



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:59 PM GMT

PDB ID : 1N0V  
Title : Crystal structure of elongation factor 2  
Authors : Joergensen, R.; Ortiz, P.A.; Carr-Schmid, A.; Nissen, P.; Kinzy, T.G.; Andersen, G.R.  
Deposited on : 2002-10-15  
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

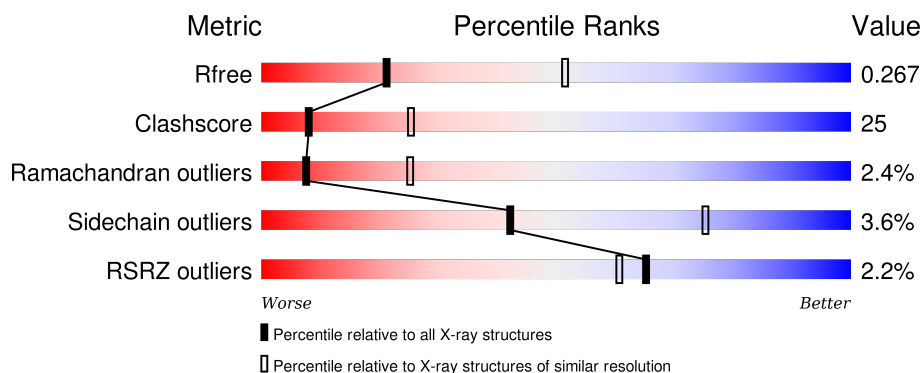
# 1 Overall quality at a glance

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	C	842	<div> <div>2%</div> <div>54%</div> <div>40%</div> <div>• •</div> </div>
1	D	842	<div> <div>2%</div> <div>54%</div> <div>41%</div> <div>• •</div> </div>

## 2 Entry composition

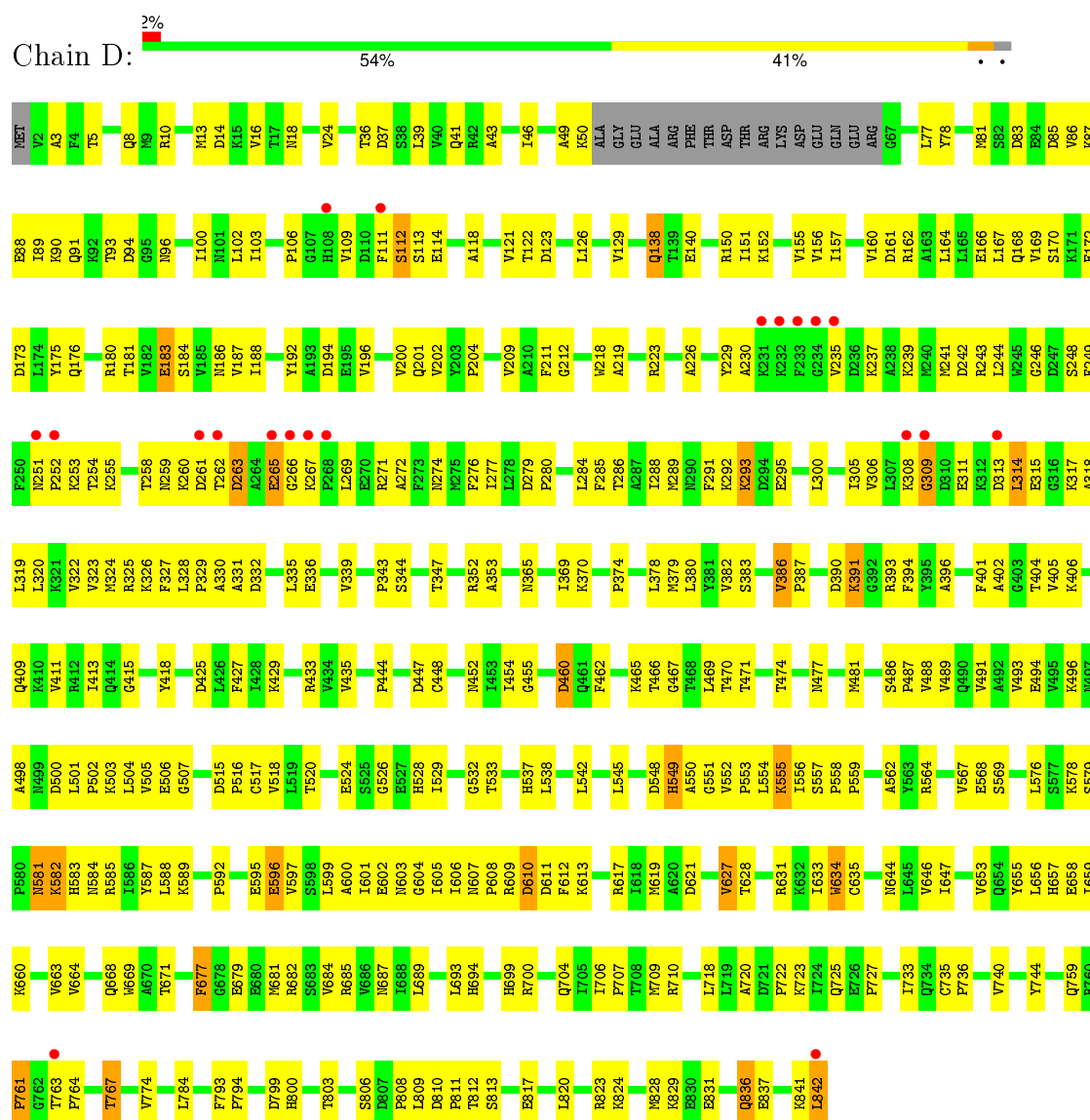
There is only 1 type of molecule in this entry. The entry contains 12838 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	825	Total	C	N	O	S	0	0	0
			6419	4084	1096	1209	30			
1	D	825	Total	C	N	O	S	0	0	0
			6419	4084	1096	1209	30			





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.83Å 114.55Å 177.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 24.94 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.85) 96.4 (24.94-2.85)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.84Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.273 0.228 , 0.267	Depositor DCC
$R_{free}$ test set	1101 reflections (2.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 45917 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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	C	0.40	0/6543	0.65	0/8859
1	D	0.41	0/6543	0.68	2/8859 (0.0%)
All	All	0.41	0/13086	0.67	2/17718 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	ASP	N-CA-C	6.78	129.29	111.00
1	D	266	GLY	N-CA-C	-5.83	98.54	113.10

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	C	6419	0	6492	321	0
1	D	6419	0	6492	317	0
All	All	12838	0	12984	638	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 25.

All (638) 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:D:644:ASN:HD22	1:D:684:VAL:H	1.15	0.95
1:C:418:TYR:HB3	1:C:477:ASN:HD21	1.27	0.95
1:D:391:LYS:HA	1:D:391:LYS:HE2	1.50	0.94
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.33	0.93
1:D:841:LYS:O	1:D:842:LEU:HB3	1.69	0.93
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.50	0.93
1:D:533:THR:H	1:D:537:HIS:HD2	1.03	0.93
1:D:258:THR:HG22	1:D:260:LYS:H	1.34	0.92
1:D:91:GLN:HE22	1:D:344:SER:H	1.07	0.92
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.10	0.92
1:C:258:THR:HG22	1:C:260:LYS:H	1.34	0.92
1:D:685:ARG:HE	1:D:687:ASN:HD21	1.09	0.91
1:C:607:ASN:HD21	1:C:609:ARG:HH21	1.16	0.91
1:D:494:GLU:HB2	1:D:555:LYS:HD3	1.52	0.91
1:C:156:VAL:HG22	1:C:210:ALA:HB3	1.52	0.89
1:D:607:ASN:HD21	1:D:609:ARG:NH2	1.69	0.89
1:D:126:LEU:HD11	1:D:156:VAL:HG23	1.54	0.89
1:D:488:VAL:HG23	1:D:489:VAL:HG23	1.56	0.88
1:D:265:GLU:HG2	1:D:267:LYS:NZ	1.89	0.88
1:D:91:GLN:NE2	1:D:344:SER:H	1.73	0.86
1:D:288:ILE:HG23	1:D:319:LEU:HD23	1.59	0.85
1:C:759:GLN:HB2	1:C:766:PHE:CE1	2.11	0.85
1:D:251:ASN:HB3	1:D:254:THR:OG1	1.77	0.84
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.60	0.84
1:D:694:HIS:O	1:D:700:ARG:HD3	1.79	0.83
1:D:140:GLU:HG3	1:D:188:ILE:HD13	1.62	0.82
1:D:262:THR:HA	1:D:267:LYS:O	1.79	0.82
1:C:391:LYS:HA	1:C:391:LYS:HE2	1.62	0.81
1:D:533:THR:H	1:D:537:HIS:CD2	1.95	0.80
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.18	0.79
1:D:186:ASN:HB3	1:D:201:GLN:HE21	1.48	0.78
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.47	0.78
1:D:784:LEU:HD23	1:D:794:PRO:HG3	1.64	0.78
1:C:607:ASN:HD21	1:C:609:ARG:NH2	1.81	0.77
1:D:3:ALA:HA	1:D:46:ILE:O	1.84	0.77
1:C:305:ILE:HG21	1:C:323:VAL:HG13	1.67	0.77
1:D:126:LEU:HD11	1:D:156:VAL:CG2	2.15	0.76
1:C:36:THR:HG22	1:C:102:LEU:HD21	1.65	0.76
1:D:487:PRO:HA	1:D:532:GLY:O	1.86	0.76
1:C:291:PHE:HE1	1:C:315:GLU:HB3	1.52	0.75
1:D:533:THR:N	1:D:537:HIS:HD2	1.83	0.75
1:D:265:GLU:HB3	1:D:267:LYS:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:VAL:HG22	1:C:170:SER:H	1.52	0.74
1:D:150:ARG:NH1	1:D:196:VAL:HG11	2.03	0.74
1:C:91:GLN:HE21	1:C:347:THR:CB	2.01	0.73
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.68	0.72
1:D:106:PRO:HG2	1:D:114:GLU:HG3	1.70	0.72
1:C:809:LEU:O	1:C:811:PRO:HD3	1.90	0.72
1:C:500:ASP:HB3	1:C:552:VAL:HG11	1.71	0.72
1:D:644:ASN:ND2	1:D:684:VAL:H	1.87	0.71
1:D:226:ALA:O	1:D:230:ALA:HB2	1.90	0.71
1:D:491:VAL:HG21	1:D:542:LEU:HD11	1.71	0.71
1:D:569:SER:O	1:D:720:ALA:HB1	1.91	0.71
1:D:91:GLN:HE22	1:D:344:SER:N	1.85	0.71
1:D:94:ASP:C	1:D:94:ASP:OD1	2.28	0.71
1:C:153:PRO:HD2	1:C:200:VAL:HG22	1.73	0.70
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.73	0.70
1:D:155:VAL:HG23	1:D:202:VAL:HG11	1.72	0.70
1:D:152:LYS:HG3	1:D:200:VAL:CG2	2.21	0.70
1:C:533:THR:H	1:C:537:HIS:HD2	1.40	0.70
1:C:49:ALA:O	1:C:50:LYS:CB	2.40	0.69
1:D:808:PRO:HG2	1:D:809:LEU:HD12	1.72	0.69
1:C:49:ALA:O	1:C:50:LYS:HB2	1.92	0.69
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.74	0.69
1:D:784:LEU:CD2	1:D:794:PRO:HG3	2.23	0.69
1:D:260:LYS:HB2	1:D:263:ASP:HB2	1.75	0.68
1:D:693:LEU:HB3	1:D:700:ARG:HD2	1.75	0.68
1:D:162:ARG:O	1:D:166:GLU:HB2	1.93	0.68
1:D:279:ASP:HB3	1:D:280:PRO:HD3	1.74	0.68
1:D:406:LYS:HB3	1:D:447:ASP:HB3	1.75	0.68
1:D:500:ASP:CB	1:D:552:VAL:HG11	2.24	0.68
1:D:305:ILE:HG21	1:D:323:VAL:HG13	1.76	0.68
1:D:265:GLU:HG2	1:D:267:LYS:HZ2	1.58	0.68
1:C:91:GLN:HE22	1:C:343:PRO:HA	1.58	0.68
1:D:669:TRP:HD1	1:D:710:ARG:NH1	1.90	0.68
1:C:581:ASN:ND2	1:C:704:GLN:HG3	2.08	0.68
1:D:507:GLY:HA3	1:D:550:ALA:HB2	1.75	0.67
1:D:186:ASN:HB3	1:D:201:GLN:NE2	2.09	0.67
1:D:284:LEU:HD13	1:D:324:MET:HE1	1.76	0.67
1:D:806:SER:HB2	1:D:813:SER:HB2	1.76	0.67
1:C:94:ASP:OD1	1:C:94:ASP:C	2.31	0.67
1:D:172:GLU:HA	1:D:274:ASN:HD21	1.60	0.66
1:D:324:MET:HE2	1:D:324:MET:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:ASP:OD2	1:C:628:THR:HB	1.96	0.66
1:D:260:LYS:HD2	1:D:263:ASP:OD1	1.96	0.66
1:D:433:ARG:HE	1:D:444:PRO:HB3	1.59	0.66
1:D:659:ILE:HD13	1:D:693:LEU:HD21	1.78	0.65
1:C:68:ILE:HD13	1:C:390:ASP:HB2	1.79	0.65
1:D:581:ASN:O	1:D:582:LYS:HB2	1.96	0.65
1:C:644:ASN:ND2	1:C:684:VAL:HB	2.10	0.65
1:C:533:THR:H	1:C:537:HIS:CD2	2.14	0.65
1:C:607:ASN:ND2	1:C:609:ARG:HH21	1.93	0.65
1:C:169:VAL:HG22	1:C:173:ASP:HB2	1.78	0.65
1:C:91:GLN:HE22	1:C:344:SER:H	1.45	0.65
1:D:496:LYS:HD2	1:D:553:PRO:HB3	1.79	0.65
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.79	0.65
1:D:394:PHE:CZ	1:D:516:PRO:HG3	2.32	0.65
1:D:579:SER:HB2	1:D:704:GLN:OE1	1.96	0.65
1:C:454:ILE:HG13	1:C:455:GLY:H	1.62	0.65
1:D:613:LYS:HE3	1:D:631:ARG:HH12	1.63	0.64
1:D:219:ALA:HB3	1:D:330:ALA:HA	1.79	0.64
1:D:235:VAL:HG11	1:D:239:LYS:CG	2.27	0.64
1:C:611:ASP:OD2	1:C:613:LYS:HB2	1.97	0.64
1:C:117:ALA:HB2	1:C:481:MET:CE	2.28	0.64
1:D:91:GLN:HE21	1:D:347:THR:CB	2.10	0.64
1:D:595:GLU:O	1:D:599:LEU:HD22	1.96	0.64
1:D:289:MET:CE	1:D:317:LYS:HG2	2.27	0.64
1:D:374:PRO:O	1:D:404:THR:HG23	1.97	0.64
1:C:153:PRO:HD2	1:C:200:VAL:CG2	2.27	0.64
1:D:600:ALA:HB1	1:D:606:ILE:HG12	1.80	0.64
1:D:647:ILE:HD12	1:D:647:ILE:N	2.13	0.64
1:C:391:LYS:HE2	1:C:391:LYS:CA	2.27	0.63
1:D:435:VAL:HG12	1:D:444:PRO:HA	1.80	0.63
1:D:581:ASN:HD21	1:D:699:HIS:HB3	1.63	0.63
1:C:83:ASP:O	1:C:87:LYS:HG3	1.99	0.63
1:C:91:GLN:NE2	1:C:344:SER:H	1.96	0.63
1:D:265:GLU:HG2	1:D:267:LYS:CD	2.27	0.63
1:C:117:ALA:HB2	1:C:481:MET:HE1	1.81	0.63
1:D:394:PHE:N	1:D:460:ASP:OD2	2.24	0.63
1:C:413:ILE:HD11	1:C:459:ILE:HD12	1.82	0.62
1:C:382:VAL:O	1:C:466:THR:HG22	1.99	0.62
1:D:109:VAL:HG21	1:D:138:GLN:HG3	1.82	0.62
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.30	0.62
1:C:500:ASP:CB	1:C:552:VAL:HG11	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:PHE:O	1:D:113:SER:N	2.33	0.62
1:C:488:VAL:HG23	1:C:489:VAL:HG23	1.82	0.62
1:C:86:VAL:HG21	1:C:96:ASN:OD1	2.00	0.62
1:D:235:VAL:HG11	1:D:239:LYS:HG2	1.82	0.61
1:C:630:ALA:O	1:C:633:ILE:HG13	1.98	0.61
1:D:194:ASP:HB3	1:D:196:VAL:HG23	1.82	0.61
1:C:578:LYS:HB3	1:C:585:ARG:HG2	1.82	0.61
1:C:600:ALA:HB1	1:C:606:ILE:HG12	1.82	0.61
1:D:194:ASP:C	1:D:196:VAL:H	2.04	0.61
1:C:823:ARG:HH11	1:C:823:ARG:HB3	1.63	0.61
1:C:581:ASN:HB3	1:C:583:HIS:H	1.64	0.61
1:C:435:VAL:HG12	1:C:444:PRO:HA	1.83	0.61
1:C:578:LYS:HA	1:C:584:ASN:O	2.01	0.61
1:D:379:MET:HB2	1:D:402:ALA:HB3	1.81	0.61
1:D:258:THR:HG22	1:D:259:ASN:N	2.15	0.60
1:C:580:PRO:HD2	1:C:704:GLN:OE1	2.00	0.60
1:D:454:ILE:HG13	1:D:455:GLY:H	1.66	0.60
1:D:588:LEU:HD12	1:D:588:LEU:C	2.21	0.60
1:D:653:VAL:HG11	1:D:656:LEU:HD13	1.83	0.60
1:D:251:ASN:ND2	1:D:269:LEU:HD21	2.16	0.60
1:D:685:ARG:HE	1:D:687:ASN:ND2	1.92	0.60
1:D:583:HIS:HB3	1:D:694:HIS:HB2	1.84	0.60
1:D:251:ASN:HD22	1:D:269:LEU:HD21	1.64	0.60
1:D:129:VAL:HG11	1:D:181:THR:HG21	1.84	0.60
1:C:569:SER:O	1:C:720:ALA:HB1	2.02	0.60
1:D:258:THR:HG22	1:D:260:LYS:N	2.12	0.60
1:C:496:LYS:HD2	1:C:553:PRO:HB3	1.82	0.60
1:C:497:ASN:HB2	1:C:500:ASP:OD2	2.00	0.60
1:C:429:LYS:HE2	1:C:462:PHE:CZ	2.36	0.60
1:D:842:LEU:HD23	1:D:842:LEU:OXT	2.00	0.59
1:D:327:PHE:O	1:D:328:LEU:HD23	2.02	0.59
1:D:429:LYS:HE3	1:D:462:PHE:CE1	2.38	0.59
1:D:106:PRO:CG	1:D:114:GLU:HG3	2.31	0.59
1:C:303:LEU:O	1:C:304:GLU:HB2	2.02	0.59
1:C:13:MET:HG2	1:C:452:ASN:ND2	2.18	0.59
1:C:296:ILE:O	1:C:300:LEU:HD13	2.03	0.59
1:C:465:LYS:NZ	1:C:517:CYS:SG	2.71	0.58
1:C:685:ARG:HE	1:C:687:ASN:ND2	1.91	0.58
1:D:391:LYS:CA	1:D:391:LYS:HE2	2.29	0.58
1:C:4:PHE:O	1:C:47:SER:HA	2.03	0.58
1:D:555:LYS:O	1:D:555:LYS:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:VAL:HG11	1:D:469:LEU:HG	1.84	0.58
1:C:717:PHE:HD2	1:C:718:LEU:CD1	2.16	0.58
1:C:155:VAL:HG12	1:C:156:VAL:N	2.19	0.58
1:D:605:ILE:H	1:D:605:ILE:HD12	1.69	0.58
1:D:465:LYS:HE3	1:D:517:CYS:SG	2.43	0.58
1:C:186:ASN:HB3	1:C:201:GLN:NE2	2.19	0.58
1:C:629:ASP:HB3	1:C:647:ILE:HG21	1.84	0.57
1:D:353:ALA:HB3	1:D:370:LYS:HG2	1.86	0.57
1:C:463:LEU:HD22	1:C:466:THR:O	2.04	0.57
1:D:454:ILE:HG13	1:D:455:GLY:N	2.20	0.57
1:C:576:LEU:HD11	1:C:585:ARG:HD3	1.87	0.57
1:D:581:ASN:HB2	1:D:704:GLN:OE1	2.04	0.57
1:C:823:ARG:HE	1:C:832:VAL:HG22	1.69	0.57
1:D:627:VAL:HG13	1:D:628:THR:N	2.20	0.57
1:C:89:ILE:HG22	1:C:91:GLN:HB3	1.87	0.57
1:D:49:ALA:O	1:D:50:LYS:HB2	2.04	0.57
1:C:291:PHE:CE1	1:C:315:GLU:HB3	2.37	0.56
1:D:5:THR:OG1	1:D:8:GLN:HG3	2.05	0.56
1:D:249:PHE:CZ	1:D:261:ASP:HB3	2.40	0.56
1:D:235:VAL:CG1	1:D:239:LYS:HB3	2.35	0.56
1:D:36:THR:HG22	1:D:102:LEU:HD21	1.86	0.56
1:D:155:VAL:HG12	1:D:156:VAL:N	2.20	0.56
1:D:578:LYS:HD3	1:D:585:ARG:NH2	2.20	0.56
1:D:24:VAL:HG23	1:D:102:LEU:HD11	1.87	0.56
1:C:722:PRO:O	1:C:723:LYS:HG3	2.05	0.56
1:C:327:PHE:O	1:C:328:LEU:HD23	2.04	0.56
1:C:232:LYS:O	1:C:232:LYS:HG2	2.05	0.56
1:D:413:ILE:HB	1:D:427:PHE:HB2	1.87	0.56
1:D:318:ALA:O	1:D:322:VAL:HG23	2.05	0.56
1:C:251:ASN:HB3	1:C:254:THR:OG1	2.04	0.56
1:C:71:LYS:HB3	1:C:386:VAL:HG23	1.86	0.56
1:C:336:GLU:HG2	1:C:340:LEU:HD12	1.88	0.56
1:C:150:ARG:NH1	1:C:196:VAL:HG21	2.21	0.56
1:C:4:PHE:HB3	1:C:8:GLN:HB2	1.86	0.56
1:D:89:ILE:HG21	1:D:93:THR:HG21	1.86	0.56
1:C:737:GLU:HB2	1:C:766:PHE:CD2	2.40	0.56
1:D:584:ASN:HD21	1:D:700:ARG:HG2	1.71	0.56
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.88	0.56
1:D:251:ASN:HB3	1:D:254:THR:HG1	1.70	0.56
1:D:300:LEU:HG	1:D:305:ILE:HB	1.87	0.55
1:C:190:SER:HB3	1:C:201:GLN:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:589:LYS:HE2	1:D:689:LEU:HD11	1.88	0.55
1:D:285:PHE:CE1	1:D:320:LEU:HD21	2.41	0.55
1:D:820:LEU:HG	1:D:824:LYS:HE2	1.87	0.55
1:D:103:ILE:HD13	1:D:121:VAL:CG2	2.36	0.55
1:C:235:VAL:HG12	1:C:236:ASP:N	2.21	0.55
1:D:277:ILE:O	1:D:280:PRO:HD2	2.07	0.55
1:D:596:GLU:OE1	1:D:596:GLU:HA	2.07	0.55
1:D:607:ASN:HD21	1:D:609:ARG:CZ	2.19	0.55
1:D:429:LYS:HG3	1:D:462:PHE:CZ	2.42	0.55
1:C:405:VAL:HA	1:C:409:GLN:OE1	2.07	0.55
1:C:485:VAL:O	1:C:485:VAL:HG22	2.06	0.55
1:D:489:VAL:HG12	1:D:538:LEU:HD22	1.88	0.55
1:C:396:ALA:HB3	1:C:456:LEU:HB2	1.88	0.55
1:C:587:TYR:O	1:C:689:LEU:N	2.35	0.55
1:D:603:ASN:O	1:D:605:ILE:HD12	2.07	0.55
1:C:588:LEU:C	1:C:588:LEU:HD12	2.27	0.55
1:D:383:SER:HA	1:D:481:MET:HE1	1.89	0.55
1:C:552:VAL:HG13	1:C:553:PRO:HD2	1.89	0.55
1:D:289:MET:HE3	1:D:317:LYS:HG2	1.89	0.55
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.71	0.55
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.90	0.54
1:C:27:HIS:CE1	1:C:29:ASP:HB2	2.42	0.54
1:D:664:VAL:O	1:D:668:GLN:HG2	2.07	0.54
1:C:366:CYS:O	1:C:370:LYS:HG3	2.08	0.54
1:C:619:MET:O	1:C:625:TRP:HB2	2.08	0.54
1:D:545:LEU:O	1:D:550:ALA:HB3	2.08	0.54
1:C:374:PRO:O	1:C:404:THR:HG23	2.08	0.54
1:D:13:MET:HB3	1:D:452:ASN:ND2	2.23	0.54
1:C:585:ARG:HG3	1:C:585:ARG:HH11	1.72	0.54
1:C:806:SER:HB3	1:C:813:SER:HB2	1.90	0.54
1:C:152:LYS:HG3	1:C:200:VAL:CG2	2.38	0.53
1:D:466:THR:CG2	1:D:481:MET:HE2	2.38	0.53
1:D:86:VAL:HG21	1:D:96:ASN:OD1	2.08	0.53
1:D:192:TYR:HA	1:D:763:THR:HG22	1.88	0.53
1:D:474:THR:O	1:D:474:THR:HG22	2.08	0.53
1:C:647:ILE:N	1:C:647:ILE:HD12	2.23	0.53
1:D:260:LYS:O	1:D:263:ASP:HB2	2.09	0.53
1:C:579:SER:OG	1:C:581:ASN:HB2	2.08	0.53
1:D:581:ASN:ND2	1:D:699:HIS:HB3	2.24	0.53
1:D:226:ALA:HB2	1:D:241:MET:HB3	1.89	0.53
1:C:493:VAL:O	1:C:528:HIS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:LEU:O	1:C:323:VAL:HG23	2.09	0.53
1:C:150:ARG:HH12	1:C:196:VAL:HG21	1.73	0.53
1:D:515:ASP:HB3	1:D:518:VAL:CG1	2.38	0.53
1:C:162:ARG:HG3	1:C:166:GLU:OE2	2.09	0.53
1:D:265:GLU:HG2	1:D:267:LYS:HZ3	1.70	0.53
1:C:150:ARG:NH1	1:C:196:VAL:HG11	2.24	0.53
1:C:155:VAL:CG1	1:C:156:VAL:N	2.71	0.53
1:C:705:ILE:O	1:C:708:THR:N	2.42	0.53
1:C:89:ILE:HD13	1:C:93:THR:HG21	1.90	0.53
1:C:178:PHE:O	1:C:182:VAL:HG23	2.09	0.53
1:D:634:TRP:O	1:D:635:CYS:HB3	2.09	0.53
1:D:169:VAL:HG22	1:D:170:SER:N	2.23	0.53
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.09	0.52
1:C:597:VAL:O	1:C:601:ILE:HG13	2.09	0.52
1:D:533:THR:HG22	1:D:533:THR:O	2.09	0.52
1:C:501:LEU:HB3	1:C:502:PRO:CD	2.37	0.52
1:C:842:LEU:HD23	1:C:842:LEU:OXT	2.09	0.52
1:C:466:THR:HG21	1:C:481:MET:SD	2.48	0.52
1:C:576:LEU:HD13	1:C:587:TYR:CE1	2.44	0.52
1:D:169:VAL:CG2	1:D:173:ASP:HB2	2.39	0.52
1:D:597:VAL:O	1:D:601:ILE:HG13	2.09	0.52
1:D:515:ASP:HB3	1:D:518:VAL:HG12	1.91	0.52
1:D:501:LEU:HB3	1:D:502:PRO:HD3	1.91	0.52
1:C:295:GLU:C	1:C:297:PRO:HD2	2.30	0.52
1:D:94:ASP:O	1:D:94:ASP:OD1	2.26	0.52
1:C:581:ASN:O	1:C:582:LYS:CB	2.57	0.52
1:D:235:VAL:HG12	1:D:239:LYS:HB3	1.91	0.52
1:C:229:TYR:O	1:C:233:PHE:HB2	2.09	0.52
1:C:378:LEU:H	1:C:471:THR:HB	1.74	0.52
1:C:129:VAL:HG11	1:C:181:THR:CG2	2.40	0.52
1:C:532:GLY:HA3	1:C:538:LEU:HD13	1.92	0.52
1:D:567:VAL:HG23	1:D:592:PRO:HG3	1.90	0.52
1:C:418:TYR:HB3	1:C:477:ASN:ND2	2.11	0.51
1:D:390:ASP:O	1:D:391:LYS:HB2	2.10	0.51
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.90	0.51
1:D:813:SER:O	1:D:817:GLU:HB2	2.10	0.51
1:D:103:ILE:HD13	1:D:121:VAL:HG23	1.91	0.51
1:C:809:LEU:H	1:C:809:LEU:HD12	1.76	0.51
1:D:89:ILE:HG21	1:D:93:THR:CG2	2.41	0.51
1:D:466:THR:HG22	1:D:467:GLY:N	2.25	0.51
1:D:727:PRO:HG2	1:D:774:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:TYR:HB2	1:C:206:ARG:HG2	1.92	0.51
1:D:603:ASN:HB2	1:D:605:ILE:HD13	1.92	0.51
1:C:152:LYS:HG3	1:C:200:VAL:HG23	1.92	0.51
1:D:226:ALA:CB	1:D:241:MET:HB3	2.40	0.51
1:D:595:GLU:O	1:D:599:LEU:CD2	2.58	0.51
1:C:111:PHE:CZ	1:C:540:ILE:HD12	2.45	0.51
1:C:615:ARG:HG2	1:C:619:MET:CE	2.41	0.51
1:D:382:VAL:O	1:D:466:THR:HG23	2.11	0.51
1:D:313:ASP:OD1	1:D:314:LEU:N	2.44	0.51
1:D:313:ASP:O	1:D:315:GLU:HG3	2.11	0.51
1:C:169:VAL:HG22	1:C:173:ASP:CB	2.41	0.51
1:C:212:GLY:HA2	1:C:218:TRP:CZ3	2.46	0.51
1:C:522:MET:HE1	1:C:528:HIS:CE1	2.46	0.51
1:C:124:GLY:HA3	1:C:342:LEU:HD22	1.93	0.51
1:D:466:THR:HG21	1:D:481:MET:HE2	1.92	0.50
1:C:290:ASN:HB3	1:C:292:LYS:HE2	1.93	0.50
1:D:496:LYS:HE3	1:D:554:LEU:O	2.11	0.50
1:D:183:GLU:OE1	1:D:183:GLU:HA	2.11	0.50
1:D:551:GLY:O	1:D:552:VAL:HG23	2.11	0.50
1:C:199:ASP:C	1:C:201:GLN:H	2.15	0.50
1:C:785:ARG:HB2	1:C:790:GLY:HA2	1.93	0.50
1:C:110:ASP:OD1	1:C:781:THR:HG21	2.11	0.50
1:D:229:TYR:CE2	1:D:276:PHE:HB3	2.46	0.50
1:C:841:LYS:O	1:C:842:LEU:HB3	2.11	0.50
1:C:520:THR:HA	1:C:529:ILE:O	2.11	0.50
1:D:37:ASP:O	1:D:41:GLN:HG2	2.11	0.50
1:D:646:VAL:C	1:D:647:ILE:HD12	2.32	0.50
1:D:501:LEU:O	1:D:505:VAL:HG23	2.12	0.50
1:D:162:ARG:HG3	1:D:166:GLU:OE2	2.11	0.49
1:D:43:ALA:HB1	1:D:78:TYR:O	2.11	0.49
1:D:237:LYS:O	1:D:241:MET:HG2	2.12	0.49
1:D:562:ALA:O	1:D:727:PRO:HD3	2.12	0.49
1:C:288:ILE:HA	1:C:296:ILE:HD11	1.95	0.49
1:C:823:ARG:NH1	1:C:829:LYS:O	2.45	0.49
1:C:111:PHE:O	1:C:113:SER:N	2.45	0.49
1:C:225:PHE:CE2	1:C:277:ILE:HG23	2.48	0.49
1:C:46:ILE:O	1:C:47:SER:C	2.50	0.49
1:C:36:THR:O	1:C:40:VAL:HG23	2.12	0.49
1:D:500:ASP:HB3	1:D:552:VAL:HG11	1.93	0.49
1:D:291:PHE:O	1:D:293:LYS:N	2.45	0.49
1:C:138:GLN:HG3	1:C:139:THR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:HB2	1:D:100:ILE:HB	1.94	0.49
1:C:831:GLU:OE1	1:C:831:GLU:N	2.42	0.49
1:D:378:LEU:O	1:D:470:THR:HA	2.12	0.49
1:C:27:HIS:ND1	1:C:29:ASP:HB2	2.26	0.49
1:D:660:LYS:O	1:D:664:VAL:HG23	2.13	0.49
1:C:420:PRO:HG2	1:C:476:HIS:CD2	2.48	0.49
1:C:581:ASN:O	1:C:582:LYS:HB2	2.13	0.49
1:C:615:ARG:HG2	1:C:619:MET:HE1	1.95	0.49
1:C:3:ALA:HA	1:C:46:ILE:O	2.12	0.49
1:C:455:GLY:O	1:C:456:LEU:HD23	2.13	0.49
1:D:600:ALA:CB	1:D:606:ILE:HG12	2.42	0.49
1:C:218:TRP:C	1:C:330:ALA:HB2	2.33	0.49
1:C:504:LEU:HD13	1:C:554:LEU:HD21	1.95	0.49
1:C:390:ASP:O	1:C:391:LYS:HB2	2.12	0.48
1:C:394:PHE:N	1:C:460:ASP:OD2	2.43	0.48
1:D:157:ILE:HD12	1:D:211:PHE:CE1	2.48	0.48
1:C:728:VAL:HB	1:C:800:HIS:CE1	2.48	0.48
1:C:453:ILE:HG22	1:C:453:ILE:O	2.13	0.48
1:C:634:TRP:O	1:C:635:CYS:HB3	2.12	0.48
1:D:289:MET:HE1	1:D:317:LYS:HG2	1.95	0.48
1:D:568:GLU:HB2	1:D:723:LYS:HD3	1.94	0.48
1:C:203:TYR:HB2	1:C:206:ARG:CG	2.44	0.48
1:C:118:ALA:O	1:C:121:VAL:HG22	2.13	0.48
1:D:265:GLU:CB	1:D:267:LYS:HD2	2.42	0.48
1:D:548:ASP:O	1:D:550:ALA:N	2.47	0.48
1:C:717:PHE:HD2	1:C:718:LEU:HD13	1.78	0.48
1:D:733:ILE:O	1:D:767:THR:HA	2.12	0.48
1:D:369:ILE:HD12	1:D:401:PHE:HB3	1.93	0.48
1:C:478:MET:O	1:C:480:VAL:HG13	2.13	0.48
1:C:156:VAL:HG21	1:C:334:LEU:CD2	2.43	0.48
1:C:454:ILE:HG13	1:C:455:GLY:N	2.26	0.48
1:C:613:LYS:HG2	1:C:631:ARG:NH1	2.27	0.48
1:D:619:MET:CE	1:D:633:ILE:HD11	2.44	0.48
1:C:727:PRO:O	1:C:774:VAL:HG23	2.13	0.48
1:C:650:THR:HG22	1:C:690:ASP:HA	1.94	0.48
1:C:315:GLU:O	1:C:318:ALA:HB3	2.14	0.48
1:C:320:LEU:C	1:C:322:VAL:H	2.17	0.48
1:D:448:CYS:SG	1:D:452:ASN:HB2	2.54	0.48
1:D:164:LEU:HD12	1:D:285:PHE:CE1	2.48	0.48
1:C:16:VAL:O	1:C:345:PRO:HD2	2.14	0.47
1:C:318:ALA:O	1:C:322:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:GLY:O	1:C:791:GLN:N	2.47	0.47
1:C:345:PRO:O	1:C:349:GLN:HG3	2.13	0.47
1:D:671:THR:HA	1:D:681:MET:HG3	1.96	0.47
1:C:127:VAL:HG21	1:C:143:LEU:HD13	1.97	0.47
1:D:10:ARG:NH1	1:D:10:ARG:O	2.47	0.47
1:C:126:LEU:HD21	1:C:334:LEU:HD22	1.96	0.47
1:D:308:LYS:O	1:D:309:GLY:C	2.51	0.47
1:D:706:ILE:HB	1:D:707:PRO:HD3	1.96	0.47
1:D:331:ALA:O	1:D:332:ASP:C	2.53	0.47
1:D:607:ASN:ND2	1:D:609:ARG:NH2	2.52	0.47
1:C:515:ASP:OD2	1:C:537:HIS:HE1	1.97	0.47
1:C:619:MET:CE	1:C:633:ILE:HD11	2.45	0.47
1:D:36:THR:HA	1:D:39:LEU:HD12	1.97	0.47
1:D:503:LYS:O	1:D:506:GLU:HB3	2.15	0.47
1:D:194:ASP:C	1:D:196:VAL:N	2.65	0.47
1:C:587:TYR:HD2	1:C:690:ASP:O	1.98	0.47
1:C:71:LYS:HB3	1:C:386:VAL:CG2	2.43	0.47
1:D:253:LYS:O	1:D:255:LYS:HG2	2.15	0.47
1:D:677:PHE:CD2	1:D:677:PHE:N	2.83	0.47
1:D:325:ARG:O	1:D:329:PRO:HG3	2.14	0.47
1:C:129:VAL:HG11	1:C:181:THR:HG21	1.97	0.47
1:C:763:THR:C	1:C:765:LEU:H	2.17	0.47
1:C:174:LEU:HD11	1:C:178:PHE:CZ	2.50	0.47
1:C:694:HIS:O	1:C:700:ARG:HD3	2.15	0.47
1:C:45:ILE:HG22	1:C:46:ILE:N	2.30	0.46
1:D:604:GLY:O	1:D:607:ASN:HB2	2.15	0.46
1:D:491:VAL:HG13	1:D:538:LEU:HD21	1.97	0.46
1:D:112:SER:HA	1:D:793:PHE:CZ	2.51	0.46
1:D:722:PRO:O	1:D:723:LYS:HD2	2.15	0.46
1:C:820:LEU:HG	1:C:824:LYS:HE3	1.98	0.46
1:D:548:ASP:O	1:D:549:HIS:C	2.54	0.46
1:D:172:GLU:HA	1:D:274:ASN:ND2	2.30	0.46
1:C:626:ASP:O	1:C:628:THR:N	2.48	0.46
1:D:647:ILE:N	1:D:647:ILE:CD1	2.77	0.46
1:D:285:PHE:CD1	1:D:320:LEU:HD21	2.50	0.46
1:C:158:ASN:O	1:C:159:LYS:HB2	2.16	0.46
1:D:391:LYS:CE	1:D:391:LYS:HA	2.34	0.46
1:D:169:VAL:HG22	1:D:170:SER:O	2.16	0.46
1:D:155:VAL:CG1	1:D:156:VAL:N	2.79	0.46
1:C:259:ASN:N	1:C:259:ASN:OD1	2.43	0.46
1:C:479:LYS:HZ2	1:C:760:ARG:HH12	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ASP:O	1:D:314:LEU:C	2.54	0.46
1:C:308:LYS:O	1:C:309:GLY:C	2.53	0.46
1:C:740:VAL:HG12	1:C:744:TYR:CE2	2.51	0.46
1:C:194:ASP:C	1:C:196:VAL:H	2.18	0.46
1:C:487:PRO:HA	1:C:532:GLY:O	2.15	0.46
1:C:585:ARG:HG3	1:C:585:ARG:NH1	2.30	0.46
1:C:429:LYS:HG3	1:C:462:PHE:CE2	2.50	0.46
1:D:160:VAL:HG23	1:D:212:GLY:O	2.16	0.46
1:C:565:GLU:OE1	1:C:674:GLY:HA3	2.16	0.46
1:D:609:ARG:O	1:D:610:ASP:O	2.33	0.46
1:D:166:GLU:HB3	1:D:167:LEU:HD12	1.98	0.46
1:C:216:HIS:HA	1:C:321:LYS:HG2	1.97	0.46
1:D:258:THR:HG22	1:D:259:ASN:H	1.79	0.46
1:C:577:SER:O	1:C:585:ARG:HA	2.16	0.46
1:D:103:ILE:HD12	1:D:122:THR:HG22	1.97	0.46
1:C:393:ARG:NH1	1:C:460:ASP:HB2	2.31	0.46
1:D:170:SER:OG	1:D:173:ASP:OD2	2.33	0.46
1:C:400:VAL:HG12	1:C:450:ALA:HA	1.98	0.46
1:C:496:LYS:HD2	1:C:553:PRO:CB	2.45	0.45
1:C:16:VAL:HG12	1:C:16:VAL:O	2.15	0.45
1:C:380:LEU:HD12	1:C:400:VAL:HG22	1.98	0.45
1:C:263:ASP:O	1:C:264:ALA:HB3	2.16	0.45
1:D:828:MET:O	1:D:829:LYS:C	2.53	0.45
1:C:408:GLY:N	1:C:431:ILE:O	2.48	0.45
1:D:644:ASN:HD21	1:D:682:ARG:CA	2.29	0.45
1:C:647:ILE:HD13	1:C:685:ARG:HG3	1.99	0.45
1:D:617:ARG:HG2	1:D:621:ASP:OD2	2.16	0.45
1:C:283:ARG:HH11	1:C:283:ARG:HG2	1.80	0.45
1:C:314:LEU:HD13	1:C:322:VAL:HG21	1.97	0.45
1:C:169:VAL:HG22	1:C:170:SER:N	2.28	0.45
1:C:223:ARG:HG3	1:C:241:MET:HE1	1.99	0.45
1:C:613:LYS:HG2	1:C:631:ARG:HH12	1.82	0.45
1:C:393:ARG:HH11	1:C:460:ASP:HB2	1.82	0.45
1:D:501:LEU:HD23	1:D:501:LEU:C	2.37	0.45
1:C:237:LYS:O	1:C:241:MET:HG2	2.17	0.45
1:C:395:TYR:CE1	1:C:457:VAL:HG13	2.52	0.45
1:D:740:VAL:HG12	1:D:744:TYR:CE2	2.52	0.45
1:D:386:VAL:HA	1:D:387:PRO:HD3	1.82	0.45
1:C:189:VAL:CG1	1:C:200:VAL:HG13	2.47	0.45
1:C:428:ILE:C	1:C:429:LYS:HD2	2.36	0.45
1:C:189:VAL:HG13	1:C:200:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:808:PRO:HG2	1:C:809:LEU:HD12	1.99	0.45
1:D:581:ASN:O	1:D:582:LYS:CB	2.63	0.45
1:C:428:ILE:O	1:C:429:LYS:HD2	2.17	0.45
1:C:109:VAL:HG21	1:C:138:GLN:HB2	1.97	0.45
1:C:138:GLN:CG	1:C:139:THR:N	2.80	0.45
1:C:459:ILE:HG22	1:C:459:ILE:O	2.16	0.45
1:C:404:THR:HG22	1:C:449:PRO:HA	1.98	0.45
1:D:799:ASP:OD1	1:D:800:HIS:HD2	2.00	0.45
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.99	0.45
1:D:605:ILE:N	1:D:605:ILE:HD12	2.30	0.45
1:C:223:ARG:HA	1:C:241:MET:HE1	1.99	0.45
1:C:183:GLU:OE1	1:C:183:GLU:HA	2.17	0.45
1:D:390:ASP:O	1:D:393:ARG:HG2	2.17	0.44
1:C:737:GLU:CD	1:C:766:PHE:HE2	2.20	0.44
1:C:479:LYS:NZ	1:C:760:ARG:NH1	2.65	0.44
1:D:576:LEU:HD13	1:D:587:TYR:CE1	2.53	0.44
1:C:296:ILE:N	1:C:297:PRO:HD2	2.32	0.44
1:D:111:PHE:CD2	1:D:111:PHE:N	2.84	0.44
1:D:49:ALA:O	1:D:50:LYS:CB	2.66	0.44
1:D:291:PHE:CE1	1:D:315:GLU:HB3	2.52	0.44
1:C:324:MET:HA	1:C:324:MET:CE	2.47	0.44
1:D:200:VAL:HG13	1:D:200:VAL:O	2.17	0.44
1:C:45:ILE:C	1:C:46:ILE:HG13	2.38	0.44
1:C:36:THR:CG2	1:C:102:LEU:HD21	2.42	0.44
1:D:578:LYS:HE3	1:D:582:LYS:HZ3	1.83	0.44
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.99	0.44
1:D:520:THR:HA	1:D:529:ILE:O	2.18	0.44
1:D:613:LYS:HE3	1:D:631:ARG:HH22	1.82	0.44
1:C:111:PHE:HE1	1:C:540:ILE:HG13	1.83	0.44
1:D:493:VAL:O	1:D:528:HIS:HB2	2.18	0.44
1:D:249:PHE:N	1:D:249:PHE:CD2	2.86	0.44
1:D:112:SER:CB	1:D:794:PRO:O	2.65	0.44
1:C:501:LEU:HD23	1:C:501:LEU:C	2.38	0.44
1:C:819:VAL:O	1:C:823:ARG:HG3	2.18	0.44
1:C:3:ALA:HB1	1:C:48:ALA:HB2	2.00	0.44
1:D:823:ARG:NH1	1:D:829:LYS:O	2.51	0.44
1:D:123:ASP:O	1:D:151:ILE:HG23	2.18	0.44
1:C:389:SER:O	1:C:391:LYS:N	2.48	0.43
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.83	0.43
1:D:235:VAL:HG21	1:D:243:ARG:NH1	2.33	0.43
1:C:111:PHE:CE1	1:C:540:ILE:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:GLU:O	1:D:187:VAL:HG23	2.18	0.43
1:D:204:PRO:HA	1:D:209:VAL:HB	1.98	0.43
1:D:81:MET:HB3	1:D:85:ASP:HB2	1.99	0.43
1:D:265:GLU:HB3	1:D:267:LYS:CD	2.45	0.43
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.78	0.43
1:D:324:MET:CE	1:D:324:MET:HA	2.46	0.43
1:C:8:GLN:O	1:C:11:SER:HB3	2.18	0.43
1:D:607:ASN:HA	1:D:608:PRO:HD3	1.77	0.43
1:C:193:ALA:O	1:C:194:ASP:C	2.56	0.43
1:C:132:ILE:HD12	1:C:162:ARG:CD	2.49	0.43
1:D:677:PHE:HD2	1:D:677:PHE:N	2.15	0.43
1:D:85:ASP:OD1	1:D:223:ARG:NH2	2.45	0.43
1:D:405:VAL:HA	1:D:409:GLN:OE1	2.19	0.43
1:D:311:GLU:OE1	1:D:326:LYS:HE3	2.19	0.43
1:D:91:GLN:HE22	1:D:343:PRO:HA	1.82	0.43
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.53	0.43
1:D:223:ARG:HH11	1:D:223:ARG:HG2	1.84	0.43
1:C:103:ILE:HD13	1:C:121:VAL:HG23	2.01	0.43
1:C:605:ILE:HD12	1:C:605:ILE:N	2.34	0.43
1:D:261:ASP:C	1:D:262:THR:HG23	2.39	0.43
1:D:658:GLU:OE1	1:D:700:ARG:NH2	2.50	0.43
1:C:186:ASN:OD1	1:C:201:GLN:HB3	2.18	0.43
1:D:382:VAL:HG13	1:D:396:ALA:HB1	2.00	0.43
1:D:415:GLY:HA3	1:D:425:ASP:OD1	2.19	0.43
1:C:261:ASP:OD1	1:C:262:THR:N	2.52	0.43
1:C:546:GLU:HB2	1:C:554:LEU:HD12	2.00	0.43
1:D:365:ASN:O	1:D:369:ILE:HG12	2.18	0.43
1:D:619:MET:HE3	1:D:633:ILE:HD11	2.00	0.43
1:C:223:ARG:HG3	1:C:241:MET:CE	2.49	0.43
1:D:558:PRO:HA	1:D:559:PRO:HD3	1.91	0.43
1:C:130:ASP:OD1	1:C:159:LYS:HD3	2.19	0.43
1:C:614:ALA:O	1:C:618:ILE:HG13	2.19	0.43
1:D:306:VAL:O	1:D:306:VAL:HG23	2.18	0.43
1:C:298:VAL:O	1:C:301:GLU:HB3	2.19	0.43
1:D:262:THR:O	1:D:262:THR:OG1	2.36	0.42
1:D:235:VAL:CG1	1:D:239:LYS:HG2	2.49	0.42
1:C:616:ALA:HA	1:C:630:ALA:HB1	2.00	0.42
1:C:243:ARG:O	1:C:272:ALA:HB3	2.19	0.42
1:C:81:MET:O	1:C:96:ASN:HB3	2.18	0.42
1:D:176:GLN:HB3	1:D:180:ARG:HH12	1.84	0.42
1:C:122:THR:O	1:C:352:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASP:N	1:C:161:ASP:OD2	2.51	0.42
1:C:168:GLN:O	1:C:168:GLN:HG3	2.18	0.42
1:D:584:ASN:HD22	1:D:693:LEU:HA	1.84	0.42
1:C:150:ARG:HH12	1:C:196:VAL:HG11	1.84	0.42
1:D:552:VAL:HG13	1:D:553:PRO:HD2	2.00	0.42
1:C:267:LYS:HA	1:C:268:PRO:HD3	1.89	0.42
1:D:292:LYS:HD3	1:D:295:GLU:OE2	2.19	0.42
1:D:611:ASP:OD2	1:D:613:LYS:HB2	2.19	0.42
1:C:103:ILE:HD12	1:C:122:THR:HG22	2.02	0.42
1:C:763:THR:HA	1:C:764:PRO:HD3	1.75	0.42
1:C:314:LEU:O	1:C:315:GLU:HG3	2.20	0.42
1:C:489:VAL:HG12	1:C:538:LEU:HD22	2.01	0.42
1:C:371:ASN:O	1:C:372:CYS:C	2.58	0.42
1:D:810:ASP:O	1:D:812:THR:N	2.52	0.42
1:C:545:LEU:HA	1:C:549:HIS:HB2	1.99	0.42
1:D:258:THR:CG2	1:D:259:ASN:N	2.82	0.42
1:D:829:LYS:HE2	1:D:831:GLU:OE1	2.19	0.42
1:D:411:VAL:CG1	1:D:469:LEU:HG	2.48	0.42
1:D:265:GLU:HG2	1:D:267:LYS:CE	2.49	0.42
1:C:4:PHE:CD1	1:C:8:GLN:NE2	2.87	0.42
1:C:176:GLN:O	1:C:180:ARG:HG3	2.20	0.42
1:D:556:ILE:HG22	1:D:557:SER:N	2.35	0.42
1:D:305:ILE:HD11	1:D:327:PHE:CD1	2.55	0.42
1:D:129:VAL:HG11	1:D:181:THR:CG2	2.48	0.42
1:C:328:LEU:O	1:C:330:ALA:N	2.53	0.42
1:D:103:ILE:HD13	1:D:121:VAL:HG21	2.02	0.42
1:D:169:VAL:CG2	1:D:170:SER:N	2.83	0.42
1:C:194:ASP:C	1:C:196:VAL:N	2.73	0.41
1:C:533:THR:HG22	1:C:533:THR:O	2.20	0.41
1:C:581:ASN:O	1:C:582:LYS:CG	2.68	0.41
1:D:504:LEU:O	1:D:507:GLY:N	2.53	0.41
1:D:118:ALA:O	1:D:122:THR:HG23	2.20	0.41
1:C:414:GLN:HB2	1:C:477:ASN:OD1	2.20	0.41
1:C:91:GLN:HE22	1:C:344:SER:N	2.13	0.41
1:D:167:LEU:O	1:D:168:GLN:C	2.57	0.41
1:C:237:LYS:O	1:C:238:ALA:C	2.59	0.41
1:D:83:ASP:O	1:D:87:LYS:HG3	2.20	0.41
1:C:149:GLU:O	1:C:150:ARG:HB2	2.20	0.41
1:D:152:LYS:HG3	1:D:200:VAL:HG21	1.99	0.41
1:C:579:SER:HB2	1:C:704:GLN:OE1	2.20	0.41
1:D:379:MET:SD	1:D:470:THR:HG22	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:VAL:HG12	1:C:236:ASP:H	1.84	0.41
1:C:479:LYS:NZ	1:C:760:ARG:HH12	2.18	0.41
1:C:561:VAL:O	1:C:563:TYR:CD2	2.73	0.41
1:C:737:GLU:OE2	1:C:766:PHE:HE2	2.03	0.41
1:D:112:SER:HB2	1:D:794:PRO:O	2.21	0.41
1:D:599:LEU:O	1:D:602:GLU:N	2.53	0.41
1:C:231:LYS:C	1:C:233:PHE:H	2.24	0.41
1:C:16:VAL:O	1:C:16:VAL:CG1	2.68	0.41
1:C:595:GLU:O	1:C:599:LEU:HD22	2.20	0.41
1:D:612:PHE:CE1	1:D:613:LYS:HG2	2.55	0.41
1:D:192:TYR:CE1	1:D:764:PRO:HD2	2.55	0.41
1:C:695:ALA:O	1:C:700:ARG:NH1	2.53	0.41
1:C:533:THR:N	1:C:537:HIS:HD2	2.14	0.41
1:D:725:GLN:HE21	1:D:803:THR:HG1	1.62	0.41
1:D:655:TYR:O	1:D:658:GLU:HB2	2.21	0.41
1:D:474:THR:CG2	1:D:474:THR:O	2.69	0.41
1:C:419:VAL:HG12	1:C:421:GLY:H	1.85	0.41
1:D:16:VAL:C	1:D:18:ASN:N	2.74	0.41
1:C:735:CYS:SG	1:C:736:PRO:HD2	2.60	0.41
1:D:655:TYR:O	1:D:656:LEU:C	2.58	0.41
1:D:486:SER:HA	1:D:487:PRO:HD3	1.87	0.41
1:C:718:LEU:N	1:C:718:LEU:HD13	2.36	0.41
1:C:300:LEU:HG	1:C:305:ILE:HB	2.02	0.41
1:C:189:VAL:O	1:C:193:ALA:HB2	2.20	0.41
1:D:218:TRP:HB3	1:D:324:MET:HB3	2.02	0.41
1:C:94:ASP:OD1	1:C:94:ASP:O	2.38	0.41
1:D:515:ASP:HA	1:D:516:PRO:HD3	1.93	0.41
1:D:613:LYS:CE	1:D:631:ARG:HH22	2.33	0.41
1:D:181:THR:O	1:D:184:SER:N	2.54	0.41
1:C:271:ARG:HG3	1:C:271:ARG:HH11	1.86	0.41
1:D:271:ARG:O	1:D:272:ALA:C	2.58	0.41
1:D:524:GLU:C	1:D:526:GLY:H	2.22	0.41
1:C:685:ARG:NE	1:C:687:ASN:HD21	1.94	0.41
1:C:314:LEU:HD22	1:C:318:ALA:HB1	2.03	0.41
1:D:88:GLU:O	1:D:90:LYS:HD2	2.21	0.41
1:D:335:LEU:O	1:D:336:GLU:C	2.58	0.41
1:D:111:PHE:HB3	1:D:114:GLU:HG2	2.03	0.40
1:C:551:GLY:O	1:C:552:VAL:HG23	2.22	0.40
1:C:491:VAL:HG12	1:C:559:PRO:HA	2.02	0.40
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.86	0.40
1:C:730:LEU:HD12	1:C:730:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:GLN:HB2	1:D:836:GLN:HE21	1.62	0.40
1:D:493:VAL:HG12	1:D:494:GLU:N	2.37	0.40
1:C:188:ILE:O	1:C:189:VAL:C	2.59	0.40
1:C:497:ASN:O	1:C:498:ALA:C	2.59	0.40
1:D:465:LYS:CE	1:D:517:CYS:SG	3.09	0.40
1:C:109:VAL:O	1:C:109:VAL:HG12	2.21	0.40
1:C:309:GLY:O	1:C:310:ASP:C	2.60	0.40
1:C:284:LEU:CD1	1:C:324:MET:HE3	2.51	0.40
1:C:836:GLN:HB2	1:C:836:GLN:HE21	1.69	0.40
1:D:418:TYR:HB3	1:D:477:ASN:HD21	1.87	0.40
1:C:571:SER:HB2	1:C:589:LYS:HG2	2.02	0.40
1:D:161:ASP:CG	1:D:162:ARG:N	2.74	0.40
1:C:436:LEU:O	1:C:442:VAL:HA	2.21	0.40
1:C:785:ARG:O	1:C:789:GLY:N	2.54	0.40
1:D:252:PRO:O	1:D:255:LYS:HG2	2.21	0.40
1:D:735:CYS:HA	1:D:736:PRO:HD3	1.97	0.40
1:D:175:TYR:OH	1:D:246:GLY:HA2	2.21	0.40
1:C:91:GLN:NE2	1:C:347:THR:CB	2.78	0.40
1:C:806:SER:HB2	1:C:815:ALA:CB	2.52	0.40
1:C:760:ARG:HA	1:C:761:PRO:HD3	1.78	0.40
1:D:380:LEU:HD23	1:D:380:LEU:C	2.42	0.40
1:D:663:VAL:HG13	1:D:709:MET:HG2	2.03	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	C	821/842 (98%)	713 (87%)	85 (10%)	23 (3%)	6	21
1	D	821/842 (98%)	735 (90%)	70 (8%)	16 (2%)	10	32
All	All	1642/1684 (98%)	1448 (88%)	155 (9%)	39 (2%)	7	25

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	112	SER
1	D	112	SER
1	D	309	GLY
1	D	549	HIS
1	D	610	ASP
1	C	309	GLY
1	C	610	ASP
1	C	627	VAL
1	C	790	GLY
1	C	795	GLN
1	D	293	LYS
1	D	314	LEU
1	D	582	LYS
1	C	329	PRO
1	C	498	ALA
1	C	582	LYS
1	D	286	THR
1	D	391	LYS
1	D	498	ALA
1	D	657	HIS
1	C	232	LYS
1	C	293	LYS
1	C	330	ALA
1	C	536	LEU
1	D	811	PRO
1	C	166	GLU
1	C	200	VAL
1	C	321	LYS
1	C	761	PRO
1	C	188	ILE
1	C	189	VAL
1	C	252	PRO
1	C	390	ASP
1	C	391	LYS
1	D	244	LEU
1	D	627	VAL
1	D	761	PRO
1	C	169	VAL
1	D	339	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	C	701/715 (98%)	674 (96%)	27 (4%)	39	73
1	D	701/715 (98%)	677 (97%)	24 (3%)	44	77
All	All	1402/1430 (98%)	1351 (96%)	51 (4%)	42	75

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	36	THR
1	C	81	MET
1	C	138	GLN
1	C	154	VAL
1	C	183	GLU
1	C	194	ASP
1	C	236	ASP
1	C	259	ASN
1	C	262	THR
1	C	313	ASP
1	C	352	ARG
1	C	411	VAL
1	C	466	THR
1	C	481	MET
1	C	564	ARG
1	C	596	GLU
1	C	599	LEU
1	C	718	LEU
1	C	730	LEU
1	C	735	CYS
1	C	761	PRO
1	C	767	THR
1	C	785	ARG
1	C	806	SER
1	C	823	ARG
1	C	836	GLN
1	C	842	LEU

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Mol	Chain	Res	Type
1	D	14	ASP
1	D	138	GLN
1	D	183	GLU
1	D	242	ASP
1	D	248	SER
1	D	265	GLU
1	D	352	ARG
1	D	386	VAL
1	D	460	ASP
1	D	471	THR
1	D	555	LYS
1	D	564	ARG
1	D	581	ASN
1	D	596	GLU
1	D	634	TRP
1	D	677	PHE
1	D	679	GLU
1	D	718	LEU
1	D	759	GLN
1	D	761	PRO
1	D	767	THR
1	D	836	GLN
1	D	837	GLU
1	D	842	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	91	GLN
1	C	101	ASN
1	C	138	GLN
1	C	201	GLN
1	C	365	ASN
1	C	414	GLN
1	C	452	ASN
1	C	537	HIS
1	C	581	ASN
1	C	644	ASN
1	C	687	ASN
1	C	748	ASN
1	C	753	GLN
1	C	759	GLN

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Mol	Chain	Res	Type
1	C	800	HIS
1	C	836	GLN
1	D	30	HIS
1	D	91	GLN
1	D	101	ASN
1	D	138	GLN
1	D	176	GLN
1	D	201	GLN
1	D	274	ASN
1	D	365	ASN
1	D	371	ASN
1	D	452	ASN
1	D	537	HIS
1	D	581	ASN
1	D	584	ASN
1	D	644	ASN
1	D	687	ASN
1	D	753	GLN
1	D	800	HIS
1	D	836	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	C	825/842 (97%)	0.02	16 (1%) 70 66	32, 55, 95, 123	0
1	D	825/842 (97%)	-0.05	20 (2%) 62 57	29, 51, 99, 127	0
All	All	1650/1684 (97%)	-0.01	36 (2%) 65 61	29, 54, 97, 127	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	762	GLY	6.1
1	D	268	PRO	5.1
1	D	266	GLY	4.0
1	D	234	GLY	3.9
1	C	764	PRO	3.9
1	D	262	THR	3.7
1	D	267	LYS	3.7
1	C	842	LEU	3.4
1	D	111	PHE	3.3
1	C	48	ALA	2.9
1	D	235	VAL	2.8
1	D	232	LYS	2.7
1	D	842	LEU	2.7
1	C	168	GLN	2.7
1	C	50	LYS	2.6
1	C	548	ASP	2.6
1	D	313	ASP	2.6
1	C	265	GLU	2.6
1	D	265	GLU	2.5
1	D	108	HIS	2.5
1	C	29	ASP	2.5
1	C	108	HIS	2.5
1	D	261	ASP	2.4
1	D	309	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	231	LYS	2.4
1	D	763	THR	2.3
1	D	308	LYS	2.3
1	C	28	VAL	2.3
1	C	391	LYS	2.2
1	D	233	PHE	2.1
1	C	210	ALA	2.1
1	C	481	MET	2.1
1	C	313	ASP	2.1
1	D	251	ASN	2.0
1	D	252	PRO	2.0
1	C	234	GLY	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 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.