



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 PM GMT

PDB ID : 3ZZ0
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

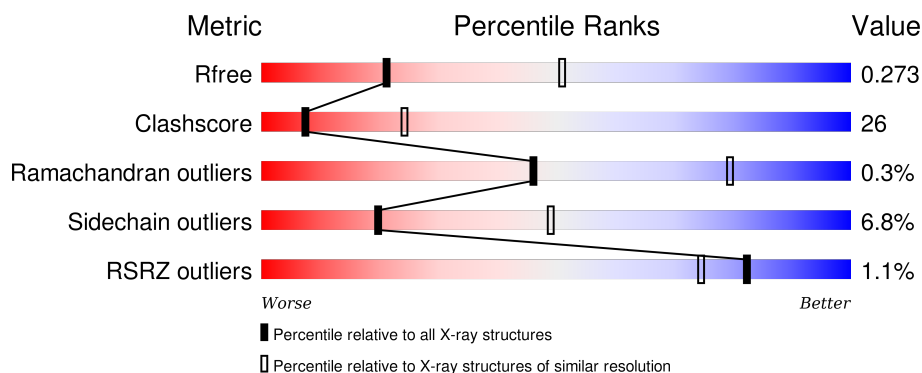
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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

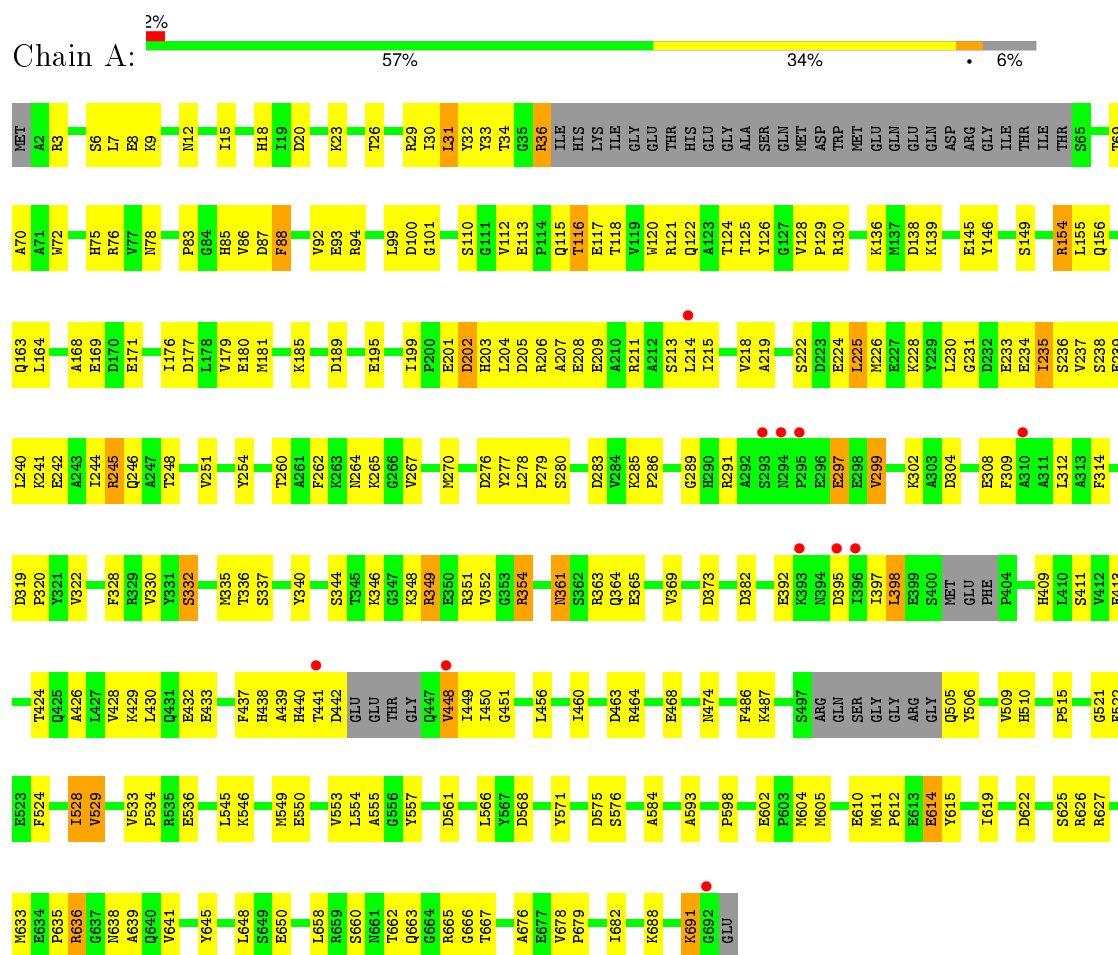
- Molecule 2 is water.

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

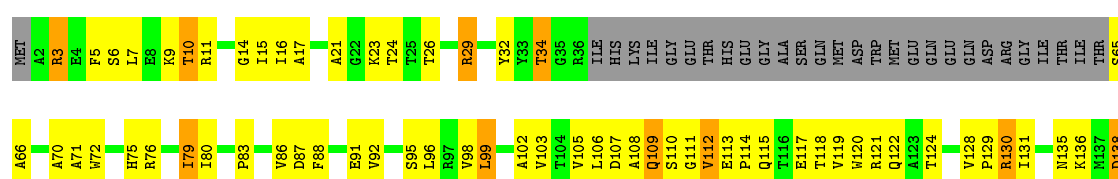
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

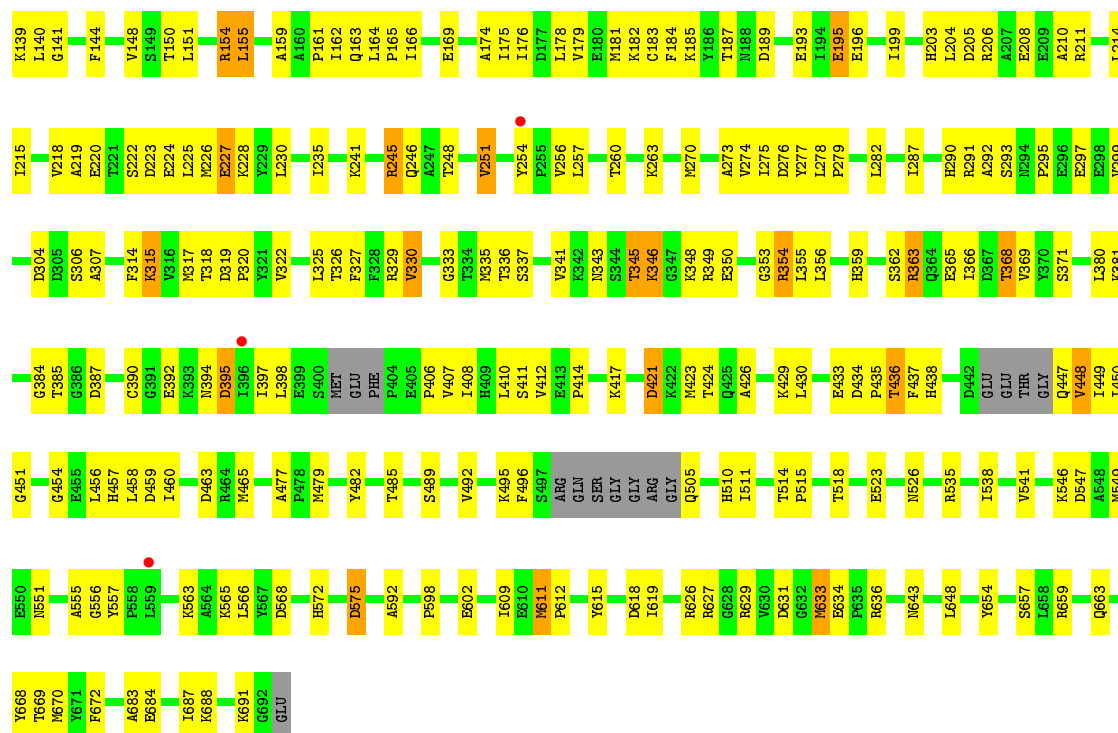
• Molecule 1: ELONGATION FACTOR G



• Molecule 1: ELONGATION FACTOR G

Chain B: 





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 0.243 , 0.273	Depositor DCC
R_{free} test set	1737 reflections (4.76%)	DCC
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.8	EDS
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36516 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.28	1/5107 (0.0%)	0.49	0/6906
1	B	0.28	1/5107 (0.0%)	0.52	0/6906
All	All	0.28	2/10214 (0.0%)	0.50	0/13812

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	691	LYS	C-N	-5.21	1.23	1.33
1	B	691	LYS	C-N	-5.16	1.23	1.33

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	5021	0	4934	235	1
1	B	5021	0	4934	275	2
2	A	11	0	0	2	0
2	B	15	0	0	1	0
All	All	10068	0	9868	509	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 26.

All (509) 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:OE1	1:B:109:GLN:N	1.80	1.12
1:A:615:TYR:OH	1:A:663:GLN:NE2	1.84	1.11
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:HH11	1:A:354:ARG:HG2	1.23	1.02
1:B:195:GLU:CD	1:B:195:GLU:H	1.62	1.01
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:OE1	1:A:614:GLU:N	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:OE1	1:A:208:GLU:N	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: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
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:A:354:ARG:HH12	1:A:365:GLU:CD	1.82	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:65:SER:OG	1:B:66:ALA:N	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:201:GLU:HA	1:A:204:LEU:HD13	1.68	0.76
1:A:3:ARG:HH12	1:A:7:LEU:H	1.32	0.76
1:B:3:ARG:NE	1:B:5:PHE:O	2.13	0.76
1:A:346:LYS:NZ	1:A:382:ASP:HB3	2.01	0.76
1:B:15:ILE:HG23	1:B:103:VAL:O	1.86	0.76
1:B:109:GLN:HE21	1:B:139:LYS:HE3	1.50	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: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:OE1	1:B:634:GLU:N	2.22	0.73
1:B:211:ARG:NH1	1:B:235:ILE:HD11	2.00	0.73
1:A:349:ARG:NH1	1:A:392:GLU:OE1	2.20	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:A:204:LEU:O	1:A:208:GLU:OE1	2.09	0.71
1:B:345:THR:HG21	1:B:387:ASP:OD1	1.90	0.71
1:A:312:LEU:HB2	1:A:398:LEU:HD13	1.73	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:B:274:VAL:HG13	1:B:278:LEU:HD12	1.73	0.69
1:A:308:GLU:O	1:A:332:SER:OG	2.09	0.69
1:A:244:ILE:O	1:A:248:THR:HG22	1.93	0.69
1:A:354:ARG:NH1	1:A:354:ARG:HG2	1.97	0.68
1:B:631:ASP:O	1:B:643:ASN:HB3	1.93	0.68
1:B:290:HIS:CD2	1:B:295:PRO:HA	2.28	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:CG	1:B:354:ARG:HH11	2.05	0.67
1:B:182:LYS:HE2	1:B:196:GLU:CD	2.14	0.67
1:B:109:GLN:HE21	1:B:139:LYS:CE	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:THR:HG21	1:A:666:GLY:N	2.09	0.66
1:A:110:SER:HB3	1:A:113:GLU:OE2	1.95	0.66
1:B:395:ASP:OD1	1:B:395:ASP:N	2.28	0.66
1:A:219:ALA:HB1	1:A:226:MET:HB2	1.78	0.66
1:B:203:HIS:CE1	1:B:206:ARG:HH11	2.13	0.66
1:A:214:LEU:O	1:A:218:VAL:HG23	1.96	0.66
1:A:354:ARG:NH1	1:A:365:GLU:CD	2.48	0.65
1:A:30:ILE:O	1:A:34:THR:OG1	2.14	0.65
1:A:553:VAL:HG11	1:A:593:ALA:HB2	1.79	0.64
1:A:464:ARG:O	1:A:468:GLU:HB3	1.97	0.64
1:A:633:MET:HB3	1:B:633:MET:HB3	1.77	0.64
1:A:120:TRP:HZ2	1:A:254:TYR:CD2	2.15	0.64
1:B:572:HIS:HD2	1:B:575:ASP:N	1.96	0.64
1:B:335:MET:HE1	1:B:341:VAL:HG11	1.78	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:A:154:ARG:HH22	1:A:610:GLU:CD	2.01	0.63
1:B:314:PHE:HE2	1:B:315:LYS:HZ3	1.45	0.63
1:B:227:GLU:N	1:B:227:GLU:OE1	2.30	0.63
1:B:343:ASN:OD1	1:B:345:THR:HG22	1.98	0.63
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:304:ASP:OD1	2:A:2005:HOH:O	2.16	0.62
1:A:34:THR:HB	1:A:70:ALA:HB1	1.81	0.62
1:A:297:GLU:CD	1:A:297:GLU:N	2.53	0.62
1:A:204:LEU:O	1:A:207:ALA:N	2.31	0.61
1:A:154:ARG:NH2	1:A:610:GLU:OE1	2.27	0.61
1:A:248:THR:HG21	1:A:277:TYR:HB3	1.82	0.61
1:A:211:ARG:O	1:A:215:ILE:HG13	2.00	0.61
1:B:304:ASP:OD1	1:B:306:SER:N	2.33	0.61
1:A:411:SER:HA	1:A:449:ILE:HD13	1.81	0.61
1:A:129:PRO:HG2	1:A:279:PRO:HG3	1.80	0.61
1:A:20:ASP:O	1:A:136:LYS:NZ	2.28	0.61
1:A:237:VAL:HG23	1:A:238:SER:H	1.65	0.61
1:A:302:LYS:HE2	1:A:304:ASP:CB	2.25	0.61
1:A:297:GLU:OE1	1:A:297:GLU:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASP:HB3	1:B:456:LEU:CD2	2.30	0.60
1:B:319:ASP:CG	1:B:320:PRO:HD2	2.21	0.60
1:B:315:LYS:HG2	1:B:327:PHE:HB2	1.82	0.60
1:B:408:ILE:HD11	1:B:454:GLY:C	2.21	0.60
1:A:115:GLN:N	1:A:115:GLN:OE1	2.31	0.60
1:A:344:SER:OG	1:A:397:ILE:HG12	2.02	0.60
1:B:226:MET:O	1:B:230:LEU:HD13	2.01	0.60
1:B:163:GLN:HA	1:B:176:ILE:O	2.02	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:B:185:LYS:HB2	1:B:195:GLU:OE1	2.02	0.60
1:A:413:GLU:HB3	1:A:474:ASN:HB2	1.84	0.60
1:B:602:GLU:CD	1:B:627:ARG:HH22	2.06	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:B:612:PRO:HG2	1:B:615:TYR:HE2	1.67	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
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:115:GLN:O	1:B:118:THR:OG1	2.12	0.59
1:B:450:ILE:HD12	1:B:450:ILE:O	2.02	0.59
1:B:366:ILE:HD11	1:B:369:VAL:HG22	1.85	0.59
1:A:291:ARG:HB3	1:A:395:ASP:OD2	2.02	0.59
1:A:319:ASP:OD1	1:A:320:PRO:HD2	2.03	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:A:340:TYR:OH	1:A:351:ARG:NH1	2.36	0.59
1:B:112:VAL:HG21	1:B:155:LEU:CD1	2.33	0.59
1:B:612:PRO:HG2	1:B:615:TYR:CE2	2.38	0.58
1:B:245:ARG:HG3	1:B:276:ASP:O	2.04	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:N	1:B:421:ASP:OD1	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:B:109:GLN:NE2	1:B:139:LYS:HE3	2.18	0.58
1:B:17:ALA:HB2	1:B:105:VAL:HB	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG22	1:A:76:ARG:NH1	2.19	0.58
1:B:602:GLU:OE2	1:B:627:ARG:NH2	2.34	0.57
1:B:335:MET:HE3	1:B:341:VAL:HG11	1.86	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:B:223:ASP:CA	1:B:226:MET:HG2	2.25	0.57
1:B:572:HIS:CD2	1:B:575:ASP:H	2.17	0.57
1:A:626:ARG:NH1	1:A:650:GLU:O	2.36	0.57
1:A:312:LEU:HB2	1:A:398:LEU:CD1	2.34	0.57
1:B:124:THR:HA	1:B:130:ARG:HH22	1.69	0.56
1:A:361:ASN:N	1:A:361:ASN:OD1	2.37	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:433:GLU:OE1	1:A:464:ARG:NH2	2.30	0.56
1:B:195:GLU:CD	1:B:195:GLU:N	2.39	0.56
1:B:359:HIS:HB2	1:B:362:SER:O	2.06	0.56
1:A:528:ILE:HG12	1:A:533:VAL:HB	1.87	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:181:MET:O	1:A:199:ILE:HD11	2.04	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:A:622:ASP:O	1:A:625:SER:OG	2.15	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: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:333:GLY:N	1:B:371:SER:OG	2.40	0.54
1:B:109:GLN:O	1:B:110:SER:CB	2.56	0.54
1:A:26:THR:O	1:A:30:ILE:HG13	2.07	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:A:662:THR:HG21	1:A:666:GLY:HA3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HD2	1:A:75:HIS:NE2	2.22	0.53
1:B:356:LEU:HD23	1:B:365:GLU:HA	1.89	0.53
1:A:460:ILE:O	1:A:463:ASP:HB3	2.07	0.53
1:A:245:ARG:HD2	1:A:276:ASP:O	2.08	0.53
1:B:211:ARG:O	1:B:214:LEU:HB3	2.09	0.53
1:B:128:VAL:O	1:B:130:ARG:NE	2.32	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:B:224:GLU:O	1:B:227:GLU:OE1	2.26	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:A:145:GLU:HA	1:A:145:GLU:OE1	2.08	0.53
1:B:684:GLU:OE1	1:B:688:LYS:NZ	2.42	0.53
1:A:627:ARG:HB3	1:A:627:ARG:HH11	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:161:PRO:HA	1:B:256:VAL:HB	1.91	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:A:155:LEU:O	1:A:156:GLN:HG2	2.10	0.52
1:A:83:PRO:HG2	1:A:92:VAL:CA	2.40	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:441:THR:O	1:A:442:ASP:C	2.48	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:636:ARG:HD3	1:A:641:VAL:HG23	1.92	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:36:ARG:O	1:A:36:ARG:HG3	2.09	0.52
1:A:208:GLU:CD	1:A:208:GLU:N	2.62	0.51
1:B:34:THR:HB	1:B:70:ALA:HB1	1.92	0.51
1:A:34:THR:HG22	1:A:72:TRP:HB2	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:636:ARG:O	1:A:639:ALA:O	2.28	0.51
1:A:177:ASP:OD2	1:A:180:GLU:HB2	2.10	0.51
1:B:317:MET:HG2	1:B:318:THR:H	1.75	0.51
1:B:346:LYS:NZ	1:B:346:LYS:HB3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:SER:H	1:B:9:LYS:CE	2.24	0.51
1:B:354:ARG:HH12	1:B:365:GLU:CD	2.13	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:345:THR:HG22	1:B:346:LYS:HG2	1.93	0.51
1:B:117:GLU:OE2	1:B:121:ARG:NH2	2.44	0.51
1:B:319:ASP:HB3	1:B:322:VAL:HG22	1.93	0.50
1:B:108:ALA:HB2	1:B:135:ASN:O	2.11	0.50
1:B:611:MET:N	1:B:611:MET:SD	2.84	0.50
1:A:413:GLU:OE1	1:A:474:ASN:ND2	2.29	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:O	1:B:260:THR:HG23	2.11	0.50
1:B:140:LEU:HD12	1:B:140:LEU:C	2.32	0.50
1:B:354:ARG:CG	1:B:354:ARG:NH1	2.69	0.49
1:B:535:ARG:HA	1:B:538:ILE:HD12	1.94	0.49
1:B:102:ALA:O	1:B:130:ARG:HA	2.12	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:B:349:ARG:CZ	1:B:392:GLU:OE2	2.60	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:113:GLU:HB3	1:B:114:PRO:CD	2.42	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:A:615:TYR:OH	1:A:665:ARG:NH1	2.44	0.49
1:B:189:ASP:CG	1:B:263:LYS:HD3	2.33	0.49
1:A:138:ASP:HA	1:A:169:GLU:O	2.12	0.49
1:B:9:LYS:HA	1:B:75:HIS:CE1	2.48	0.48
1:A:534:PRO:HD3	1:A:571:TYR:CD1	2.48	0.48
1:B:109:GLN:HB3	1:B:141:GLY:O	2.12	0.48
1:A:438:HIS:NE2	1:A:440:HIS:NE2	2.62	0.48
1:B:454:GLY:O	1:B:457:HIS:HB3	2.13	0.48
1:A:228:LYS:NZ	1:A:233:GLU:HB3	2.27	0.48
1:B:612:PRO:CG	1:B:615:TYR:HE2	2.25	0.48
1:B:23:LYS:O	1:B:23:LYS:HD3	2.14	0.48
1:B:505:GLN:HA	1:B:575:ASP:O	2.14	0.48
1:B:304:ASP:O	1:B:333:GLY:N	2.44	0.48
1:A:237:VAL:HG23	1:A:238:SER:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:HD3	1:A:314:PHE:HA	1.94	0.48
1:B:407:VAL:HG11	1:B:672:PHE:CD1	2.48	0.48
1:A:340:TYR:OH	1:A:351:ARG:CZ	2.62	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
1:B:32:TYR:CD1	1:B:32:TYR:C	2.87	0.48
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:A:222:SER:C	1:A:225:LEU:HD11	2.34	0.48
1:B:219:ALA:O	1:B:222:SER:O	2.31	0.48
1:A:224:GLU:HG2	1:A:225:LEU:N	2.28	0.47
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:B:121:ARG:CZ	1:B:636:ARG:HD3	2.44	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:A:163:GLN:O	1:A:164:LEU:HD23	2.15	0.47
1:B:477:ALA:O	1:B:479:MET:HG3	2.13	0.47
1:A:32:TYR:CD1	1:A:32:TYR:C	2.88	0.47
1:B:322:VAL:CG2	1:B:325:LEU:HD21	2.45	0.47
1:A:424:THR:O	1:A:428:VAL:HG23	2.14	0.47
1:B:450:ILE:CD1	1:B:458:LEU:HD22	2.44	0.47
1:B:88:PHE:O	1:B:92:VAL:HG23	2.14	0.47
1:A:426:ALA:O	1:A:430:LEU:HG	2.15	0.47
1:B:235:ILE:O	1:B:235:ILE:HD12	2.15	0.46
1:A:635:PRO:O	1:A:636:ARG:HD2	2.14	0.46
1:B:6:SER:OG	1:B:9:LYS:HE2	2.15	0.46
1:A:605:MET:HG2	1:A:648:LEU:HB2	1.97	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: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:B:211:ARG:NH2	1:B:235:ILE:CD1	2.74	0.46
1:A:348:LYS:HD3	1:A:349:ARG:N	2.22	0.46
1:B:423:MET:HG3	1:B:465:MET:HE2	1.97	0.46
1:A:679:PRO:CG	1:A:682:ILE:HD12	2.45	0.46
1:A:241:LYS:HG3	1:A:277:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TRP:CZ2	1:A:254:TYR:CD2	2.99	0.46
1:B:15:ILE:HG21	1:B:23:LYS:HE2	1.98	0.46
1:B:9:LYS:HA	1:B:75:HIS:ND1	2.31	0.46
1:B:423:MET:HG3	1:B:465:MET:CE	2.46	0.46
1:B:322:VAL:HG21	1:B:325:LEU:HD21	1.96	0.46
1:A:163:GLN:HA	1:A:176:ILE:O	2.16	0.46
1:A:85:HIS:O	1:A:88:PHE:HB2	2.16	0.46
1:A:260:THR:O	1:A:260:THR:HG23	2.16	0.46
1:B:429:LYS:NZ	1:B:433:GLU:OE2	2.42	0.45
1:B:337:SER:HB2	1:B:353:GLY:O	2.17	0.45
1:B:408:ILE:HG23	1:B:648:LEU:HD21	1.97	0.45
1:A:506:TYR:O	1:A:576:SER:HA	2.16	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:A:222:SER:CB	1:A:225:LEU:HD11	2.36	0.45
1:A:289:GLY:C	1:A:299:VAL:HG23	2.36	0.45
1:A:86:VAL:C	1:A:88:PHE:H	2.20	0.45
1:A:168:ALA:O	1:A:171:GLU:N	2.49	0.45
1:A:437:PHE:HD1	1:A:438:HIS:N	2.15	0.45
1:A:260:THR:HG22	1:A:265:LYS:HB2	1.98	0.45
1:B:485:THR:O	1:B:598:PRO:HA	2.17	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:128:VAL:HA	1:B:129:PRO:HD3	1.75	0.45
1:B:185:LYS:HB2	1:B:195:GLU:CD	2.38	0.45
1:A:437:PHE:HB2	1:A:451:GLY:O	2.16	0.45
1:A:3:ARG:CZ	1:A:6:SER:HA	2.46	0.45
1:B:626:ARG:O	1:B:627:ARG:HB3	2.17	0.45
1:A:441:THR:CA	1:A:448:VAL:HG23	2.37	0.45
1:B:96:LEU:HD22	1:B:128:VAL:HG21	1.98	0.45
1:A:248:THR:CG2	1:A:277:TYR:O	2.65	0.45
1:B:546:LYS:O	1:B:549:MET:N	2.50	0.45
1:A:509:VAL:HG22	1:A:584:ALA:HB1	1.99	0.45
1:A:204:LEU:O	1:A:206:ARG:N	2.50	0.45
1:B:162:ILE:HG13	1:B:256:VAL:O	2.17	0.44
1:B:23:LYS:HG3	1:B:24:THR:N	2.32	0.44
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:A:9:LYS:HD2	1:A:75:HIS:CD2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:NH2	1:A:283:ASP:OD2	2.50	0.44
1:B:659:ARG:O	1:B:663:GLN:N	2.50	0.44
1:B:329:ARG:HD2	1:B:330:VAL:N	2.32	0.44
1:A:204:LEU:O	1:A:205:ASP:C	2.53	0.44
1:B:615:TYR:O	1:B:618:ASP:N	2.51	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: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:B:21:ALA:HB1	1:B:105:VAL:HG12	2.00	0.44
1:B:10:THR:HG22	1:B:76:ARG:CG	2.48	0.44
1:A:602:GLU:HG2	1:A:678:VAL:HG22	1.98	0.44
1:B:546:LYS:HG3	1:B:547:ASP:N	2.33	0.44
1:A:614:GLU:CD	1:A:614:GLU:H	2.10	0.43
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:203:HIS:HE1	1:B:206:ARG:NH1	2.14	0.43
1:B:112:VAL:HG21	1:B:155:LEU:HD12	2.00	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:B:215:ILE:HG23	1:B:225:LEU:HD21	1.99	0.43
1:A:429:LYS:HG3	1:A:432:GLU:OE2	2.18	0.43
1:B:362:SER:HA	1:B:363:ARG:HH21	1.83	0.43
1:B:669:THR:HG22	1:B:670:MET:N	2.33	0.43
1:B:366:ILE:CD1	1:B:369:VAL:HG22	2.48	0.43
1:A:8:GLU:CD	1:A:8:GLU:N	2.71	0.43
1:B:411:SER:HA	1:B:449:ILE:HD12	2.00	0.43
1:B:163:GLN:HE22	1:B:257:LEU:HD23	1.84	0.43
1:B:96:LEU:HD23	1:B:99:LEU:HD11	2.01	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:330:VAL:HG23	1:A:330:VAL:O	2.18	0.43
1:A:278:LEU:HA	1:A:278:LEU:HD23	1.88	0.43
1:B:434:ASP:C	1:B:434:ASP:OD1	2.56	0.43
1:B:166:ILE:HD12	1:B:174:ALA:HB3	2.00	0.43
1:A:15:ILE:CG2	1:A:23:LYS:HG3	2.49	0.43
1:B:629:ARG:NH1	1:B:631:ASP:HB2	2.34	0.43
1:A:615:TYR:CZ	1:A:663:GLN:NE2	2.82	0.43
1:A:117:GLU:O	1:A:121:ARG:HG2	2.19	0.43
1:B:314:PHE:C	1:B:385:THR:HG23	2.40	0.42
1:B:346:LYS:HB2	1:B:348:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ARG:NH1	1:A:299:VAL:HG13	2.34	0.42
1:A:528:ILE:HD12	1:A:528:ILE:HA	1.77	0.42
1:A:369:VAL:HG12	1:A:373:ASP:HB3	2.00	0.42
1:B:227:GLU:OE2	1:B:228:LYS:NZ	2.43	0.42
1:A:93:GLU:HG3	1:A:126:TYR:OH	2.19	0.42
1:A:612:PRO:HG3	1:A:665:ARG:NE	2.34	0.42
1:B:291:ARG:NH1	1:B:395:ASP:OD1	2.50	0.42
1:A:8:GLU:H	1:A:8:GLU:CD	2.23	0.42
1:B:251:VAL:O	1:B:251:VAL:HG12	2.19	0.42
1:B:16:ILE:O	1:B:17:ALA:HB2	2.19	0.42
1:B:292:ALA:HA	1:B:397:ILE:HD11	2.00	0.42
1:A:245:ARG:NH1	1:A:276:ASP:O	2.51	0.42
1:A:179:VAL:O	1:A:179:VAL:HG12	2.20	0.42
1:B:492:VAL:HG21	1:B:592:ALA:HB2	2.02	0.42
1:A:6:SER:OG	1:A:9:LYS:HG2	2.19	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:B:138:ASP:C	1:B:169:GLU:HA	2.40	0.42
1:A:83:PRO:HG2	1:A:92:VAL:CB	2.50	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:184:PHE:CE1	1:B:196:GLU:HG2	2.55	0.42
1:B:304:ASP:C	1:B:304:ASP:OD1	2.58	0.42
1:B:10:THR:HG22	1:B:76:ARG:HG2	2.01	0.42
1:A:688:LYS:O	1:A:691:LYS:NZ	2.30	0.42
1:A:545:LEU:O	1:A:549:MET:N	2.50	0.42
1:A:99:LEU:HD13	1:A:101:GLY:O	2.20	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:B:214:LEU:O	1:B:218:VAL:HG23	2.19	0.42
1:A:678:VAL:HG13	1:A:679:PRO:HD2	2.02	0.42
1:A:409:HIS:HB2	1:A:450:ILE:O	2.20	0.42
1:A:348:LYS:CD	1:A:349:ARG:N	2.73	0.41
1:A:291:ARG:NH1	1:A:299:VAL:CG1	2.83	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:309:PHE:CZ	1:A:335:MET:HE2	2.55	0.41
1:B:107:ASP:O	1:B:111:GLY:HA2	2.20	0.41
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.73	0.41
1:A:222:SER:O	1:A:225:LEU:HD11	2.19	0.41
1:B:71:ALA:HA	1:B:75:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:TRP:CD1	1:B:130:ARG:NH1	2.88	0.41
1:A:308:GLU:N	1:A:308:GLU:OE1	2.49	0.41
1:B:412:VAL:HG12	1:B:448:VAL:O	2.20	0.41
1:A:180:GLU:O	1:A:181:MET:HB2	2.20	0.41
1:A:88:PHE:HA	1:A:88:PHE:HD1	1.79	0.41
1:B:555:ALA:HB3	1:B:557:TYR:CD2	2.55	0.41
1:B:414:PRO:HD2	1:B:447:GLN:HG2	2.02	0.41
1:B:355:LEU:O	1:B:365:GLU:HA	2.21	0.41
1:B:290:HIS:HD2	1:B:291:ARG:O	2.04	0.41
1:B:87:ASP:HB3	1:B:456:LEU:HD22	2.02	0.41
1:B:437:PHE:C	1:B:438:HIS:CD2	2.94	0.41
1:A:29:ARG:CD	1:A:33:TYR:CE2	3.03	0.41
1:B:66:ALA:HB1	1:B:315:LYS:HD2	2.01	0.41
1:B:350:GLU:HA	1:B:350:GLU:OE1	2.21	0.41
1:B:609:ILE:HD13	1:B:654:TYR:OH	2.20	0.41
1:B:163:GLN:C	1:B:164:LEU:HG	2.39	0.41
1:B:290:HIS:HA	1:B:297:GLU:O	2.20	0.41
1:A:319:ASP:HB3	1:A:322:VAL:HG22	2.03	0.41
1:A:164:LEU:HB2	1:A:176:ILE:HD12	2.01	0.41
1:B:164:LEU:CD1	1:B:178:LEU:HD21	2.45	0.41
1:B:23:LYS:C	1:B:23:LYS:HD3	2.41	0.41
1:B:390:CYS:SG	1:B:394:ASN:O	2.77	0.41
1:B:362:SER:CA	1:B:363:ARG:HH21	2.34	0.41
1:A:555:ALA:HB3	1:A:557:TYR:CD2	2.56	0.41
1:A:336:THR:HG22	1:A:337:SER:O	2.21	0.41
1:B:511:ILE:HA	1:B:565:LYS:O	2.21	0.41
1:B:270:MET:O	1:B:273:ALA:HB3	2.21	0.41
1:B:164:LEU:HA	1:B:165:PRO:HD3	1.76	0.41
1:B:17:ALA:CB	1:B:105:VAL:HB	2.51	0.41
1:B:314:PHE:O	1:B:385:THR:HG23	2.20	0.41
1:A:18:HIS:HD2	1:A:115:GLN:HB2	1.86	0.41
1:B:199:ILE:H	1:B:199:ILE:HG13	1.62	0.41
1:A:604:MET:HG3	1:A:676:ALA:HB2	2.03	0.41
1:A:230:LEU:C	1:A:230:LEU:HD12	2.42	0.41
1:B:175:ILE:O	1:B:183:CYS:HA	2.21	0.41
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:A:604:MET:CE	1:A:645:TYR:HB3	2.51	0.40
1:B:79:ILE:C	1:B:79:ILE:HD12	2.41	0.40
1:A:529:VAL:HG23	1:A:529:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:463:ASP:OD1	1:A:463:ASP:C	2.60	0.40
1:B:495:LYS:HG3	1:B:496:PHE:N	2.36	0.40
1:B:335:MET:HE2	1:B:335:MET:HB2	1.78	0.40
1:A:185:LYS:HE2	1:A:195:GLU:OE1	2.22	0.40
1:A:354:ARG:NH1	1:A:365:GLU:OE2	2.54	0.40
1:A:29:ARG:NE	1:A:29:ARG:HA	2.37	0.40
1:B:354:ARG:NH1	1:B:365:GLU:CD	2.75	0.40
1:B:129:PRO:HG2	1:B:279:PRO:HG3	2.04	0.40
1:A:211:ARG:O	1:A:214:LEU:HB3	2.21	0.40
1:B:119:VAL:O	1:B:122:GLN:HB2	2.21	0.40
1:A:228:LYS:HZ2	1:A:233:GLU:HB3	1.87	0.40
1:B:482:TYR:O	1:B:557:TYR:HB3	2.22	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:A:505:GLN:HA	1:A:575:ASP:O	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 ⓘ

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	639/693 (92%)	600 (94%)	38 (6%)	1 (0%)	52 84
1	B	639/693 (92%)	588 (92%)	48 (8%)	3 (0%)	34 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1278/1386 (92%)	1188 (93%)	86 (7%)	4 (0%)	46 79

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%)	507 (93%)	36 (7%)	21 51
1	B	543/579 (94%)	505 (93%)	38 (7%)	19 47
All	All	1086/1158 (94%)	1012 (93%)	74 (7%)	20 49

All (74) 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	88	PHE
1	A	116	THR
1	A	139	LYS
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
1	A	245	ARG

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	262	PHE
1	A	270	MET
1	A	280	SER
1	A	297	GLU
1	A	299	VAL
1	A	332	SER
1	A	349	ARG
1	A	352	VAL
1	A	354	ARG
1	A	361	ASN
1	A	363	ARG
1	A	364	GLN
1	A	398	LEU
1	A	448	VAL
1	A	528	ILE
1	A	529	VAL
1	A	536	GLU
1	A	614	GLU
1	A	636	ARG
1	A	660	SER
1	A	667	THR
1	B	3	ARG
1	B	10	THR
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	227	GLU
1	B	245	ARG
1	B	246	GLN
1	B	299	VAL
1	B	315	LYS

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Mol	Chain	Res	Type
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	421	ASP
1	B	424	THR
1	B	436	THR
1	B	448	VAL
1	B	459	ASP
1	B	514	THR
1	B	518	THR
1	B	575	ASP
1	B	611	MET
1	B	633	MET
1	B	657	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	663	GLN
1	B	163	GLN
1	B	290	HIS
1	B	438	HIS
1	B	510	HIS
1	B	572	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.05	11 (1%) 73 63	41, 82, 141, 252	0
1	B	649/693 (93%)	-0.02	3 (0%) 91 88	47, 87, 137, 274	0
All	All	1298/1386 (93%)	0.02	14 (1%) 82 74	41, 85, 139, 274	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	ALA	3.9
1	A	295	PRO	3.8
1	A	395	ASP	3.0
1	A	293	SER	2.7
1	B	559	LEU	2.6
1	A	396	ILE	2.6
1	A	692	GLY	2.4
1	A	441	THR	2.4
1	A	294	ASN	2.4
1	A	393	LYS	2.4
1	B	396	ILE	2.3
1	A	214	LEU	2.2
1	B	254	TYR	2.2
1	A	448	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.