



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:38 PM GMT

PDB ID : 1PWV  
Title : Crystal structure of Anthrax Lethal Factor wild-type protein complexed with an optimised peptide substrate.  
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.  
Deposited on : 2003-07-02  
Resolution : 2.85 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](mailto: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.

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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

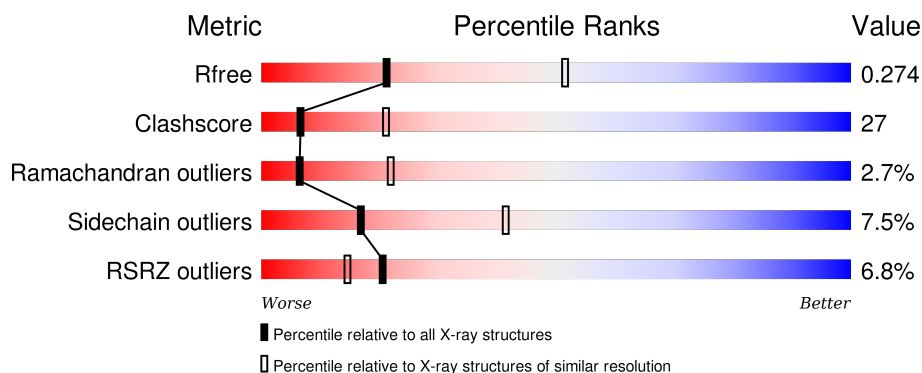
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	776	<div> <div>6%</div> <div>47%</div> <div>41%</div> <div>6%</div> <div>6%</div> </div>
1	B	776	<div> <div>6%</div> <div>49%</div> <div>41%</div> <div>5%</div> <div>5%</div> </div>
2	C	20	<div> <div>10%</div> <div>20%</div> <div>15%</div> <div>55%</div> </div>
2	D	20	<div> <div>10%</div> <div>15%</div> <div>20%</div> <div>10%</div> <div>55%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12230 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 Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			6028	3833	1015	1173	7			
1	B	736	Total	C	N	O	S	0	0	0
			6050	3848	1014	1181	7			

- Molecule 2 is a protein called LF20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	S	0	0	0
			76	52	9	14	1			
2	D	9	Total	C	N	O	S	0	0	0
			76	52	9	14	1			





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.70 Å   137.40 Å   98.30 Å 90.00°   98.00°   90.00°	Depositor
Resolution (Å)	46.06 – 2.85 46.05 – 2.85	Depositor EDS
% Data completeness (in resolution range)	85.8 (46.06-2.85) 85.8 (46.05-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.86 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.231 , 0.279 0.229 , 0.274	Depositor DCC
$R_{free}$ test set	2578 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	EDS
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 56961 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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	0.40	0/6136	0.65	1/8263 (0.0%)
1	B	0.41	0/6158	0.66	2/8294 (0.0%)
2	C	0.49	0/80	0.97	1/111 (0.9%)
2	D	0.41	0/80	0.75	0/111
All	All	0.40	0/12454	0.66	4/16779 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	PRO	CA-N-CD	-6.97	101.74	111.50
2	C	15	PRO	CA-N-CD	-6.07	103.00	111.50
1	A	97	LEU	CA-C-N	-5.86	104.31	117.20
1	B	126	GLU	N-CA-C	-5.02	97.44	111.00

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	6028	0	6018	357	0
1	B	6050	0	6034	311	0
2	C	76	0	69	12	0
2	D	76	0	69	7	0
All	All	12230	0	12190	664	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (664) 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:352:GLU:O	1:B:356:LEU:HG	1.40	1.18
1:B:304:LYS:HD3	1:B:304:LYS:H	0.99	1.15
1:A:319:LEU:HA	1:A:322:ILE:HD11	1.20	1.12
1:A:516:ASN:HD21	1:A:518:LYS:HD2	1.20	1.05
1:B:675:VAL:HG22	2:D:14:GLU:HG2	1.39	1.04
1:A:434:LYS:HZ2	1:A:434:LYS:HB3	1.20	1.04
1:B:366:ASN:HB2	1:B:367:PRO:HD3	1.41	1.02
1:A:268:TYR:HB3	1:B:125:TYR:CE2	1.96	1.01
1:B:483:TYR:HB3	1:B:520:ILE:HD11	1.40	1.00
1:A:304:LYS:HD3	1:A:304:LYS:H	1.27	0.97
1:A:49:LYS:HG3	1:A:50:GLY:H	1.28	0.96
1:A:577:PRO:O	1:A:580:THR:HG22	1.65	0.95
1:B:712:LYS:HD2	1:B:712:LYS:H	1.27	0.94
1:B:510:ARG:H	1:B:522:GLN:HE21	1.11	0.94
1:B:304:LYS:HD3	1:B:304:LYS:N	1.81	0.94
1:B:708:VAL:HG21	1:B:769:GLN:HE21	1.36	0.91
1:A:104:ILE:HG22	1:A:105:LYS:H	1.36	0.90
1:A:92:ILE:HD12	1:A:92:ILE:H	1.37	0.89
1:A:516:ASN:ND2	1:A:518:LYS:HD2	1.86	0.89
1:B:304:LYS:CD	1:B:304:LYS:H	1.86	0.89
1:B:498:ARG:HH21	1:B:540:LYS:HE3	1.39	0.88
1:B:712:LYS:HA	1:B:715:ILE:HD12	1.56	0.88
1:A:107:ILE:HG21	1:A:145:LEU:HD12	1.56	0.87
1:A:563:GLN:NE2	1:A:585:PHE:H	1.72	0.86
1:B:711:SER:O	1:B:715:ILE:HG13	1.76	0.86
1:A:87:ASP:OD1	1:A:115:HIS:HB2	1.76	0.86
1:A:268:TYR:HB3	1:B:125:TYR:HE2	1.37	0.85
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.57	0.85
1:A:434:LYS:HB3	1:A:434:LYS:NZ	1.92	0.85
1:B:43:ILE:HD11	1:B:75:LYS:HB2	1.58	0.84
1:A:675:VAL:HA	2:C:14:GLU:HG3	1.59	0.83
1:A:322:ILE:HG23	1:A:372:GLU:OE1	1.76	0.83
1:B:90:LYS:HE3	1:B:90:LYS:HA	1.61	0.83
1:B:324:ILE:H	1:B:324:ILE:HD12	1.41	0.83
1:A:46:ILE:H	1:A:46:ILE:HD12	1.44	0.82
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.62	0.81
1:A:368:LEU:HD23	1:A:369:SER:N	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:HD23	1:B:237:ALA:HB3	1.62	0.81
1:B:77:ILE:HD11	1:B:162:LYS:HG3	1.61	0.80
1:A:104:ILE:HD11	1:A:114:LEU:HG	1.63	0.80
1:B:97:LEU:HB2	1:B:102:LYS:NZ	1.96	0.80
1:A:766:ILE:O	1:A:770:ILE:HG12	1.82	0.80
1:B:496:ASN:H	1:B:496:ASN:HD22	1.26	0.80
1:B:349:LEU:HG	1:B:350:SER:H	1.47	0.79
1:A:304:LYS:H	1:A:304:LYS:CD	1.95	0.79
1:A:368:LEU:HD23	1:A:369:SER:H	1.49	0.78
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.13	0.78
1:A:686:HIS:HB2	1:A:742:ARG:HD3	1.65	0.78
1:B:516:ASN:HD22	1:B:516:ASN:H	1.32	0.77
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.66	0.77
1:A:263:ARG:HB3	1:A:263:ARG:HH11	1.49	0.77
1:A:754:LYS:O	1:A:758:ASN:HB2	1.85	0.77
1:A:426:SER:HA	1:A:510:ARG:HA	1.67	0.77
1:B:708:VAL:HG21	1:B:769:GLN:NE2	2.01	0.76
1:B:712:LYS:CD	1:B:712:LYS:H	1.98	0.76
1:B:34:GLU:O	1:B:38:GLU:HB2	1.85	0.76
1:B:483:TYR:CB	1:B:520:ILE:HD11	2.17	0.75
1:B:628:ARG:H	1:B:665:SER:HB3	1.51	0.75
1:A:312:SER:HB3	1:A:315:GLU:HG3	1.68	0.74
1:B:510:ARG:H	1:B:522:GLN:NE2	1.86	0.74
1:B:454:LEU:HA	1:B:467:ILE:HG21	1.70	0.74
1:A:66:VAL:HG12	1:A:70:VAL:HG21	1.70	0.74
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.68	0.73
1:A:510:ARG:HB2	1:A:522:GLN:HG2	1.70	0.73
1:B:564:LEU:O	1:B:568:GLN:HG3	1.88	0.73
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.23	0.73
1:A:49:LYS:HG3	1:A:50:GLY:N	2.02	0.73
1:A:65:LYS:HE2	1:A:227:PRO:HG3	1.69	0.73
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.71	0.73
1:B:366:ASN:CB	1:B:367:PRO:HD3	2.18	0.72
1:B:165:GLN:HE21	1:B:166:PRO:HA	1.54	0.72
1:A:319:LEU:HA	1:A:322:ILE:CD1	2.11	0.72
1:B:677:LEU:HD11	2:D:11:TYR:CE1	2.25	0.72
1:B:516:ASN:HD22	1:B:516:ASN:N	1.86	0.72
1:A:263:ARG:HD3	1:B:264:MET:HE2	1.72	0.71
1:A:79:GLY:HA2	1:A:127:PRO:HG2	1.72	0.71
1:A:598:SER:O	1:A:602:ILE:HG13	1.90	0.71
1:A:411:GLN:HE21	1:A:411:GLN:HA	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ASN:HB2	1:B:367:PRO:CD	2.19	0.70
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.56	0.70
1:A:296:LEU:O	1:A:296:LEU:HD22	1.90	0.70
1:A:676:GLU:HG2	2:C:14:GLU:OE2	1.91	0.70
1:B:406:LEU:HD12	1:B:406:LEU:O	1.91	0.70
1:A:318:LEU:HG	1:A:372:GLU:CD	2.12	0.70
1:B:258:GLU:HG3	1:B:502:ARG:NH1	2.07	0.70
1:B:258:GLU:HG3	1:B:502:ARG:HH12	1.56	0.70
1:B:121:ALA:HB1	1:B:154:ILE:HD11	1.74	0.69
1:B:346:ARG:HE	1:B:356:LEU:HD13	1.56	0.69
1:B:496:ASN:N	1:B:496:ASN:HD22	1.89	0.69
1:A:412:TYR:O	1:A:416:ILE:HG13	1.93	0.69
1:A:244:MET:HE3	1:A:244:MET:HA	1.73	0.69
1:A:741:PHE:O	1:A:745:HIS:HD2	1.74	0.69
1:B:107:ILE:HG21	1:B:145:LEU:CD1	2.22	0.69
1:B:352:GLU:O	1:B:356:LEU:CG	2.31	0.68
1:A:123:GLU:HG2	1:A:124:GLY:H	1.58	0.68
1:A:118:TYR:CD2	1:A:143:LYS:HD3	2.28	0.68
1:A:410:LYS:HE2	1:A:414:ARG:HH21	1.59	0.68
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.29	0.68
1:B:331:SER:OG	1:B:334:GLU:HG3	1.94	0.68
1:A:370:GLU:HG3	1:A:373:LYS:HD3	1.77	0.67
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.29	0.67
1:A:346:ARG:O	1:A:348:SER:N	2.23	0.67
1:A:449:THR:HA	1:A:673:LYS:HD3	1.76	0.67
1:A:658:LEU:HD21	2:C:8:VAL:HB	1.75	0.67
1:B:107:ILE:HB	1:B:146:ASN:ND2	2.10	0.67
1:A:156:SER:HB3	1:A:217:PHE:CD2	2.29	0.66
1:A:675:VAL:O	1:A:675:VAL:HG13	1.94	0.66
1:A:173:VAL:O	1:A:177:ILE:HG12	1.96	0.66
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.30	0.66
1:B:401:SER:CB	1:B:638:ASN:HD22	2.07	0.66
1:A:410:LYS:HE2	1:A:414:ARG:NH2	2.11	0.66
1:B:553:SER:O	1:B:557:THR:HG23	1.95	0.66
1:A:567:ASN:HD21	1:A:583:ILE:H	1.43	0.66
1:B:516:ASN:ND2	1:B:516:ASN:H	1.93	0.66
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.78	0.65
1:B:392:LEU:HD21	1:B:416:ILE:HD12	1.77	0.65
1:B:312:SER:OG	1:B:315:GLU:HG3	1.95	0.65
1:A:338:LEU:HA	1:A:341:LEU:HD12	1.77	0.65
1:B:679:ASN:C	1:B:679:ASN:HD22	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:HB3	1:B:136:ASP:OD1	1.96	0.65
1:B:483:TYR:HB3	1:B:520:ILE:CD1	2.23	0.65
1:B:754:LYS:O	1:B:758:ASN:HB2	1.95	0.65
1:A:491:ARG:HH21	1:B:539:GLU:HG3	1.62	0.65
1:A:94:LEU:HD22	1:A:97:LEU:CD1	2.26	0.65
1:A:340:LYS:HG3	1:A:343:ILE:HD12	1.78	0.65
1:A:333:GLU:H	1:A:333:GLU:CD	1.99	0.65
1:B:165:GLN:NE2	1:B:166:PRO:HA	2.11	0.65
1:B:611:GLN:NE2	1:B:774:ILE:HD13	2.11	0.65
1:A:732:ASN:ND2	1:A:735:GLU:HG2	2.12	0.64
1:B:712:LYS:HD2	1:B:712:LYS:N	2.09	0.64
1:B:237:ALA:N	1:B:238:PRO:CD	2.60	0.64
1:A:595:ILE:HD11	1:A:633:ASP:HB3	1.79	0.64
1:A:250:GLN:HG3	1:A:251:GLU:H	1.63	0.64
1:B:97:LEU:HB2	1:B:102:LYS:HZ1	1.61	0.64
1:A:460:ASN:N	1:A:460:ASN:HD22	1.96	0.64
1:A:66:VAL:CG1	1:A:70:VAL:HG21	2.27	0.64
1:A:711:SER:O	1:A:715:ILE:HG13	1.98	0.64
1:B:207:GLU:HB3	1:B:208:GLN:HE21	1.63	0.64
1:A:94:LEU:HD22	1:A:97:LEU:HD12	1.79	0.64
1:B:722:GLY:HA3	1:B:730:ARG:HH11	1.62	0.64
1:B:721:GLU:OE1	1:B:761:LYS:HB2	1.98	0.63
1:A:99:GLU:O	1:A:103:LYS:HD3	1.97	0.63
1:A:500:LYS:HE2	1:A:537:GLN:NE2	2.14	0.63
1:A:319:LEU:CA	1:A:322:ILE:HD11	2.12	0.63
1:B:84:VAL:HG22	1:B:85:ASP:N	2.12	0.63
1:B:324:ILE:HD13	1:B:339:LYS:HG2	1.80	0.63
1:B:300:ILE:HB	1:B:386:TYR:HB3	1.79	0.63
1:A:179:ASN:ND2	1:A:200:ASP:OD1	2.29	0.63
1:B:156:SER:HB2	1:B:217:PHE:CD2	2.34	0.63
1:A:437:LEU:HD12	1:A:505:LEU:HG	1.80	0.62
1:A:679:ASN:C	1:A:679:ASN:HD22	2.03	0.62
1:A:625:GLY:HA3	1:A:664:ARG:HD2	1.81	0.62
1:B:759:ALA:N	1:B:760:PRO:HD3	2.14	0.62
1:A:332:THR:HG22	1:A:336:GLU:OE2	2.00	0.62
1:A:67:PRO:O	1:A:70:VAL:HG22	1.99	0.62
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.15	0.62
1:A:206:LEU:HD13	1:A:213:VAL:HG21	1.82	0.62
1:A:343:ILE:O	1:A:346:ARG:HG3	2.00	0.62
1:A:37:LYS:O	1:A:41:LYS:HG3	2.00	0.61
1:A:107:ILE:HD13	1:A:107:ILE:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASN:ND2	1:B:496:ASN:HB2	2.15	0.61
1:A:702:LYS:H	1:A:702:LYS:HD2	1.65	0.61
1:A:140:ASN:OD1	1:A:143:LYS:HG3	2.01	0.61
1:B:125:TYR:CE2	1:B:162:LYS:HE3	2.36	0.61
1:A:107:ILE:HD11	1:A:219:LYS:HG3	1.81	0.61
1:B:496:ASN:H	1:B:496:ASN:ND2	1.98	0.61
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.33	0.61
1:B:47:GLU:O	1:B:84:VAL:HG23	2.01	0.61
1:A:57:GLU:HA	1:A:60:GLU:OE2	2.00	0.61
1:A:118:TYR:CD2	1:A:119:VAL:HG23	2.36	0.60
1:B:107:ILE:HG12	1:B:149:TYR:CG	2.36	0.60
1:B:256:LEU:HD22	1:B:260:LYS:HE2	1.82	0.60
1:A:392:LEU:HD21	1:A:416:ILE:HD13	1.83	0.60
1:B:555:ILE:N	1:B:555:ILE:HD12	2.17	0.60
1:A:373:LYS:HE2	1:A:377:LYS:HE3	1.83	0.60
1:B:169:LYS:O	1:B:172:ASP:HB2	2.02	0.60
1:A:55:LYS:HE2	1:A:85:ASP:OD2	2.01	0.60
1:A:323:GLN:O	1:A:326:SER:N	2.33	0.60
1:A:578:LYS:HG2	1:A:579:TYR:CD2	2.37	0.60
1:A:300:ILE:HD12	1:A:300:ILE:N	2.17	0.60
1:B:304:LYS:O	1:B:308:ILE:HG13	2.01	0.60
1:A:710:ASN:O	1:A:715:ILE:HD11	2.02	0.59
1:B:304:LYS:HE2	1:B:305:ASP:OD2	2.02	0.59
1:A:315:GLU:HB3	1:A:375:PHE:HE1	1.67	0.59
1:B:107:ILE:H	1:B:146:ASN:HD21	1.50	0.59
1:B:733:GLU:CD	1:B:733:GLU:H	2.05	0.59
1:A:491:ARG:HH21	1:B:539:GLU:CG	2.16	0.59
1:B:740:ALA:O	1:B:744:MET:HG3	2.02	0.59
1:A:136:ASP:OD1	1:A:139:GLU:N	2.35	0.59
1:A:102:LYS:O	1:A:114:LEU:HB2	2.01	0.59
1:A:578:LYS:HG2	1:A:579:TYR:CE2	2.38	0.59
1:A:679:ASN:ND2	1:A:682:GLU:HG3	2.18	0.59
1:B:85:ASP:OD1	1:B:133:SER:HB3	2.03	0.59
1:A:677:LEU:HD21	2:C:11:TYR:CE1	2.37	0.58
1:B:478:SER:HB2	1:B:590:ARG:O	2.03	0.58
1:B:587:VAL:HA	1:B:633:ASP:OD1	2.04	0.58
1:A:268:TYR:CB	1:B:125:TYR:HE2	2.11	0.58
1:B:679:ASN:ND2	1:B:682:GLU:H	2.01	0.58
1:B:36:LEU:HG	1:B:40:MET:HE1	1.85	0.58
1:A:615:ILE:O	1:A:619:THR:HB	2.04	0.58
1:A:656:LYS:O	1:A:668:LEU:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ARG:O	1:B:665:SER:HB2	2.03	0.58
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.19	0.58
1:B:187:ASP:HA	1:B:195:LYS:HE2	1.84	0.58
1:A:178:LYS:HG3	1:A:179:ASN:N	2.18	0.58
1:A:156:SER:HA	1:A:160:LEU:HD12	1.86	0.58
1:B:557:THR:O	1:B:561:GLU:HG3	2.04	0.58
1:A:411:GLN:NE2	1:A:411:GLN:HA	2.18	0.58
1:B:122:LYS:HB3	1:B:128:VAL:HG22	1.86	0.57
1:A:611:GLN:OE1	1:A:770:ILE:HG21	2.04	0.57
1:A:500:LYS:HE2	1:A:537:GLN:HE22	1.68	0.57
1:B:529:ILE:N	1:B:529:ILE:HD12	2.20	0.57
1:B:555:ILE:HD12	1:B:555:ILE:H	1.69	0.57
1:B:510:ARG:N	1:B:522:GLN:HE21	1.91	0.57
1:B:123:GLU:HG2	1:B:124:GLY:H	1.70	0.57
1:A:635:THR:OG1	1:A:637:PRO:HD2	2.04	0.57
1:B:658:LEU:HD12	1:B:659:TYR:H	1.70	0.57
1:A:574:LEU:HD23	1:A:619:THR:HG21	1.86	0.57
1:B:636:LEU:O	1:B:642:GLN:NE2	2.38	0.57
1:A:198:PRO:HG2	1:A:199:THR:H	1.69	0.57
1:A:435:ILE:HD12	1:A:435:ILE:N	2.19	0.56
1:B:683:GLY:O	1:B:687:GLU:HG2	2.05	0.56
1:A:315:GLU:HB3	1:A:375:PHE:CE1	2.41	0.56
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.41	0.56
1:B:65:LYS:HB3	1:B:65:LYS:NZ	2.19	0.56
1:A:717:ILE:HG23	1:A:761:LYS:HB3	1.88	0.56
1:A:675:VAL:HA	2:C:14:GLU:CG	2.34	0.56
1:B:401:SER:HB3	1:B:638:ASN:HD22	1.70	0.56
1:A:455:VAL:CG1	1:A:460:ASN:HA	2.35	0.56
1:B:36:LEU:O	1:B:40:MET:HE3	2.06	0.56
1:B:126:GLU:N	1:B:127:PRO:HD3	2.19	0.56
1:B:319:LEU:O	1:B:322:ILE:HG22	2.06	0.56
1:A:732:ASN:HD21	1:A:735:GLU:HG2	1.70	0.56
1:B:524:ASN:HD22	1:B:552:LYS:HE3	1.70	0.56
1:A:304:LYS:HD3	1:A:304:LYS:N	2.09	0.56
1:A:99:GLU:OE1	1:A:99:GLU:HA	2.06	0.55
1:A:455:VAL:HG12	1:A:460:ASN:HA	1.88	0.55
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.87	0.55
1:A:234:GLN:HB2	1:A:241:PHE:CD2	2.41	0.55
1:B:476:LYS:C	1:B:529:ILE:HD13	2.27	0.55
1:B:63:LEU:O	1:B:65:LYS:N	2.39	0.55
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:HD22	1:A:682:GLU:HB2	1.88	0.55
1:B:67:PRO:HB2	1:B:70:VAL:HG23	1.88	0.55
1:B:346:ARG:NE	1:B:356:LEU:HD13	2.21	0.55
1:B:677:LEU:HD22	1:B:682:GLU:HB3	1.89	0.55
1:A:437:LEU:HD12	1:A:505:LEU:CG	2.36	0.55
1:A:83:ILE:N	1:A:83:ILE:HD12	2.21	0.55
1:B:107:ILE:HD13	1:B:219:LYS:HG2	1.89	0.54
1:A:396:GLY:HA3	1:A:588:HIS:HD2	1.71	0.54
1:A:66:VAL:HG12	1:A:70:VAL:CG2	2.37	0.54
1:A:79:GLY:CA	1:A:127:PRO:HG2	2.37	0.54
1:A:653:VAL:HG21	1:A:658:LEU:HG	1.90	0.54
1:B:90:LYS:CA	1:B:90:LYS:HE3	2.35	0.54
1:A:67:PRO:HD3	1:A:225:ILE:HD12	1.90	0.54
1:B:74:TYR:HA	1:B:159:ILE:HD11	1.88	0.54
1:B:460:ASN:O	1:B:498:ARG:NH2	2.37	0.54
1:A:656:LYS:CE	1:A:680:ASP:OD2	2.55	0.54
1:A:140:ASN:HD21	1:A:142:GLU:HB2	1.73	0.54
1:A:370:GLU:HA	1:A:373:LYS:HB3	1.88	0.54
1:A:247:PHE:HA	1:A:251:GLU:HB2	1.89	0.54
1:A:252:ILE:O	1:A:255:SER:HB2	2.08	0.54
1:A:182:ASP:OD1	1:A:184:ASP:HB2	2.08	0.54
1:B:693:ASP:OD2	1:B:708:VAL:HG12	2.08	0.53
1:A:677:LEU:HD11	2:C:11:TYR:CE1	2.43	0.53
1:A:739:GLU:HA	1:A:739:GLU:OE1	2.07	0.53
1:A:586:ASN:HB3	1:A:632:THR:HB	1.88	0.53
1:A:289:GLY:HA2	1:A:422:LEU:HD11	1.90	0.53
1:B:64:GLU:O	1:B:64:GLU:HG2	2.08	0.53
1:A:319:LEU:HD12	1:A:322:ILE:CD1	2.39	0.53
1:A:566:ILE:HG23	1:A:583:ILE:HD12	1.90	0.53
1:A:648:GLU:HB2	1:A:651:GLU:HG3	1.91	0.53
1:A:730:ARG:O	1:A:730:ARG:HG2	2.08	0.53
1:B:77:ILE:HG13	1:B:162:LYS:HE2	1.90	0.53
1:B:95:GLU:C	1:B:97:LEU:H	2.11	0.53
1:B:349:LEU:HG	1:B:350:SER:N	2.22	0.53
1:A:277:HIS:CE1	1:A:425:GLN:HE21	2.27	0.53
1:B:36:LEU:HG	1:B:40:MET:CE	2.38	0.53
1:B:669:HIS:CE1	1:B:671:PRO:HD2	2.44	0.53
1:A:648:GLU:HB3	1:A:650:TYR:CE1	2.43	0.53
1:A:674:GLY:O	1:A:676:GLU:N	2.42	0.53
1:A:332:THR:O	1:A:336:GLU:HG3	2.09	0.53
1:B:618:VAL:O	1:B:621:TYR:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ALA:HB1	1:B:497:GLU:HB2	1.90	0.53
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.73	0.53
1:B:311:LEU:HD22	1:B:315:GLU:HB3	1.91	0.52
1:B:456:ASP:HB3	1:B:459:ASP:O	2.09	0.52
1:A:103:LYS:HD2	1:A:103:LYS:N	2.23	0.52
1:A:440:ASN:HD21	1:A:500:LYS:NZ	2.07	0.52
1:A:104:ILE:CG2	1:A:105:LYS:H	2.16	0.52
1:A:563:GLN:HE21	1:A:585:PHE:H	1.54	0.52
1:B:693:ASP:OD2	1:B:709:THR:HG23	2.09	0.52
1:B:67:PRO:HG2	1:B:248:ASN:OD1	2.10	0.52
1:A:640:ALA:O	1:A:642:GLN:N	2.42	0.52
1:A:658:LEU:HD22	1:A:659:TYR:N	2.25	0.52
1:A:254:LEU:HD13	1:A:502:ARG:NH2	2.25	0.52
1:B:605:GLU:HG3	1:B:681:SER:OG	2.10	0.52
1:B:95:GLU:O	1:B:97:LEU:HD23	2.10	0.52
1:A:196:GLU:O	1:A:197:HIS:C	2.49	0.51
1:A:437:LEU:HD11	1:A:519:LEU:HD12	1.92	0.51
1:A:167:TYR:CZ	1:A:536:LYS:HB2	2.45	0.51
1:B:630:VAL:HG11	1:B:639:ILE:HD13	1.91	0.51
1:A:318:LEU:HD21	1:A:372:GLU:HG2	1.91	0.51
1:A:319:LEU:HD12	1:A:322:ILE:HD11	1.92	0.51
1:B:675:VAL:HG12	1:B:676:GLU:HG2	1.92	0.51
1:B:477:TYR:CD1	1:B:555:ILE:HG23	2.45	0.51
1:A:203:VAL:HG21	1:A:465:ARG:NH2	2.24	0.51
1:A:165:GLN:HA	1:A:166:PRO:C	2.31	0.51
1:A:373:LYS:HE2	1:A:377:LYS:CE	2.39	0.51
1:A:656:LYS:HE2	1:A:680:ASP:OD2	2.11	0.51
1:A:435:ILE:H	1:A:435:ILE:HD12	1.76	0.51
1:B:287:GLU:CA	1:B:290:ARG:HH21	2.23	0.51
1:A:399:ILE:CD1	1:A:413:LYS:HG3	2.40	0.51
1:B:598:SER:O	1:B:602:ILE:HG13	2.11	0.51
1:A:285:LEU:HD22	1:A:290:ARG:HD3	1.93	0.51
1:A:313:GLN:O	1:A:317:GLU:HG2	2.10	0.51
1:A:490:GLU:OE2	1:A:500:LYS:HE3	2.11	0.51
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.11	0.51
1:B:426:SER:HA	1:B:510:ARG:HA	1.93	0.51
1:B:84:VAL:CG2	1:B:85:ASP:N	2.73	0.51
1:A:319:LEU:HD23	1:A:345:ILE:CD1	2.41	0.51
1:B:149:TYR:HA	1:B:222:ALA:HB2	1.92	0.51
1:A:697:GLY:HA3	1:A:706:ASP:O	2.11	0.50
1:A:119:VAL:CG2	1:A:147:VAL:HG22	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LEU:HD11	2:D:11:TYR:CZ	2.47	0.50
1:A:460:ASN:N	1:A:460:ASN:ND2	2.58	0.50
1:B:637:PRO:HA	1:B:642:GLN:NE2	2.26	0.50
1:A:669:HIS:CD2	1:A:671:PRO:HD2	2.47	0.50
1:A:175:ASN:OD1	1:A:200:ASP:HB3	2.12	0.50
1:A:595:ILE:CD1	1:A:633:ASP:HB3	2.40	0.50
1:A:690:HIS:HB3	2:C:9:TYR:HD2	1.75	0.50
1:A:491:ARG:HB3	1:A:492:PRO:HD2	1.94	0.50
1:A:437:LEU:CD1	1:A:519:LEU:HD12	2.42	0.50
1:B:287:GLU:HA	1:B:290:ARG:HH21	1.76	0.50
1:A:65:LYS:CE	1:A:227:PRO:HG3	2.41	0.50
1:A:675:VAL:HG12	2:C:11:TYR:HE2	1.76	0.50
1:B:150:GLU:O	1:B:153:LYS:HB2	2.11	0.50
1:B:197:HIS:HD2	1:B:199:THR:O	1.95	0.50
1:B:48:VAL:HB	1:B:85:ASP:OD2	2.12	0.50
1:A:676:GLU:HA	1:A:676:GLU:OE1	2.12	0.49
1:B:206:LEU:O	1:B:206:LEU:HD13	2.11	0.49
1:B:453:ASP:HB2	1:B:467:ILE:HG12	1.94	0.49
1:B:107:ILE:HG21	1:B:145:LEU:HD11	1.92	0.49
1:B:446:LEU:HG	1:B:591:TYR:HB2	1.93	0.49
1:A:653:VAL:CG2	1:A:658:LEU:HG	2.43	0.49
1:B:93:SER:HB2	1:B:128:VAL:HG11	1.93	0.49
1:A:647:ASP:HB2	1:A:651:GLU:OE1	2.12	0.49
1:A:31:THR:HA	1:A:34:GLU:HB2	1.94	0.49
1:B:472:LYS:HG3	1:B:532:VAL:HB	1.94	0.49
1:B:107:ILE:CD1	1:B:219:LYS:HG2	2.43	0.49
1:B:437:LEU:HD11	1:B:519:LEU:HD12	1.94	0.49
1:B:563:GLN:O	1:B:567:ASN:ND2	2.37	0.49
1:A:104:ILE:HG22	1:A:105:LYS:N	2.15	0.49
1:B:308:ILE:O	1:B:311:LEU:HB2	2.13	0.49
1:A:49:LYS:CG	1:A:50:GLY:H	2.13	0.49
1:A:165:GLN:HA	1:A:166:PRO:O	2.13	0.49
1:A:154:ILE:HG22	1:A:159:ILE:HD13	1.94	0.49
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.93	0.49
1:B:682:GLU:HG2	1:B:742:ARG:HH11	1.77	0.49
1:A:178:LYS:HG3	1:A:179:ASN:H	1.78	0.49
1:A:399:ILE:HD12	1:A:413:LYS:HG3	1.94	0.49
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.78	0.48
1:A:472:LYS:HG3	1:A:532:VAL:HB	1.95	0.48
1:A:612:SER:O	1:A:616:LYS:HG3	2.13	0.48
1:A:346:ARG:C	1:A:348:SER:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:VAL:O	2:C:8:VAL:HG23	2.13	0.48
1:B:91:HIS:HD2	1:B:93:SER:OG	1.96	0.48
1:A:300:ILE:H	1:A:300:ILE:HD12	1.78	0.48
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.96	0.48
1:A:571:ASN:OD1	1:A:580:THR:HG23	2.13	0.48
1:B:678:ARG:HH11	1:B:678:ARG:HB3	1.78	0.48
1:A:210:SER:O	1:A:214:GLN:HG3	2.13	0.48
1:A:122:LYS:HE2	1:A:128:VAL:HG23	1.95	0.48
1:A:627:GLY:HA3	1:A:664:ARG:O	2.14	0.48
1:B:129:LEU:HD13	1:B:131:ILE:HD11	1.94	0.48
1:A:643:TYR:HA	1:A:646:GLN:CG	2.38	0.48
1:A:424:HIS:O	1:A:510:ARG:HD2	2.14	0.48
1:B:578:LYS:O	1:B:579:TYR:HB2	2.14	0.48
1:B:323:GLN:NE2	1:B:325:ASP:HB2	2.28	0.48
1:B:250:GLN:O	1:B:252:ILE:N	2.47	0.48
1:A:49:LYS:O	1:A:51:GLU:N	2.46	0.48
1:A:453:ASP:HB2	1:A:467:ILE:HG12	1.95	0.48
1:A:321:ARG:O	1:A:321:ARG:HG3	2.13	0.48
1:B:608:ASN:HD22	1:B:608:ASN:N	2.10	0.48
1:B:325:ASP:O	1:B:326:SER:HB2	2.14	0.48
1:B:233:LEU:CD2	1:B:237:ALA:HB3	2.40	0.48
1:A:277:HIS:CD2	1:A:429:SER:CB	2.96	0.48
1:A:107:ILE:CD1	1:A:219:LYS:HG3	2.44	0.47
1:A:67:PRO:HD3	1:A:225:ILE:CD1	2.43	0.47
1:A:81:ILE:HG12	1:A:129:LEU:HD23	1.96	0.47
1:A:256:LEU:HD21	1:A:260:LYS:HE3	1.96	0.47
1:A:396:GLY:HA3	1:A:588:HIS:CD2	2.49	0.47
1:A:298:ILE:O	1:A:298:ILE:HG13	2.14	0.47
1:B:212:GLU:O	1:B:216:VAL:HG23	2.14	0.47
1:A:323:GLN:O	1:A:325:ASP:N	2.47	0.47
1:B:722:GLY:HA3	1:B:730:ARG:NH1	2.30	0.47
1:B:721:GLU:OE2	1:B:759:ALA:HA	2.13	0.47
1:B:640:ALA:HA	1:B:643:TYR:CE1	2.49	0.47
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.50	0.47
1:A:387:ASP:CG	1:A:390:GLN:HB2	2.35	0.47
1:B:748:ASP:OD2	1:B:751:GLU:HG2	2.14	0.47
1:B:276:GLN:O	1:B:277:HIS:C	2.51	0.47
1:B:117:HIS:ND1	1:B:118:TYR:N	2.61	0.47
1:A:318:LEU:HG	1:A:372:GLU:OE2	2.14	0.47
1:A:119:VAL:HG12	1:A:120:TYR:N	2.29	0.47
1:A:660:VAL:HG22	2:C:8:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD22	1:A:97:LEU:HD11	1.97	0.47
1:B:381:LEU:HD11	1:B:650:TYR:HA	1.96	0.47
1:B:50:GLY:C	1:B:51:GLU:HG2	2.34	0.47
1:A:264:MET:O	1:A:268:TYR:HD2	1.96	0.47
1:A:92:ILE:H	1:A:92:ILE:CD1	2.14	0.47
1:B:121:ALA:HB1	1:B:154:ILE:CD1	2.42	0.47
1:A:567:ASN:O	1:A:571:ASN:HB2	2.15	0.47
1:A:392:LEU:HD13	1:A:482:ASN:HA	1.96	0.47
1:A:732:ASN:OD1	1:A:734:ALA:N	2.48	0.47
1:A:319:LEU:HD23	1:A:345:ILE:HD12	1.96	0.47
1:A:268:TYR:CB	1:B:125:TYR:CE2	2.83	0.47
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.37	0.47
1:B:370:GLU:OE1	1:B:373:LYS:HD3	2.15	0.46
1:B:550:VAL:HB	1:B:551:PRO:CD	2.46	0.46
1:A:488:ILE:HG13	1:A:517:GLY:O	2.15	0.46
2:D:8:VAL:O	2:D:8:VAL:HG23	2.13	0.46
1:A:373:LYS:HE2	1:A:377:LYS:NZ	2.31	0.46
1:B:723:SER:HB3	1:B:730:ARG:HD3	1.96	0.46
1:A:725:LEU:O	1:A:726:THR:O	2.33	0.46
1:B:420:ASP:OD1	1:B:523:ARG:HD3	2.15	0.46
1:B:608:ASN:N	1:B:608:ASN:ND2	2.63	0.46
1:A:243:TYR:C	1:A:243:TYR:CD1	2.88	0.46
1:B:606:TRP:CZ2	1:B:615:ILE:HG23	2.51	0.46
1:B:47:GLU:OE1	1:B:91:HIS:HE1	1.97	0.46
1:B:658:LEU:HD12	1:B:659:TYR:N	2.30	0.46
1:B:437:LEU:CD2	1:B:488:ILE:HA	2.45	0.46
1:A:610:ILE:CG2	1:A:614:LEU:HD23	2.45	0.46
1:B:678:ARG:HG2	1:B:682:GLU:OE1	2.15	0.46
1:A:125:TYR:O	1:A:126:GLU:HG3	2.16	0.46
1:B:524:ASN:HB3	1:B:552:LYS:CD	2.46	0.46
1:A:634:ILE:HD11	1:A:639:ILE:HD12	1.98	0.46
1:A:683:GLY:O	1:A:687:GLU:HG2	2.16	0.46
1:B:80:LYS:O	1:B:128:VAL:HA	2.16	0.46
1:B:62:LEU:O	1:B:148:TYR:OH	2.29	0.46
1:B:610:ILE:HB	1:B:615:ILE:HD11	1.96	0.46
1:B:505:LEU:HD23	1:B:549:VAL:HG21	1.97	0.46
1:A:294:LYS:HA	1:A:294:LYS:HD3	1.77	0.46
1:A:43:ILE:HG13	1:A:44:VAL:N	2.31	0.46
1:B:114:LEU:HD11	1:B:120:TYR:HB2	1.98	0.46
1:B:449:THR:HA	1:B:673:LYS:HD3	1.97	0.46
1:A:226:GLU:OE1	1:A:229:HIS:ND1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:HE1	1:A:93:SER:HG	1.63	0.45
1:A:324:ILE:C	1:A:326:SER:H	2.19	0.45
1:A:33:GLU:O	1:A:37:LYS:HG3	2.16	0.45
1:B:713:LYS:O	1:B:717:ILE:HG12	2.16	0.45
1:A:402:PRO:HA	1:A:409:ARG:CZ	2.46	0.45
1:B:63:LEU:C	1:B:65:LYS:H	2.20	0.45
1:A:241:PHE:CD1	1:A:241:PHE:C	2.88	0.45
1:B:210:SER:O	1:B:214:GLN:HG3	2.17	0.45
1:A:373:LYS:O	1:A:377:LYS:HG3	2.15	0.45
1:B:748:ASP:OD2	1:B:750:ALA:HB3	2.16	0.45
1:A:477:TYR:H	1:A:593:SER:HB3	1.81	0.45
1:A:123:GLU:HG2	1:A:124:GLY:N	2.27	0.45
1:B:412:TYR:O	1:B:416:ILE:HG12	2.17	0.45
1:B:323:GLN:HE22	1:B:325:ASP:HB2	1.81	0.45
1:A:465:ARG:O	1:A:469:ASN:ND2	2.49	0.45
1:A:107:ILE:HG13	1:A:145:LEU:CD1	2.46	0.45
1:A:674:GLY:HA3	1:A:677:LEU:HD12	1.98	0.45
1:A:65:LYS:HE2	1:A:227:PRO:CG	2.44	0.45
1:A:124:GLY:C	1:A:126:GLU:H	2.19	0.45
1:A:55:LYS:HD3	1:A:133:SER:HB2	1.99	0.45
1:B:636:LEU:HD13	1:B:669:HIS:HB2	1.99	0.45
1:B:237:ALA:N	1:B:238:PRO:HD2	2.32	0.45
1:B:63:LEU:C	1:B:65:LYS:N	2.70	0.45
1:A:252:ILE:HG23	1:A:253:ASN:N	2.32	0.45
1:B:119:VAL:HG21	1:B:147:VAL:HG13	1.99	0.45
1:B:478:SER:HB2	1:B:590:ARG:C	2.38	0.45
1:B:126:GLU:N	1:B:127:PRO:CD	2.79	0.45
1:A:441:MET:HG2	1:A:442:ASN:N	2.32	0.45
1:A:192:ASN:HA	1:A:195:LYS:HB2	1.99	0.45
1:A:749:HIS:CE1	1:A:752:ARG:HH11	2.34	0.45
1:A:567:ASN:ND2	1:A:582:LEU:H	2.14	0.44
1:A:244:MET:CE	1:A:244:MET:HA	2.45	0.44
1:A:346:ARG:NH1	1:A:347:ASP:HB3	2.32	0.44
1:B:48:VAL:CG2	1:B:52:GLU:HG2	2.46	0.44
1:A:84:VAL:HG11	1:A:91:HIS:HD2	1.82	0.44
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.78	0.44
1:A:330:LEU:HD13	1:A:338:LEU:CD1	2.47	0.44
1:B:247:PHE:HA	1:B:251:GLU:HB2	1.99	0.44
1:B:594:ASN:O	1:B:598:SER:HB3	2.17	0.44
1:B:168:GLN:HA	1:B:171:LEU:HD12	1.99	0.44
1:A:479:ILE:HD11	1:A:555:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG2	1:A:64:GLU:O	2.16	0.44
1:B:234:GLN:O	1:B:238:PRO:HG3	2.17	0.44
1:A:656:LYS:HE3	1:A:680:ASP:OD2	2.17	0.44
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.90	0.44
1:A:114:LEU:C	1:A:116:GLU:H	2.21	0.44
1:B:379:LEU:O	1:B:383:ILE:HG23	2.17	0.44
1:A:459:ASP:OD2	1:A:461:THR:HG23	2.18	0.44
1:B:765:PHE:O	1:B:768:ASP:HB2	2.17	0.44
1:B:324:ILE:HD12	1:B:324:ILE:N	2.23	0.44
1:B:401:SER:CB	1:B:638:ASN:ND2	2.79	0.44
1:A:614:LEU:HD22	1:A:770:ILE:HD12	1.98	0.44
1:B:398:LEU:H	1:B:398:LEU:HD22	1.83	0.44
1:A:675:VAL:O	1:A:675:VAL:CG1	2.64	0.44
1:B:51:GLU:HG3	1:B:55:LYS:HE3	2.00	0.44
2:D:13:MET:H	2:D:13:MET:HG3	1.48	0.44
1:A:102:LYS:C	1:A:103:LYS:HD2	2.36	0.44
1:A:46:ILE:O	1:A:47:GLU:HG3	2.17	0.44
1:B:387:ASP:HB3	1:B:390:GLN:HB3	2.00	0.44
1:A:442:ASN:C	1:A:442:ASN:OD1	2.56	0.44
1:A:267:ARG:CZ	1:A:489:ASN:HB3	2.48	0.44
1:A:204:GLU:OE2	1:A:204:GLU:N	2.39	0.44
1:A:202:SER:HB2	1:A:204:GLU:OE2	2.17	0.43
1:B:635:THR:HA	1:B:654:HIS:CE1	2.53	0.43
1:B:325:ASP:OD2	1:B:339:LYS:HD3	2.18	0.43
1:B:178:LYS:HD2	1:B:201:PHE:CZ	2.52	0.43
1:B:149:TYR:CA	1:B:222:ALA:HB2	2.49	0.43
1:A:290:ARG:O	1:A:294:LYS:HB2	2.18	0.43
1:A:173:VAL:HG21	1:A:243:TYR:CD2	2.53	0.43
1:B:603:LEU:O	1:B:606:TRP:HB3	2.19	0.43
1:B:669:HIS:HE1	1:B:671:PRO:HB2	1.84	0.43
1:B:524:ASN:HB3	1:B:552:LYS:HD2	2.00	0.43
1:A:707:LEU:CB	1:A:709:THR:HG22	2.48	0.43
1:B:444:ASN:ND2	1:B:451:GLY:HA3	2.34	0.43
1:B:50:GLY:O	1:B:51:GLU:HG2	2.19	0.43
1:B:35:HIS:NE2	1:B:72:GLU:OE2	2.48	0.43
1:A:159:ILE:N	1:A:159:ILE:HD12	2.32	0.43
1:A:328:ASP:C	1:A:330:LEU:H	2.22	0.43
1:B:443:ILE:CD1	1:B:454:LEU:HD22	2.49	0.43
1:A:91:HIS:CE1	1:A:93:SER:H	2.37	0.43
1:A:749:HIS:CE1	1:A:752:ARG:NH1	2.85	0.43
1:A:499:LEU:HD12	1:A:543:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASN:HD22	1:B:164:ASN:N	2.15	0.43
1:A:330:LEU:HB2	1:A:335:LYS:HE3	1.99	0.43
1:B:223:TYR:O	1:B:230:ARG:HA	2.19	0.43
1:A:443:ILE:HG21	1:A:451:GLY:HA2	2.01	0.43
1:B:268:TYR:O	1:B:272:GLU:HG2	2.19	0.43
1:B:447:THR:HG23	1:B:447:THR:O	2.19	0.43
1:B:88:ILE:HG22	1:B:130:VAL:HG12	2.01	0.43
1:A:621:TYR:HE2	1:A:694:ASP:OD2	2.02	0.43
2:C:13:MET:HG3	2:C:13:MET:H	1.48	0.43
1:A:330:LEU:O	1:A:335:LYS:HE3	2.19	0.43
1:B:89:THR:HG22	1:B:90:LYS:NZ	2.34	0.43
1:B:628:ARG:H	1:B:665:SER:CB	2.24	0.43
1:A:243:TYR:HD1	1:A:244:MET:N	2.17	0.43
1:A:122:LYS:HB3	1:A:128:VAL:HB	2.01	0.43
1:A:237:ALA:N	1:A:238:PRO:HD3	2.33	0.43
1:A:503:ILE:N	1:A:503:ILE:HD13	2.34	0.43
1:A:450:LEU:HB3	1:A:467:ILE:HG23	2.01	0.43
1:B:96:ALA:O	1:B:98:SER:N	2.52	0.43
1:B:311:LEU:HD22	1:B:315:GLU:CB	2.49	0.42
1:A:330:LEU:HD13	1:A:338:LEU:HD12	2.01	0.42
1:A:87:ASP:OD2	1:A:87:ASP:C	2.58	0.42
1:B:406:LEU:O	1:B:410:LYS:HG2	2.19	0.42
1:B:123:GLU:OE1	1:B:157:ARG:HD2	2.19	0.42
1:B:177:ILE:C	1:B:179:ASN:H	2.23	0.42
1:A:305:ASP:O	1:A:309:HIS:HB2	2.19	0.42
1:A:642:GLN:OE1	1:A:653:VAL:HG22	2.19	0.42
1:A:710:ASN:ND2	1:A:710:ASN:O	2.51	0.42
1:A:370:GLU:HA	1:A:373:LYS:CB	2.48	0.42
1:B:65:LYS:HB2	1:B:148:TYR:OH	2.19	0.42
1:B:119:VAL:HA	1:B:130:VAL:O	2.20	0.42
1:B:164:ASN:ND2	1:B:164:ASN:N	2.65	0.42
1:B:236:TYR:C	1:B:238:PRO:HD2	2.39	0.42
1:A:522:GLN:HE21	1:A:522:GLN:HB2	1.60	0.42
1:A:460:ASN:H	1:A:460:ASN:ND2	2.17	0.42
1:B:84:VAL:CG2	1:B:85:ASP:H	2.32	0.42
1:A:574:LEU:HD12	1:A:574:LEU:N	2.34	0.42
1:B:643:TYR:HA	1:B:646:GLN:HG3	2.02	0.42
1:B:707:LEU:HD11	2:D:9:TYR:CZ	2.54	0.42
1:A:636:LEU:HA	1:A:636:LEU:HD12	1.86	0.42
1:A:193:GLN:CA	1:A:193:GLN:HE21	2.32	0.42
1:A:149:TYR:HA	1:A:222:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:O	1:B:145:LEU:HD22	2.19	0.42
1:B:193:GLN:NE2	1:B:212:GLU:HG3	2.35	0.42
1:B:177:ILE:C	1:B:179:ASN:N	2.73	0.42
1:A:29:ASN:O	1:A:32:GLN:HB2	2.20	0.42
1:B:90:LYS:CE	1:B:90:LYS:HA	2.41	0.42
1:B:122:LYS:HE2	1:B:128:VAL:HG22	2.01	0.42
1:A:693:ASP:OD1	1:A:709:THR:CG2	2.68	0.42
1:B:94:LEU:O	1:B:97:LEU:N	2.53	0.42
1:B:401:SER:HB3	1:B:638:ASN:ND2	2.33	0.42
1:A:136:ASP:CG	1:A:139:GLU:H	2.23	0.42
1:A:693:ASP:OD1	1:A:709:THR:HB	2.20	0.42
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.54	0.42
1:B:136:ASP:O	1:B:140:ASN:HB3	2.20	0.42
1:B:303:LYS:O	1:B:307:ILE:HG12	2.19	0.42
1:A:338:LEU:O	1:A:341:LEU:HB2	2.19	0.42
1:A:263:ARG:CB	1:A:263:ARG:HH11	2.27	0.42
1:B:732:ASN:OD1	1:B:734:ALA:HB3	2.20	0.42
1:B:662:GLU:H	1:B:662:GLU:CD	2.23	0.42
1:B:144:ALA:C	1:B:146:ASN:N	2.73	0.42
1:A:38:GLU:O	1:A:41:LYS:HB2	2.19	0.42
1:B:679:ASN:C	1:B:679:ASN:ND2	2.70	0.41
1:A:346:ARG:HD2	1:A:346:ARG:C	2.39	0.41
1:A:500:LYS:HZ2	1:A:500:LYS:HG2	1.72	0.41
1:B:169:LYS:NZ	1:B:251:GLU:OE2	2.53	0.41
1:A:433:ASN:O	1:A:435:ILE:HD11	2.19	0.41
1:B:293:LEU:O	1:B:296:LEU:HB3	2.20	0.41
1:B:366:ASN:CB	1:B:367:PRO:CD	2.91	0.41
1:B:95:GLU:C	1:B:97:LEU:HD23	2.40	0.41
1:B:674:GLY:HA3	1:B:677:LEU:HD12	2.02	0.41
1:A:435:ILE:N	1:A:435:ILE:CD1	2.82	0.41
1:A:264:MET:CE	1:A:265:LEU:HD13	2.51	0.41
1:A:83:ILE:HG22	1:A:83:ILE:O	2.20	0.41
1:B:632:THR:HG21	1:B:639:ILE:HD11	2.02	0.41
1:B:338:LEU:HD22	1:B:379:LEU:HD13	2.02	0.41
1:A:618:VAL:O	1:A:621:TYR:HB3	2.20	0.41
1:A:271:TRP:O	1:A:271:TRP:HD1	2.03	0.41
1:A:311:LEU:HD11	1:A:319:LEU:HD22	2.02	0.41
1:B:675:VAL:CG2	2:D:14:GLU:HG2	2.28	0.41
1:B:693:ASP:CG	1:B:709:THR:HG23	2.40	0.41
1:B:659:TYR:O	1:B:661:PRO:HD3	2.21	0.41
1:A:696:ALA:HB2	1:A:773:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:SER:C	1:B:288:GLU:N	2.73	0.41
1:A:89:THR:HG22	1:A:114:LEU:HD13	2.01	0.41
1:B:436:TYR:CE2	1:B:504:GLN:HB2	2.55	0.41
1:A:156:SER:HB3	1:A:217:PHE:HD2	1.80	0.41
1:B:190:PHE:O	1:B:195:LYS:HE3	2.21	0.41
1:A:725:LEU:O	1:A:726:THR:C	2.59	0.41
1:B:439:GLU:HB2	1:B:486:VAL:HG12	2.01	0.41
1:B:394:ASP:O	1:B:634:ILE:HB	2.21	0.41
1:A:88:ILE:H	1:A:88:ILE:HG12	1.69	0.41
1:A:118:TYR:N	1:A:118:TYR:CD1	2.88	0.41
1:A:226:GLU:HA	1:A:227:PRO:HD2	1.77	0.41
1:A:174:LEU:HD11	1:A:213:VAL:HG13	2.02	0.41
1:B:123:GLU:HG2	1:B:124:GLY:N	2.35	0.41
1:A:165:GLN:HB3	1:A:166:PRO:HA	2.01	0.41
1:A:77:ILE:C	1:B:265:LEU:HD21	2.41	0.41
1:B:772:PHE:O	1:B:776:SER:HB3	2.20	0.41
1:B:353:GLU:HA	1:B:356:LEU:HD12	2.03	0.41
1:A:324:ILE:HG22	1:A:335:LYS:HD3	2.02	0.41
1:B:252:ILE:HG23	1:B:253:ASN:N	2.35	0.41
1:A:322:ILE:HD12	1:A:324:ILE:HD11	2.03	0.41
1:A:263:ARG:HB2	1:A:266:SER:HB2	2.03	0.41
1:A:347:ASP:O	1:A:347:ASP:CG	2.58	0.41
1:B:263:ARG:HB2	1:B:266:SER:HB2	2.02	0.41
1:B:512:GLY:O	1:B:520:ILE:HG22	2.20	0.41
1:A:676:GLU:CG	2:C:14:GLU:OE2	2.66	0.41
1:A:739:GLU:CD	1:A:742:ARG:HH21	2.24	0.41
1:A:440:ASN:ND2	1:A:500:LYS:HZ2	2.19	0.41
1:A:440:ASN:ND2	1:A:500:LYS:NZ	2.68	0.41
1:B:196:GLU:O	1:B:197:HIS:C	2.58	0.41
1:A:718:PHE:O	1:A:722:GLY:HA3	2.21	0.41
1:A:571:ASN:HD22	1:A:571:ASN:HA	1.66	0.41
1:B:498:ARG:NH2	1:B:540:LYS:HE3	2.21	0.41
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.21	0.41
1:A:348:SER:O	1:A:349:LEU:C	2.59	0.41
1:B:477:TYR:CA	1:B:529:ILE:HD13	2.51	0.41
1:A:83:ILE:N	1:A:83:ILE:CD1	2.84	0.41
1:A:264:MET:HE3	1:A:265:LEU:HD13	2.03	0.40
1:A:51:GLU:O	1:A:52:GLU:C	2.59	0.40
1:B:160:LEU:O	1:B:165:GLN:HB2	2.21	0.40
1:B:322:ILE:HD13	1:B:376:LEU:HD21	2.03	0.40
1:B:533:GLN:HE21	1:B:533:GLN:HB2	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:VAL:HG12	1:A:85:ASP:OD1	2.21	0.40
1:A:321:ARG:O	1:A:321:ARG:CG	2.68	0.40
1:B:54:VAL:O	1:B:58:ALA:HB2	2.20	0.40
1:B:436:TYR:HA	1:B:503:ILE:O	2.21	0.40
1:B:118:TYR:CD1	1:B:118:TYR:N	2.89	0.40
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.21	0.40
1:A:285:LEU:CD2	1:A:290:ARG:HD3	2.51	0.40
1:B:698:TYR:CE1	1:B:702:LYS:HG3	2.56	0.40
1:B:297:GLN:NE2	1:B:514:LEU:HD13	2.36	0.40
1:B:39:ILE:CG2	1:B:43:ILE:HD12	2.51	0.40
1:A:223:TYR:CD2	1:A:229:HIS:HB3	2.56	0.40
1:A:433:ASN:O	1:A:435:ILE:CD1	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	729/776 (94%)	634 (87%)	73 (10%)	22 (3%)	5	19
1	B	732/776 (94%)	633 (86%)	83 (11%)	16 (2%)	8	27
2	C	7/20 (35%)	3 (43%)	3 (43%)	1 (14%)	0	0
2	D	7/20 (35%)	2 (29%)	4 (57%)	1 (14%)	0	0
All	All	1475/1592 (93%)	1272 (86%)	163 (11%)	40 (3%)	6	22

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	GLY
1	A	198	PRO
1	A	324	ILE

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Mol	Chain	Res	Type
1	A	327	SER
1	A	700	LEU
1	A	726	THR
1	B	53	ALA
1	B	97	LEU
1	B	326	SER
1	B	758	ASN
1	A	51	GLU
1	A	188	LEU
1	A	209	ASN
1	A	460	ASN
1	A	473	LYS
1	A	641	GLU
1	A	675	VAL
1	B	64	GLU
1	B	251	GLU
1	B	664	ARG
1	B	722	GLY
2	C	12	PRO
2	D	12	PRO
1	A	347	ASP
1	A	702	LYS
1	B	123	GLU
1	A	41	LYS
1	A	125	TYR
1	A	250	GLN
1	A	578	LYS
1	A	592	ALA
1	B	41	LYS
1	B	349	LEU
1	B	609	ASN
1	A	179	ASN
1	B	210	SER
1	B	250	GLN
1	B	616	LYS
1	A	36	LEU
1	B	138	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	672/710 (95%)	619 (92%)	53 (8%)	15	38
1	B	675/710 (95%)	631 (94%)	44 (6%)	21	49
2	C	9/17 (53%)	6 (67%)	3 (33%)	0	0
2	D	9/17 (53%)	7 (78%)	2 (22%)	1	2
All	All	1365/1454 (94%)	1263 (92%)	102 (8%)	17	41

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	46	ILE
1	A	64	GLU
1	A	102	LYS
1	A	103	LYS
1	A	107	ILE
1	A	114	LEU
1	A	140	ASN
1	A	192	ASN
1	A	193	GLN
1	A	207	GLU
1	A	211	ASN
1	A	215	GLU
1	A	233	LEU
1	A	256	LEU
1	A	259	LEU
1	A	263	ARG
1	A	265	LEU
1	A	275	LYS
1	A	294	LYS
1	A	296	LEU
1	A	301	GLU
1	A	304	LYS
1	A	314	GLU
1	A	322	ILE
1	A	329	PHE
1	A	346	ARG
1	A	372	GLU

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Mol	Chain	Res	Type
1	A	435	ILE
1	A	446	LEU
1	A	447	THR
1	A	460	ASN
1	A	462	LYS
1	A	491	ARG
1	A	494	LEU
1	A	505	LEU
1	A	522	GLN
1	A	555	ILE
1	A	564	LEU
1	A	580	THR
1	A	581	LYS
1	A	582	LEU
1	A	619	THR
1	A	635	THR
1	A	636	LEU
1	A	656	LYS
1	A	658	LEU
1	A	679	ASN
1	A	702	LYS
1	A	703	ASN
1	A	706	ASP
1	A	710	ASN
1	A	739	GLU
1	B	66	VAL
1	B	68	SER
1	B	90	LYS
1	B	97	LEU
1	B	99	GLU
1	B	107	ILE
1	B	129	LEU
1	B	146	ASN
1	B	156	SER
1	B	165	GLN
1	B	228	GLN
1	B	233	LEU
1	B	238	PRO
1	B	256	LEU
1	B	292	LEU
1	B	304	LYS
1	B	305	ASP

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Mol	Chain	Res	Type
1	B	314	GLU
1	B	323	GLN
1	B	329	PHE
1	B	350	SER
1	B	355	GLU
1	B	366	ASN
1	B	391	ARG
1	B	430	THR
1	B	446	LEU
1	B	478	SER
1	B	496	ASN
1	B	515	GLU
1	B	516	ASN
1	B	523	ARG
1	B	533	GLN
1	B	538	SER
1	B	557	THR
1	B	598	SER
1	B	611	GLN
1	B	613	ASP
1	B	643	TYR
1	B	679	ASN
1	B	682	GLU
1	B	710	ASN
1	B	758	ASN
1	B	767	ASN
1	B	769	GLN
2	C	11	TYR
2	C	13	MET
2	C	15	PRO
2	D	11	TYR
2	D	13	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	164	ASN
1	A	186	GLN
1	A	193	GLN
1	A	214	GLN
1	A	242	ASN

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Mol	Chain	Res	Type
1	A	253	ASN
1	A	262	GLN
1	A	276	GLN
1	A	277	HIS
1	A	411	GLN
1	A	440	ASN
1	A	460	ASN
1	A	469	ASN
1	A	474	ASN
1	A	522	GLN
1	A	524	ASN
1	A	537	GLN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	589	ASN
1	A	608	ASN
1	A	646	GLN
1	A	652	GLN
1	A	679	ASN
1	A	703	ASN
1	A	710	ASN
1	A	745	HIS
1	A	749	HIS
1	A	767	ASN
1	B	91	HIS
1	B	146	ASN
1	B	164	ASN
1	B	165	GLN
1	B	193	GLN
1	B	197	HIS
1	B	208	GLN
1	B	214	GLN
1	B	228	GLN
1	B	242	ASN
1	B	262	GLN
1	B	276	GLN
1	B	277	HIS
1	B	297	GLN
1	B	323	GLN
1	B	390	GLN
1	B	411	GLN

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Mol	Chain	Res	Type
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	608	ASN
1	B	638	ASN
1	B	646	GLN
1	B	654	HIS
1	B	679	ASN
1	B	710	ASN
1	B	756	GLN
1	B	758	ASN
1	B	767	ASN
1	B	769	GLN
1	B	775	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	733/776 (94%)	0.10	49 (6%)	21	15	13, 43, 108, 126	0
1	B	736/776 (94%)	0.06	48 (6%)	22	16	13, 40, 95, 115	0
2	C	9/20 (45%)	1.46	2 (22%)	1	0	94, 101, 104, 107	0
2	D	9/20 (45%)	1.65	2 (22%)	1	0	93, 101, 104, 107	0
All	All	1487/1592 (93%)	0.10	101 (6%)	20	14	13, 42, 103, 126	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	VAL	5.9
1	B	54	VAL	5.5
1	A	48	VAL	5.3
1	B	356	LEU	5.2
2	D	10	PRO	4.9
1	A	319	LEU	4.9
1	A	311	LEU	4.8
1	A	345	ILE	4.8
1	A	318	LEU	4.7
1	A	322	ILE	4.6
1	A	372	GLU	4.6
1	B	352	GLU	4.3
1	A	348	SER	4.3
1	A	310	SER	4.3
1	A	324	ILE	4.2
1	A	53	ALA	4.2
1	A	314	GLU	4.0
1	B	34	GLU	3.9
1	A	321	ARG	3.9
1	B	353	GLU	3.8
1	A	320	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	341	LEU	3.8
1	B	349	LEU	3.7
1	A	367	PRO	3.6
1	A	327	SER	3.6
1	B	348	SER	3.6
1	A	703	ASN	3.5
1	B	51	GLU	3.5
1	B	35	HIS	3.4
1	A	344	ASP	3.4
1	A	312	SER	3.3
1	A	307	ILE	3.2
1	B	49	LYS	3.2
1	A	313	GLN	3.2
1	A	316	LYS	3.1
1	B	33	GLU	3.0
1	A	52	GLU	3.0
1	A	306	ASP	3.0
1	A	198	PRO	3.0
1	A	368	LEU	3.0
1	A	29	ASN	2.9
1	B	702	LYS	2.9
2	D	9	TYR	2.8
1	B	357	LEU	2.8
1	B	350	SER	2.8
1	B	58	ALA	2.8
1	B	367	PRO	2.8
1	B	703	ASN	2.8
1	B	46	ILE	2.8
1	B	137	TYR	2.7
1	B	366	ASN	2.7
1	B	36	LEU	2.7
1	B	60	GLU	2.7
1	B	88	ILE	2.7
1	B	351	GLU	2.6
1	A	338	LEU	2.6
1	B	705	SER	2.6
1	A	343	ILE	2.6
1	A	30	LYS	2.6
1	B	45	LYS	2.6
1	A	32	GLN	2.6
1	A	330	LEU	2.6
1	A	49	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	44	VAL	2.5
1	B	321	ARG	2.5
1	B	355	GLU	2.5
1	B	56	LYS	2.5
1	B	354	LYS	2.5
1	A	315	GLU	2.5
1	B	93	SER	2.5
1	B	132	GLN	2.5
1	B	52	GLU	2.5
1	A	51	GLU	2.5
1	A	309	HIS	2.5
2	C	8	VAL	2.4
1	A	308	ILE	2.4
1	A	303	LYS	2.4
1	B	83	ILE	2.4
1	A	305	ASP	2.4
1	B	131	ILE	2.3
1	A	54	VAL	2.3
2	C	9	TYR	2.3
1	A	27	GLU	2.3
1	B	324	ILE	2.2
1	B	368	LEU	2.2
1	A	199	THR	2.2
1	B	53	ALA	2.2
1	A	346	ARG	2.2
1	B	329	PHE	2.2
1	A	347	ASP	2.2
1	A	28	ARG	2.2
1	A	33	GLU	2.2
1	B	37	LYS	2.2
1	B	135	GLU	2.2
1	B	326	SER	2.1
1	B	84	VAL	2.1
1	B	97	LEU	2.1
1	B	50	GLY	2.0
1	A	31	THR	2.0
1	A	349	LEU	2.0
1	B	345	ILE	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.