	1:B:155:LEU:HD12	2.00	0.43
1:B:203:HIS:HE1	1:B:206:ARG:NH1	2.14	0.43
1:A:35:GLY:O	1:A:36:ARG:C	2.60	0.43
1:B:107:ASP:OD1	1:B:109:GLN:NE2	2.51	0.43
1:B:546:LYS:CG	1:B:547:ASP:N	2.81	0.43
1:A:429:LYS:HG3	1:A:432:GLU:OE2	2.18	0.43
1:B:215:ILE:HG23	1:B:225:LEU:HD21	1.99	0.43
1:B:362:SER:HA	1:B:363:ARG:HH21	1.83	0.43
1:B:366:ILE:CD1	1:B:369:VAL:HG22	2.48	0.43
1:B:411:SER:HA	1:B:449:ILE:HD12	2.00	0.43
1:A:118:THR:O	1:A:122:GLN:HG3	2.19	0.43
1:A:124:THR:CG2	1:A:130:ARG:HH22	2.32	0.43
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.88	0.43
1:B:96:LEU:HD23	1:B:99:LEU:HD11	2.01	0.43
1:B:163:GLN:HE22	1:B:257:LEU:HD23	1.84	0.43
1:B:669:THR:HG22	1:B:670:MET:N	2.33	0.43
1:A:230:LEU:C	1:A:232:ASP:H	2.27	0.43
1:A:15:ILE:CG2	1:A:23:LYS:HG3	2.49	0.43
1:B:166:ILE:HD12	1:B:174:ALA:HB3	2.00	0.43
1:A:309:PHE:HZ	1:A:335:MET:HE3	1.75	0.43
1:B:441:THR:O	1:B:442:ASP:C	2.62	0.43
1:B:629:ARG:NH1	1:B:631:ASP:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:O	1:A:121:ARG:HG2	2.19	0.43
1:A:615:TYR:CZ	1:A:663:GLN:NE2	2.82	0.43
1:A:291:ARG:NH1	1:A:299:VAL:HG13	2.34	0.42
1:A:369:VAL:HG12	1:A:373:ASP:HB3	2.00	0.42
1:A:528:ILE:HA	1:A:528:ILE:HD12	1.77	0.42
1:B:346:LYS:HB2	1:B:348:LYS:HE3	2.00	0.42
1:A:484:GLU:C	1:A:559:LEU:HD12	2.43	0.42
1:A:93:GLU:HG3	1:A:126:TYR:OH	2.19	0.42
1:B:227:GLU:OE2	1:B:228:LYS:NZ	2.43	0.42
1:B:423:MET:HG3	1:B:465:MET:HE2	2.00	0.42
1:A:612:PRO:HG3	1:A:665:ARG:NE	2.34	0.42
1:B:251:VAL:HG12	1:B:251:VAL:O	2.19	0.42
1:B:291:ARG:NH1	1:B:395:ASP:OD1	2.50	0.42
1:A:179:VAL:HG12	1:A:179:VAL:O	2.20	0.42
1:A:245:ARG:NH1	1:A:276:ASP:O	2.51	0.42
1:B:292:ALA:HA	1:B:397:ILE:HD11	2.00	0.42
1:B:492:VAL:HG21	1:B:592:ALA:HB2	2.02	0.42
1:A:3:ARG:NH1	1:A:7:LEU:H	2.08	0.42
1:A:3:ARG:NH1	1:A:7:LEU:N	2.64	0.42
1:A:6:SER:OG	1:A:9:LYS:HG2	2.19	0.42
1:A:83:PRO:HG2	1:A:92:VAL:CB	2.50	0.42
1:A:422:LYS:HZ2	1:A:470:ASN:HB2	1.83	0.42
1:A:330:VAL:HG23	1:A:330:VAL:O	2.18	0.42
1:A:438:HIS:HE2	1:A:440:HIS:CD2	2.37	0.42
1:B:3:ARG:HD3	1:B:6:SER:HA	2.01	0.42
1:B:10:THR:HG22	1:B:76:ARG:HG2	2.01	0.42
1:B:184:PHE:CE1	1:B:196:GLU:HG2	2.55	0.42
1:A:99:LEU:HD13	1:A:101:GLY:O	2.20	0.42
1:A:545:LEU:O	1:A:549:MET:N	2.50	0.42
1:B:16:ILE:O	1:B:17:ALA:HB2	2.19	0.42
1:B:83:PRO:HG3	1:B:91:GLU:HB3	2.02	0.42
1:B:326:THR:HB	1:B:380:LEU:HD22	2.02	0.42
1:A:409:HIS:HB2	1:A:450:ILE:O	2.20	0.42
1:A:678:VAL:HG13	1:A:679:PRO:HD2	2.02	0.42
1:B:214:LEU:O	1:B:218:VAL:HG23	2.19	0.42
1:A:291:ARG:NH1	1:A:299:VAL:CG1	2.83	0.41
1:A:348:LYS:CD	1:A:349:ARG:N	2.73	0.41
1:B:276:ASP:HB3	1:B:277:TYR:CE1	2.55	0.41
1:B:546:LYS:HA	1:B:549:MET:HB2	2.01	0.41
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.73	0.41
1:B:107:ASP:O	1:B:111:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:SER:O	1:A:225:LEU:HD11	2.19	0.41
1:A:308:GLU:OE1	1:A:308:GLU:N	2.49	0.41
1:A:437:PHE:CD1	1:A:437:PHE:C	2.99	0.41
1:A:614:GLU:N	1:A:614:GLU:CD	2.73	0.41
1:B:71:ALA:HA	1:B:75:HIS:O	2.20	0.41
1:B:120:TRP:CD1	1:B:130:ARG:NH1	2.88	0.41
1:B:412:VAL:HG12	1:B:448:VAL:O	2.20	0.41
1:A:88:PHE:HD1	1:A:88:PHE:HA	1.79	0.41
1:A:180:GLU:O	1:A:181:MET:HB2	2.20	0.41
1:B:414:PRO:HD2	1:B:447:GLN:HG2	2.02	0.41
1:B:555:ALA:HB3	1:B:557:TYR:CD2	2.55	0.41
1:B:87:ASP:HB3	1:B:456:LEU:HD22	2.02	0.41
1:B:290:HIS:HD2	1:B:291:ARG:O	2.04	0.41
1:B:355:LEU:O	1:B:365:GLU:HA	2.21	0.41
1:A:29:ARG:CD	1:A:33:TYR:CE2	3.03	0.41
1:A:604:MET:HE3	1:A:604:MET:HB3	1.85	0.41
1:B:66:ALA:HB1	1:B:315:LYS:HD2	2.01	0.41
1:B:350:GLU:OE1	1:B:350:GLU:HA	2.21	0.41
1:B:609:ILE:HD13	1:B:654:TYR:OH	2.20	0.41
1:A:164:LEU:HB2	1:A:176:ILE:HD12	2.01	0.41
1:A:319:ASP:HB3	1:A:322:VAL:HG22	2.03	0.41
1:B:290:HIS:HA	1:B:297:GLU:O	2.20	0.41
1:B:616:MET:CE	1:B:633:MET:HE1	2.51	0.41
1:A:336:THR:HG22	1:A:337:SER:O	2.21	0.41
1:A:555:ALA:HB3	1:A:557:TYR:CD2	2.56	0.41
1:B:164:LEU:CD1	1:B:178:LEU:HD21	2.45	0.41
1:B:362:SER:CA	1:B:363:ARG:HH21	2.34	0.41
1:B:390:CYS:SG	1:B:394:ASN:O	2.77	0.41
1:B:511:ILE:HA	1:B:565:LYS:O	2.21	0.41
1:A:18:HIS:HD2	1:A:115:GLN:HB2	1.86	0.41
1:A:604:MET:HG3	1:A:676:ALA:HB2	2.03	0.41
1:B:17:ALA:CB	1:B:105:VAL:HB	2.51	0.41
1:B:164:LEU:HA	1:B:165:PRO:HD3	1.76	0.41
1:B:199:ILE:H	1:B:199:ILE:HG13	1.62	0.41
1:B:270:MET:O	1:B:273:ALA:HB3	2.21	0.41
1:B:314:PHE:O	1:B:385:THR:HG23	2.20	0.41
1:A:436:THR:HB	1:A:453:MET:HE3	2.02	0.41
1:A:616:MET:HG3	1:A:620:MET:HE3	2.03	0.41
1:B:175:ILE:O	1:B:183:CYS:HA	2.21	0.41
1:A:529:VAL:O	1:A:529:VAL:HG23	2.22	0.40
1:A:604:MET:CE	1:A:645:TYR:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLY:HA3	1:B:99:LEU:HD23	2.03	0.40
1:B:131:ILE:HG23	1:B:278:LEU:CD2	2.51	0.40
1:B:293:SER:O	1:B:295:PRO:HD3	2.19	0.40
1:B:359:HIS:O	1:B:360:ALA:C	2.65	0.40
1:B:579:MET:HE2	1:B:579:MET:HB3	1.95	0.40
1:A:312:LEU:O	1:A:328:PHE:HA	2.22	0.40
1:B:140:LEU:HD12	1:B:140:LEU:O	2.22	0.40
1:B:495:LYS:HG3	1:B:496:PHE:N	2.36	0.40
1:A:185:LYS:HE2	1:A:195:GLU:OE1	2.22	0.40
1:A:29:ARG:NE	1:A:29:ARG:HA	2.37	0.40
1:A:211:ARG:O	1:A:214:LEU:HB3	2.21	0.40
1:A:228:LYS:HZ2	1:A:233:GLU:HB3	1.87	0.40
1:A:354:ARG:NH1	1:A:365:GLU:OE2	2.54	0.40
1:A:505:GLN:HA	1:A:575:ASP:O	2.22	0.40
1:B:119:VAL:O	1:B:122:GLN:HB2	2.21	0.40
1:B:129:PRO:HG2	1:B:279:PRO:HG3	2.04	0.40
1:B:187:THR:OG1	1:B:193:GLU:HB2	2.21	0.40
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.90	0.40
1:B:482:TYR:O	1:B:557:TYR:HB3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:NZ	1:B:205:ASP:OD1[2_555]	1.95	0.25
1:B:535:ARG:NH2	1:B:618:ASP:OD1[1_455]	2.13	0.07

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	639/693 (92%)	600 (94%)	38 (6%)	1 (0%)	43 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	639/693 (92%)	588 (92%)	48 (8%)	3 (0%)	24	55
All	All	1278/1386 (92%)	1188 (93%)	86 (7%)	4 (0%)	36	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	VAL
1	B	435	PRO
1	B	381	LYS
1	A	251	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	543/579 (94%)	509 (94%)	34 (6%)	16	45
1	B	543/579 (94%)	496 (91%)	47 (9%)	9	30
All	All	1086/1158 (94%)	1005 (92%)	81 (8%)	12	37

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	36	ARG
1	A	87	ASP
1	A	109	GLN
1	A	116	THR
1	A	154	ARG
1	A	202	ASP
1	A	209	GLU
1	A	213	SER
1	A	225	LEU
1	A	234	GLU
1	A	235	ILE

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Mol	Chain	Res	Type
1	A	249	THR
1	A	270	MET
1	A	280	SER
1	A	297	GLU
1	A	299	VAL
1	A	332	SER
1	A	336	THR
1	A	349	ARG
1	A	352	VAL
1	A	354	ARG
1	A	361	ASN
1	A	363	ARG
1	A	398	LEU
1	A	448	VAL
1	A	460	ILE
1	A	518	THR
1	A	528	ILE
1	A	529	VAL
1	A	536	GLU
1	A	614	GLU
1	A	660	SER
1	A	667	THR
1	B	3	ARG
1	B	10	THR
1	B	15	ILE
1	B	29	ARG
1	B	34	THR
1	B	79	ILE
1	B	86	VAL
1	B	99	LEU
1	B	109	GLN
1	B	112	VAL
1	B	130	ARG
1	B	138	ASP
1	B	154	ARG
1	B	155	LEU
1	B	195	GLU
1	B	220	GLU
1	B	224	GLU
1	B	227	GLU
1	B	235	ILE
1	B	245	ARG

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Mol	Chain	Res	Type
1	B	246	GLN
1	B	268	GLN
1	B	299	VAL
1	B	300	ILE
1	B	315	LYS
1	B	330	VAL
1	B	345	THR
1	B	346	LYS
1	B	354	ARG
1	B	363	ARG
1	B	368	THR
1	B	395	ASP
1	B	399	GLU
1	B	421	ASP
1	B	424	THR
1	B	433	GLU
1	B	436	THR
1	B	448	VAL
1	B	449	ILE
1	B	459	ASP
1	B	514	THR
1	B	518	THR
1	B	532	VAL
1	B	611	MET
1	B	633	MET
1	B	634	GLU
1	B	657	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	643	ASN
1	A	663	GLN
1	B	156	GLN
1	B	163	GLN
1	B	290	HIS
1	B	359	HIS
1	B	438	HIS
1	B	505	GLN
1	B	526	ASN
1	B	572	HIS

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Mol	Chain	Res	Type
1	B	690	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

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	649/693 (93%)	0.36	19 (2%)	53 43	41, 82, 141, 252	0
1	B	649/693 (93%)	0.50	26 (4%)	42 33	47, 87, 137, 274	0
All	All	1298/1386 (93%)	0.43	45 (3%)	47 38	41, 85, 139, 274	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	PRO	3.2
1	B	360	ALA	3.2
1	A	310	ALA	3.1
1	B	254	TYR	3.1
1	B	138	ASP	3.1
1	B	639	ALA	2.8
1	A	86	VAL	2.8
1	A	441	THR	2.7
1	B	166	ILE	2.7
1	A	535	ARG	2.7
1	B	380	LEU	2.7
1	B	506	TYR	2.6
1	A	394	ASN	2.6
1	B	303	ALA	2.5
1	A	225	LEU	2.5
1	B	185	LYS	2.5
1	B	559	LEU	2.4
1	A	641	VAL	2.4
1	B	400	SER	2.3
1	A	285	LYS	2.3
1	B	384	GLY	2.3
1	B	433	GLU	2.3
1	A	339	SER	2.3
1	A	404	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	399	GLU	2.3
1	B	160	ALA	2.2
1	B	331	TYR	2.2
1	B	172	PHE	2.2
1	B	164	LEU	2.2
1	B	472	GLU	2.2
1	A	370	TYR	2.2
1	B	118	THR	2.1
1	B	300	ILE	2.1
1	A	393	LYS	2.1
1	A	323	GLY	2.1
1	A	391	GLY	2.1
1	A	88	PHE	2.1
1	A	398	LEU	2.1
1	B	173	GLU	2.1
1	A	448	VAL	2.1
1	A	539	PRO	2.1
1	B	140	LEU	2.1
1	B	379	GLY	2.1
1	B	345	THR	2.1
1	B	542	GLU	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.