



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:31 PM GMT

PDB ID : 4FB8  
Title : Crystal Structure of apo Acyl-CoA Carboxylase  
Authors : Reddy, M.C.M.; Bruning, J.B.; Sherekar, M.; Valluru, S.; Ehrenfeld, H.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2012-05-22  
Resolution : 3.00 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

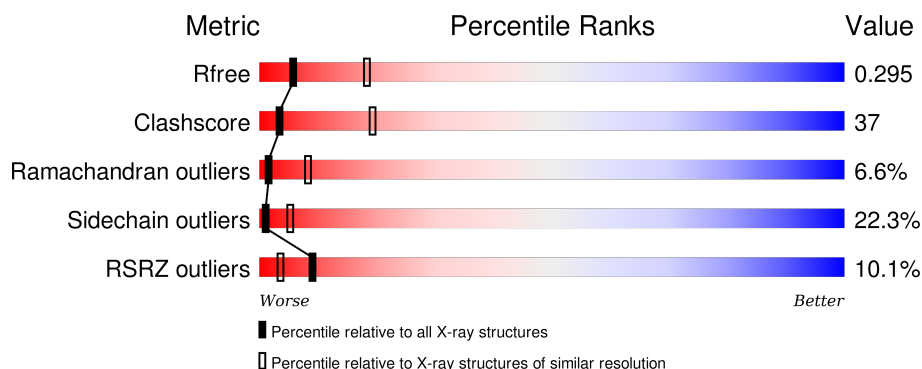
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	473	
1	B	473	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6220 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 Probable propionyl-CoA carboxylase beta chain 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3135	1959	577	585	14			
1	B	427	Total	C	N	O	S	0	0	0
			3080	1933	561	572	14			

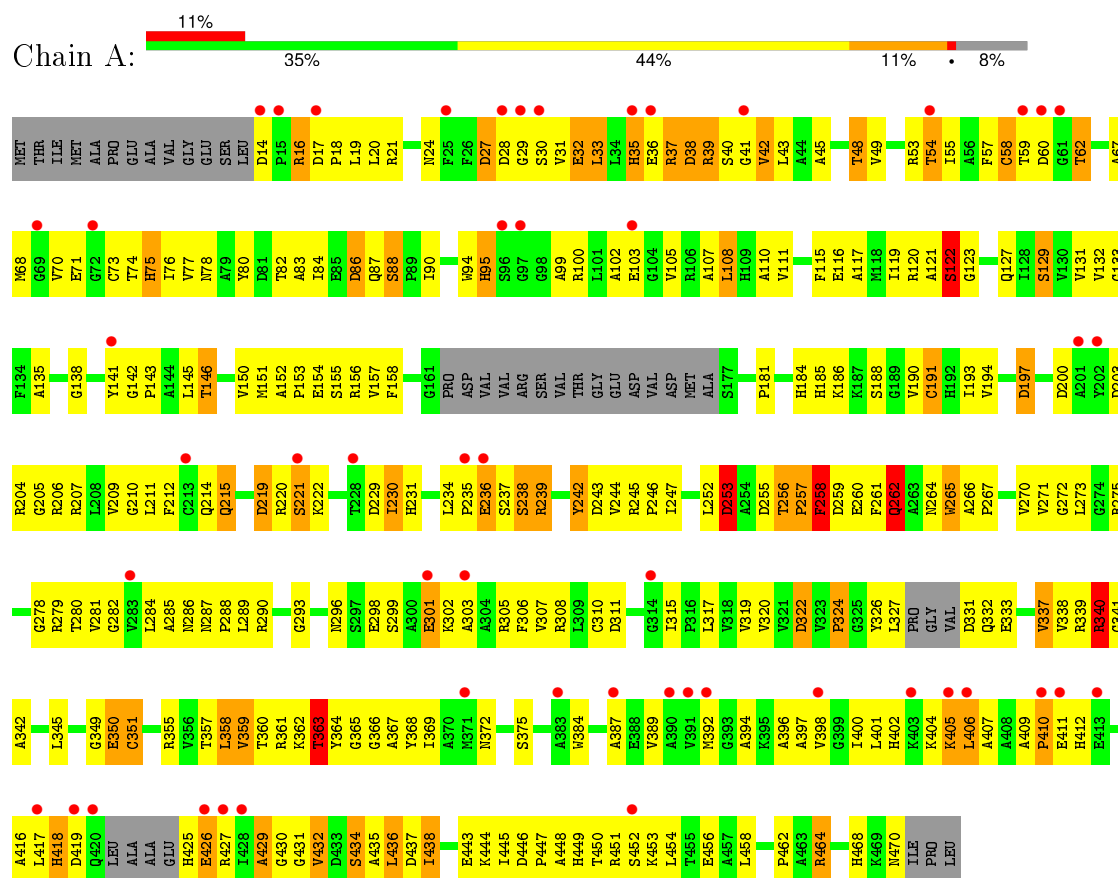
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	3	Total	O	0	0
			3	3		

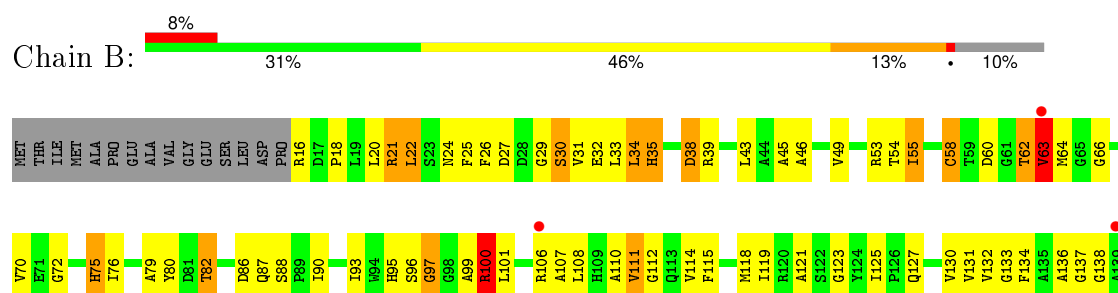
### 3 Residue-property plots

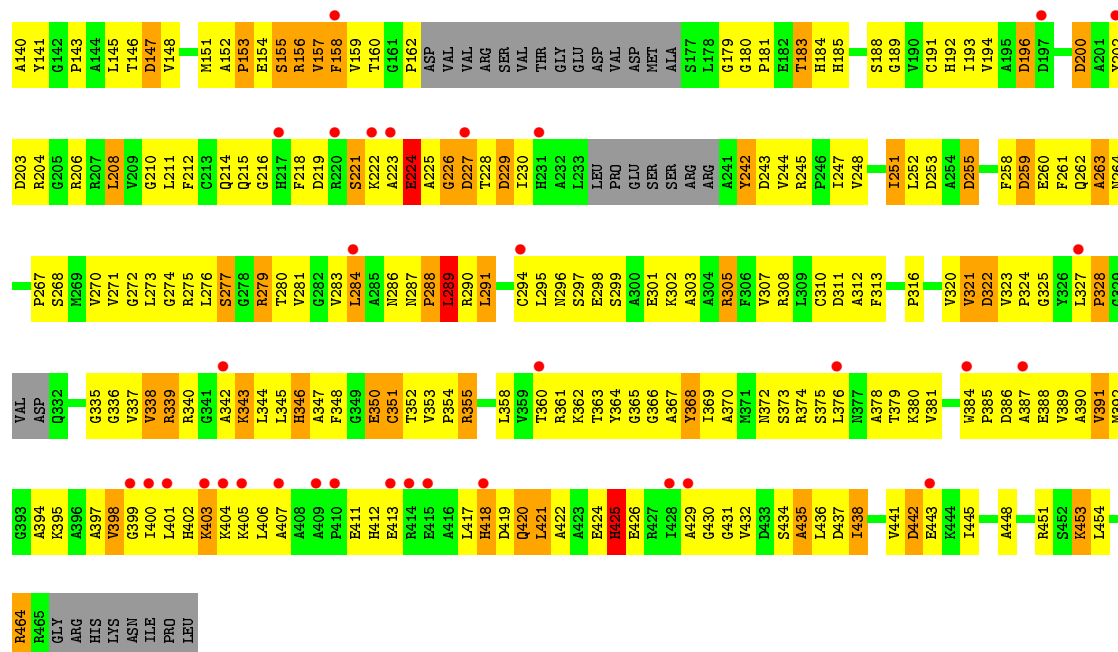
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Probable propionyl-CoA carboxylase beta chain 6



- Molecule 1: Probable propionyl-CoA carboxylase beta chain 6





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.28Å 82.36Å 157.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.85 – 3.00 46.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.85-3.00) 93.3 (46.85-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.233 , 0.304 0.234 , 0.295	Depositor DCC
$R_{free}$ test set	1041 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.0	EDS
Estimated twinning fraction	0.479 for K,H,-L 0.429 for k,h,-l	Xtriage
Reported twinning fraction	0.479 for K,H,-L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 20652 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	6220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.14 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8635e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [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	0.39	0/3191	0.63	0/4337
1	B	0.39	0/3137	0.64	0/4267
All	All	0.39	0/6328	0.63	0/8604

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	THR	Peptide

### 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	3135	0	3012	230	1
1	B	3080	0	2982	236	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
All	All	6220	0	5994	447	1

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 37.

All (447) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PHE:N	1:A:259:ASP:HB2	1.58	1.19
1:A:258:PHE:CD1	1:A:260:GLU:HB3	1.89	1.07
1:A:258:PHE:CA	1:A:259:ASP:HB2	1.85	1.04
1:A:257:PRO:O	1:A:258:PHE:HB2	1.60	0.98
1:A:258:PHE:CE1	1:A:260:GLU:HB3	2.02	0.95
1:B:339:ARG:HE	1:B:340:ARG:HG2	1.31	0.95
1:A:256:THR:N	1:A:257:PRO:HD3	1.82	0.94
1:B:344:LEU:HD23	1:B:370:ALA:HB1	1.55	0.88
1:B:151:MET:HE3	1:B:157:VAL:H	1.42	0.85
1:B:402:HIS:O	1:B:404:LYS:N	2.10	0.84
1:A:184:HIS:HB3	1:A:191:CYS:H	1.43	0.83
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.41	0.83
1:A:258:PHE:H	1:A:259:ASP:HB2	1.39	0.81
1:A:181:PRO:HB2	1:A:194:VAL:HG22	1.61	0.81
1:A:258:PHE:HA	1:A:259:ASP:HB2	1.62	0.80
1:A:108:LEU:HD12	1:B:369:ILE:HD11	1.63	0.79
1:B:358:LEU:HD22	1:B:454:LEU:HD11	1.64	0.79
1:B:296:ASN:H	1:B:299:SER:HB2	1.47	0.78
1:B:227:ASP:HB3	1:B:451:ARG:H	1.47	0.78
1:B:215:GLN:NE2	1:B:313:PHE:O	2.17	0.77
1:A:234:LEU:HD22	1:A:235:PRO:HD2	1.67	0.76
1:B:305:ARG:H	1:B:305:ARG:HD3	1.51	0.76
1:B:435:ALA:HA	1:B:438:ILE:HG13	1.68	0.76
1:A:188:SER:HB2	1:A:190:VAL:HG23	1.69	0.75
1:A:214:GLN:O	1:A:275:ARG:NH2	2.18	0.74
1:A:42:VAL:HG11	1:A:76:ILE:HD11	1.67	0.74
1:A:446:ASP:HB3	1:A:449:HIS:CE1	2.22	0.73
1:A:58:CYS:SG	1:A:59:THR:N	2.62	0.73
1:B:305:ARG:HB2	1:B:305:ARG:HH11	1.54	0.73
1:A:296:ASN:N	1:A:299:SER:OG	2.20	0.72
1:B:96:SER:OG	1:B:97:GLY:N	2.22	0.72
1:A:49:VAL:HG13	1:A:206:ARG:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PRO:O	1:A:258:PHE:CB	2.34	0.72
1:B:355:ARG:NH2	1:B:376:LEU:O	2.22	0.72
1:B:185:HIS:HD2	1:B:264:ASN:HB2	1.53	0.71
1:A:243:ASP:HB2	1:A:289:LEU:HD13	1.72	0.71
1:B:53:ARG:NH2	1:B:86:ASP:OD2	2.19	0.71
1:A:310:CYS:HB3	1:A:315:ILE:HB	1.73	0.71
1:A:120:ARG:HG3	1:A:120:ARG:HH11	1.54	0.71
1:B:398:VAL:HG13	1:B:425:HIS:NE2	2.04	0.70
1:A:122:SER:HA	1:A:127:GLN:HE22	1.56	0.70
1:A:186:LYS:HG3	1:A:264:ASN:HB3	1.74	0.70
1:A:266:ALA:HB3	1:A:302:LYS:HD2	1.72	0.70
1:A:153:PRO:HG3	1:A:197:ASP:HA	1.73	0.69
1:A:275:ARG:NH1	1:A:278:GLY:O	2.24	0.69
1:A:40:SER:O	1:A:100:ARG:NH2	2.26	0.69
1:A:67:ALA:O	1:A:100:ARG:NE	2.22	0.69
1:A:416:ALA:HB3	1:A:417:LEU:HA	1.74	0.68
1:A:394:ALA:HB1	1:A:426:GLU:HA	1.74	0.68
1:B:262:GLN:HB2	1:B:302:LYS:HE3	1.74	0.68
1:B:294:CYS:HA	1:B:323:VAL:HG23	1.76	0.68
1:A:331:ASP:O	1:A:333:GLU:N	2.27	0.67
1:A:366:GLY:HA2	1:A:369:ILE:HD12	1.76	0.67
1:A:150:VAL:HG13	1:A:193:ILE:HG22	1.76	0.67
1:B:321:VAL:O	1:B:360:THR:OG1	2.11	0.67
1:A:143:PRO:O	1:A:146:THR:OG1	2.13	0.67
1:A:73:CYS:HA	1:A:76:ILE:HD12	1.75	0.67
1:B:127:GLN:HG3	1:B:147:ASP:H	1.60	0.67
1:B:308:ARG:HH12	1:B:350:GLU:HB2	1.60	0.66
1:B:180:GLY:N	1:B:183:THR:OG1	2.27	0.66
1:B:179:GLY:HA3	1:B:184:HIS:CE1	2.30	0.66
1:A:405:LYS:O	1:A:407:ALA:N	2.29	0.66
1:A:94:TRP:HB2	1:A:131:VAL:HG22	1.77	0.66
1:A:255:ASP:HA	1:A:256:THR:CB	2.26	0.65
1:B:58:CYS:HB2	1:B:93:ILE:HB	1.76	0.65
1:B:395:LYS:HE2	1:B:419:ASP:HA	1.78	0.65
1:A:351:CYS:SG	1:A:355:ARG:NH2	2.70	0.65
1:B:361:ARG:HA	1:B:387:ALA:HA	1.79	0.65
1:A:17:ASP:HB3	1:A:20:LEU:HB3	1.77	0.65
1:A:145:LEU:HD23	1:B:342:ALA:HB1	1.77	0.65
1:A:339:ARG:NH2	1:B:188:SER:O	2.30	0.64
1:B:361:ARG:O	1:B:388:GLU:N	2.30	0.64
1:A:320:VAL:HG13	1:A:358:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:N	1:A:253:ASP:OD2	2.30	0.64
1:A:253:ASP:N	1:A:451:ARG:HH12	1.95	0.64
1:A:326:TYR:O	1:B:162:PRO:HD3	1.99	0.63
1:A:41:GLY:O	1:A:60:ASP:N	2.29	0.63
1:A:409:ALA:HB3	1:A:410:PRO:HD3	1.79	0.63
1:A:258:PHE:HA	1:A:259:ASP:CB	2.24	0.62
1:B:97:GLY:HA2	1:B:136:ALA:H	1.64	0.62
1:A:155:SER:O	1:A:156:ARG:NH1	2.32	0.62
1:B:185:HIS:CD2	1:B:264:ASN:HB2	2.34	0.62
1:B:355:ARG:NH1	1:B:355:ARG:HG3	2.15	0.62
1:A:152:ALA:O	1:A:155:SER:OG	2.10	0.62
1:B:425:HIS:O	1:B:429:ALA:N	2.25	0.61
1:B:398:VAL:HG21	1:B:421:LEU:HB2	1.82	0.61
1:B:188:SER:OG	1:B:189:GLY:N	2.33	0.61
1:B:348:PHE:HB2	1:B:376:LEU:HD13	1.83	0.61
1:A:446:ASP:HB3	1:A:449:HIS:NE2	2.16	0.61
1:A:270:VAL:N	1:A:285:ALA:O	2.29	0.61
1:A:262:GLN:O	1:A:302:LYS:NZ	2.23	0.61
1:B:219:ASP:H	1:B:277:SER:HB2	1.65	0.61
1:A:16:ARG:NH2	1:A:62:THR:HG23	2.16	0.61
1:A:108:LEU:HD21	1:B:391:VAL:HB	1.83	0.61
1:A:234:LEU:HD11	1:A:361:ARG:HD3	1.82	0.60
1:B:373:SER:OG	1:B:375:SER:OG	2.19	0.60
1:B:134:PHE:HB3	1:B:158:PHE:CE2	2.36	0.60
1:A:117:ALA:HA	1:A:120:ARG:HH12	1.67	0.60
1:A:308:ARG:NH2	1:A:350:GLU:OE2	2.34	0.60
1:B:381:VAL:HG12	1:B:441:VAL:HG13	1.84	0.60
1:A:145:LEU:HD21	1:B:345:LEU:HD12	1.84	0.60
1:B:112:GLY:HA2	1:B:115:PHE:CD2	2.37	0.60
1:A:138:GLY:O	1:A:142:GLY:N	2.25	0.60
1:B:248:VAL:HG13	1:B:283:VAL:HG11	1.84	0.59
1:B:148:VAL:HG11	1:B:208:LEU:HD11	1.84	0.59
1:A:55:ILE:HB	1:A:83:ALA:HB2	1.84	0.59
1:A:210:GLY:O	1:A:214:GLN:N	2.33	0.59
1:B:244:VAL:HG11	1:B:286:ASN:O	2.02	0.59
1:A:229:ASP:HA	1:A:448:ALA:HA	1.84	0.59
1:A:200:ASP:O	1:A:204:ARG:N	2.31	0.59
1:A:258:PHE:CA	1:A:259:ASP:CB	2.63	0.59
1:B:20:LEU:O	1:B:24:ASN:N	2.34	0.59
1:B:260:GLU:HA	1:B:272:GLY:HA3	1.84	0.59
1:A:266:ALA:HB1	1:A:299:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:C	1:A:38:ASP:H	2.07	0.58
1:A:115:PHE:O	1:A:119:ILE:HG13	2.03	0.58
1:B:252:LEU:HD13	1:B:274:GLY:HA3	1.86	0.58
1:B:191:CYS:SG	1:B:192:HIS:N	2.77	0.58
1:B:355:ARG:O	1:B:372:ASN:ND2	2.30	0.58
1:A:35:HIS:NE2	1:A:43:LEU:HA	2.18	0.58
1:A:342:ALA:HA	1:A:345:LEU:HD12	1.83	0.58
1:A:324:PRO:HG3	1:A:362:LYS:HZ3	1.69	0.58
1:B:328:PRO:HA	1:B:337:VAL:HG11	1.86	0.58
1:A:184:HIS:CG	1:A:190:VAL:HB	2.39	0.57
1:A:127:GLN:O	1:A:146:THR:HB	2.04	0.57
1:A:359:VAL:HG22	1:A:387:ALA:HB1	1.86	0.57
1:B:151:MET:HG2	1:B:181:PRO:HB3	1.85	0.57
1:B:127:GLN:NE2	1:B:145:LEU:O	2.37	0.57
1:A:365:GLY:HA2	1:B:108:LEU:HD11	1.87	0.57
1:A:462:PRO:HG2	1:A:464:ARG:HE	1.69	0.57
1:A:35:HIS:NE2	1:A:43:LEU:HD12	2.20	0.57
1:A:243:ASP:O	1:A:246:PRO:HD2	2.04	0.57
1:A:230:ILE:HG13	1:A:450:THR:HB	1.86	0.57
1:B:358:LEU:HD11	1:B:445:ILE:HD11	1.86	0.57
1:B:227:ASP:OD2	1:B:227:ASP:N	2.37	0.56
1:B:252:LEU:HD21	1:B:283:VAL:HG21	1.86	0.56
1:B:210:GLY:O	1:B:275:ARG:NH2	2.38	0.56
1:B:224:GLU:O	1:B:226:GLY:N	2.37	0.56
1:A:258:PHE:H	1:A:259:ASP:CB	2.14	0.56
1:B:261:PHE:O	1:B:263:ALA:N	2.37	0.56
1:B:200:ASP:HA	1:B:203:ASP:OD2	2.05	0.56
1:A:73:CYS:O	1:A:76:ILE:HB	2.06	0.56
1:B:321:VAL:N	1:B:358:LEU:O	2.39	0.56
1:B:328:PRO:O	1:B:337:VAL:HG11	2.05	0.56
1:B:131:VAL:HG12	1:B:155:SER:HB2	1.87	0.56
1:B:445:ILE:HG21	1:B:453:LYS:HG2	1.88	0.56
1:B:196:ASP:N	1:B:196:ASP:OD1	2.37	0.56
1:A:74:THR:HG22	1:A:78:ASN:OD1	2.06	0.56
1:B:123:GLY:HA2	1:B:312:ALA:HB1	1.88	0.56
1:A:429:ALA:O	1:A:431:GLY:N	2.38	0.55
1:B:380:LYS:HG3	1:B:442:ASP:OD1	2.06	0.55
1:A:215:GLN:O	1:A:279:ARG:HA	2.05	0.55
1:B:339:ARG:NE	1:B:340:ARG:HG2	2.11	0.55
1:A:105:VAL:HG22	1:B:438:ILE:HD12	1.88	0.55
1:B:358:LEU:HD13	1:B:454:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TYR:CZ	1:B:118:MET:HG2	2.42	0.54
1:A:303:ALA:O	1:A:306:PHE:N	2.40	0.54
1:A:256:THR:N	1:A:257:PRO:CD	2.61	0.54
1:A:432:VAL:O	1:A:435:ALA:N	2.29	0.54
1:A:319:VAL:HG21	1:A:372:ASN:HB3	1.89	0.54
1:A:258:PHE:N	1:A:259:ASP:CB	2.52	0.54
1:A:151:MET:HB3	1:A:181:PRO:HB3	1.90	0.54
1:A:320:VAL:HA	1:A:358:LEU:HD23	1.89	0.53
1:A:49:VAL:HG11	1:A:209:VAL:HG13	1.90	0.53
1:B:151:MET:CE	1:B:157:VAL:H	2.16	0.53
1:B:394:ALA:HB1	1:B:422:ALA:HA	1.90	0.53
1:A:454:LEU:O	1:A:458:LEU:N	2.36	0.53
1:A:37:ARG:O	1:A:39:ARG:N	2.42	0.53
1:A:107:ALA:O	1:A:111:VAL:N	2.29	0.53
1:A:432:VAL:O	1:A:436:LEU:N	2.41	0.53
1:B:301:GLU:OE1	1:B:340:ARG:HD2	2.09	0.53
1:B:397:ALA:C	1:B:425:HIS:HE2	2.12	0.53
1:A:219:ASP:OD2	1:A:222:LYS:HE3	2.08	0.53
1:B:364:TYR:HA	1:B:390:ALA:O	2.08	0.53
1:A:288:PRO:HA	1:A:293:GLY:N	2.24	0.53
1:B:402:HIS:O	1:B:404:LYS:HG2	2.09	0.53
1:B:361:ARG:NH1	1:B:362:LYS:HE3	2.23	0.53
1:A:360:THR:HB	1:A:384:TRP:CE3	2.44	0.52
1:B:335:GLY:O	1:B:338:VAL:HG23	2.09	0.52
1:B:152:ALA:HB3	1:B:155:SER:HB3	1.90	0.52
1:B:259:ASP:OD1	1:B:259:ASP:N	2.39	0.52
1:A:394:ALA:HB3	1:A:426:GLU:OE2	2.09	0.52
1:A:296:ASN:OD1	1:A:298:GLU:N	2.43	0.52
1:B:156:ARG:HB2	1:B:158:PHE:HB3	1.91	0.52
1:B:216:GLY:O	1:B:279:ARG:NH1	2.43	0.52
1:B:153:PRO:HA	1:B:181:PRO:HG3	1.92	0.52
1:A:402:HIS:HB2	1:A:406:LEU:HD12	1.91	0.52
1:A:151:MET:N	1:A:193:ILE:O	2.41	0.52
1:B:398:VAL:HG11	1:B:421:LEU:HB3	1.90	0.52
1:A:470:ASN:OD1	1:B:308:ARG:HD3	2.10	0.51
1:A:77:VAL:HG22	1:A:117:ALA:HB2	1.92	0.51
1:B:25:PHE:O	1:B:206:ARG:HD2	2.10	0.51
1:B:29:GLY:HA3	1:B:30:SER:HB2	1.91	0.51
1:B:255:ASP:OD2	1:B:255:ASP:N	2.36	0.51
1:B:127:GLN:HB2	1:B:146:THR:HG22	1.92	0.51
1:B:111:VAL:O	1:B:114:VAL:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:O	1:A:123:GLY:N	2.43	0.51
1:B:328:PRO:O	1:B:337:VAL:CG1	2.58	0.51
1:A:35:HIS:CE1	1:A:43:LEU:HA	2.46	0.51
1:A:94:TRP:HE1	1:A:129:SER:HG	1.43	0.51
1:B:219:ASP:H	1:B:277:SER:CB	2.23	0.51
1:B:16:ARG:HG2	1:B:95:HIS:CE1	2.45	0.51
1:A:205:GLY:O	1:A:209:VAL:HG12	2.11	0.51
1:A:219:ASP:OD2	1:A:222:LYS:HB2	2.11	0.51
1:B:154:GLU:O	1:B:156:ARG:HG2	2.10	0.51
1:A:214:GLN:C	1:A:275:ARG:HH22	2.12	0.50
1:A:200:ASP:O	1:A:204:ARG:HG2	2.10	0.50
1:A:237:SER:O	1:A:239:ARG:N	2.44	0.50
1:A:38:ASP:O	1:A:40:SER:N	2.41	0.50
1:B:155:SER:OG	1:B:155:SER:O	2.28	0.50
1:B:366:GLY:HA2	1:B:369:ILE:HD12	1.93	0.50
1:A:122:SER:HA	1:A:127:GLN:NE2	2.25	0.50
1:A:215:GLN:HA	1:A:280:THR:OG1	2.12	0.50
1:A:443:GLU:HG2	1:A:444:LYS:N	2.26	0.50
1:B:210:GLY:O	1:B:214:GLN:HB2	2.12	0.50
1:A:14:ASP:N	1:A:16:ARG:HH21	2.10	0.50
1:B:301:GLU:O	1:B:305:ARG:HD3	2.12	0.50
1:A:238:SER:HA	1:A:361:ARG:NH1	2.27	0.50
1:B:248:VAL:HA	1:B:251:ILE:HG13	1.93	0.50
1:A:200:ASP:HA	1:A:203:ASP:HB2	1.94	0.50
1:B:95:HIS:CD2	1:B:133:GLY:HA3	2.47	0.50
1:B:137:GLY:O	1:B:140:ALA:N	2.45	0.50
1:B:368:TYR:CD2	1:B:369:ILE:HG13	2.46	0.49
1:A:154:GLU:HA	1:A:156:ARG:NH2	2.26	0.49
1:A:211:LEU:HB3	1:A:280:THR:HG21	1.94	0.49
1:B:32:GLU:N	1:B:46:ALA:O	2.40	0.49
1:B:431:GLY:O	1:B:434:SER:HB3	2.12	0.49
1:A:119:ILE:HD13	1:B:346:HIS:HA	1.93	0.49
1:A:55:ILE:HG12	1:A:82:THR:HB	1.93	0.49
1:B:355:ARG:HB2	1:B:372:ASN:ND2	2.27	0.49
1:A:308:ARG:HA	1:A:311:ASP:HB3	1.95	0.49
1:A:42:VAL:HG21	1:A:76:ILE:HG13	1.95	0.49
1:A:143:PRO:HA	1:A:146:THR:HG23	1.94	0.49
1:A:185:HIS:O	1:A:264:ASN:HB2	2.12	0.49
1:B:286:ASN:ND2	1:B:323:VAL:HB	2.28	0.49
1:A:252:LEU:O	1:A:253:ASP:O	2.30	0.48
1:B:395:LYS:HD3	1:B:418:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ARG:HA	1:B:378:ALA:HB3	1.94	0.48
1:B:464:ARG:HA	1:B:464:ARG:HD2	1.54	0.48
1:A:244:VAL:HA	1:A:247:ILE:HD13	1.94	0.48
1:B:33:LEU:HD23	1:B:35:HIS:O	2.13	0.48
1:A:188:SER:HB3	1:B:335:GLY:HA3	1.95	0.48
1:B:296:ASN:OD1	1:B:299:SER:OG	2.13	0.48
1:A:100:ARG:HB3	1:A:103:GLU:HG3	1.94	0.48
1:A:270:VAL:HG23	1:A:287:ASN:HB2	1.95	0.48
1:A:86:ASP:OD1	1:A:86:ASP:N	2.46	0.48
1:B:211:LEU:HD13	1:B:273:LEU:HB3	1.94	0.48
1:A:324:PRO:N	1:A:362:LYS:HD2	2.29	0.48
1:A:150:VAL:HG13	1:A:193:ILE:CG2	2.43	0.48
1:A:37:ARG:HA	1:A:37:ARG:HD3	1.62	0.48
1:B:21:ARG:HD2	1:B:202:TYR:OH	2.12	0.48
1:A:375:SER:OG	1:B:112:GLY:HA3	2.14	0.48
1:A:18:PRO:HB3	1:A:43:LEU:HB3	1.95	0.48
1:B:60:ASP:O	1:B:66:GLY:HA2	2.14	0.47
1:B:95:HIS:CG	1:B:133:GLY:HA3	2.48	0.47
1:A:443:GLU:HG2	1:A:444:LYS:H	1.79	0.47
1:B:370:ALA:O	1:B:372:ASN:N	2.47	0.47
1:A:417:LEU:CB	1:A:418:HIS:C	2.83	0.47
1:B:323:VAL:HG22	1:B:325:GLY:H	1.79	0.47
1:A:80:TYR:O	1:A:84:ILE:HG13	2.14	0.47
1:B:399:GLY:C	1:B:401:LEU:H	2.17	0.47
1:A:116:GLU:HB2	1:B:376:LEU:HD23	1.94	0.47
1:B:365:GLY:H	1:B:391:VAL:HA	1.79	0.47
1:A:42:VAL:HA	1:A:59:THR:HA	1.96	0.47
1:B:258:PHE:CE2	1:B:260:GLU:HB2	2.49	0.47
1:B:394:ALA:HB2	1:B:425:HIS:HB3	1.97	0.47
1:B:308:ARG:HH12	1:B:350:GLU:CB	2.26	0.47
1:A:186:LYS:O	1:A:188:SER:N	2.48	0.47
1:A:154:GLU:HA	1:A:156:ARG:HH22	1.80	0.47
1:A:105:VAL:O	1:A:108:LEU:N	2.47	0.47
1:A:260:GLU:HA	1:A:272:GLY:HA2	1.97	0.47
1:A:445:ILE:HG21	1:A:453:LYS:HG3	1.96	0.47
1:A:267:PRO:HB2	1:A:290:ARG:HG3	1.97	0.47
1:B:324:PRO:HA	1:B:364:TYR:HD2	1.80	0.47
1:A:431:GLY:O	1:A:434:SER:OG	2.31	0.47
1:B:227:ASP:HB2	1:B:448:ALA:O	2.15	0.46
1:B:132:VAL:HA	1:B:155:SER:HB3	1.97	0.46
1:B:336:GLY:O	1:B:340:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.80	0.46
1:A:116:GLU:OE1	1:A:120:ARG:NH1	2.48	0.46
1:B:114:VAL:O	1:B:118:MET:HG3	2.14	0.46
1:B:218:PHE:CD1	1:B:279:ARG:HB3	2.50	0.46
1:B:157:VAL:O	1:B:159:VAL:HG23	2.16	0.46
1:B:296:ASN:HD21	1:B:298:GLU:HB2	1.81	0.46
1:B:275:ARG:NH1	1:B:280:THR:OG1	2.48	0.46
1:A:438:ILE:HG23	1:B:106:ARG:NH1	2.30	0.46
1:A:184:HIS:HA	1:A:188:SER:OG	2.15	0.46
1:A:94:TRP:NE1	1:A:129:SER:OG	2.31	0.46
1:B:215:GLN:HA	1:B:280:THR:OG1	2.16	0.46
1:B:253:ASP:HB3	1:B:255:ASP:OD2	2.16	0.46
1:A:398:VAL:HA	1:A:401:LEU:HD12	1.98	0.46
1:B:367:ALA:HA	1:B:370:ALA:HB3	1.98	0.46
1:A:267:PRO:HB2	1:A:290:ARG:CB	2.46	0.46
1:B:347:ALA:O	1:B:351:CYS:HB2	2.15	0.46
1:B:26:PHE:HD2	1:B:31:VAL:HG22	1.80	0.46
1:A:265:TRP:O	1:A:302:LYS:NZ	2.43	0.46
1:B:34:LEU:O	1:B:35:HIS:HB3	2.16	0.46
1:B:62:THR:OG1	1:B:63:VAL:N	2.48	0.46
1:B:303:ALA:O	1:B:307:VAL:HG23	2.16	0.46
1:B:66:GLY:HA3	1:B:96:SER:HA	1.97	0.46
1:A:416:ALA:CB	1:A:417:LEU:HA	2.40	0.46
1:A:394:ALA:O	1:A:396:ALA:HA	2.16	0.46
1:B:218:PHE:CE2	1:B:279:ARG:HD3	2.52	0.46
1:B:268:SER:OG	1:B:299:SER:OG	2.33	0.45
1:A:36:GLU:C	1:A:38:ASP:N	2.70	0.45
1:B:80:TYR:OH	1:B:118:MET:HG2	2.16	0.45
1:B:343:LYS:HA	1:B:343:LYS:HD2	1.55	0.45
1:B:106:ARG:O	1:B:110:ALA:N	2.49	0.45
1:A:342:ALA:HB1	1:B:145:LEU:CD2	2.47	0.45
1:A:410:PRO:HD2	1:A:411:GLU:H	1.81	0.45
1:A:301:GLU:H	1:A:301:GLU:HG2	1.50	0.45
1:B:417:LEU:HA	1:B:420:GLN:HB2	1.99	0.45
1:A:445:ILE:HG22	1:A:453:LYS:HZ3	1.81	0.45
1:A:339:ARG:C	1:A:341:GLY:H	2.20	0.45
1:A:324:PRO:O	1:A:364:TYR:HB2	2.16	0.45
1:A:271:VAL:HA	1:A:284:LEU:HA	1.98	0.45
1:B:311:ASP:HA	1:B:353:VAL:HG13	1.99	0.45
1:A:133:GLY:HA2	1:A:155:SER:HA	1.99	0.45
1:A:107:ALA:O	1:A:111:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HA	1:A:120:ARG:NH1	2.30	0.45
1:B:244:VAL:HB	1:B:288:PRO:HD2	1.99	0.45
1:B:399:GLY:O	1:B:401:LEU:N	2.46	0.45
1:B:221:SER:C	1:B:223:ALA:H	2.21	0.45
1:A:33:LEU:HA	1:A:45:ALA:HA	1.99	0.45
1:B:391:VAL:HG22	1:B:392:MET:HG2	1.99	0.44
1:A:67:ALA:HB3	1:A:100:ARG:HG3	1.99	0.44
1:B:111:VAL:HG11	1:B:138:GLY:HA3	1.99	0.44
1:B:307:VAL:O	1:B:310:CYS:N	2.50	0.44
1:A:363:THR:CG2	1:A:389:VAL:HG22	2.47	0.44
1:B:267:PRO:O	1:B:287:ASN:ND2	2.44	0.44
1:A:271:VAL:HG22	1:A:302:LYS:HE2	1.99	0.44
1:B:143:PRO:HA	1:B:146:THR:OG1	2.18	0.44
1:B:401:LEU:C	1:B:403:LYS:H	2.21	0.44
1:B:157:VAL:C	1:B:159:VAL:H	2.21	0.44
1:B:268:SER:HA	1:B:287:ASN:HB3	2.00	0.44
1:A:266:ALA:CB	1:A:299:SER:HA	2.47	0.44
1:B:55:ILE:HG12	1:B:82:THR:HG22	2.00	0.44
1:B:227:ASP:CB	1:B:451:ARG:HB3	2.48	0.44
1:A:42:VAL:HG22	1:A:75:HIS:HD2	1.82	0.44
1:B:218:PHE:HE1	1:B:276:LEU:HB3	1.83	0.44
1:B:211:LEU:HD22	1:B:280:THR:HG23	2.00	0.43
1:B:286:ASN:OD1	1:B:322:ASP:N	2.40	0.43
1:B:204:ARG:O	1:B:208:LEU:HB2	2.19	0.43
1:B:270:VAL:O	1:B:284:LEU:HA	2.18	0.43
1:B:344:LEU:HD12	1:B:344:LEU:HA	1.91	0.43
1:B:348:PHE:O	1:B:355:ARG:NH2	2.51	0.43
1:B:212:PHE:O	1:B:215:GLN:HG3	2.19	0.43
1:B:18:PRO:HG3	1:B:60:ASP:HA	2.00	0.43
1:B:388:GLU:OE2	1:B:430:GLY:HA3	2.19	0.43
1:B:33:LEU:HD11	1:B:43:LEU:HD11	2.00	0.43
1:B:328:PRO:CA	1:B:337:VAL:HG11	2.49	0.43
1:A:84:ILE:HD11	1:A:121:ALA:HB2	2.01	0.43
1:B:88:SER:O	1:B:125:ILE:HD12	2.18	0.43
1:B:411:GLU:C	1:B:413:GLU:H	2.21	0.43
1:A:260:GLU:HA	1:A:272:GLY:CA	2.49	0.43
1:B:258:PHE:O	1:B:260:GLU:N	2.51	0.43
1:B:321:VAL:HG23	1:B:358:LEU:O	2.18	0.43
1:B:294:CYS:SG	1:B:324:PRO:HD2	2.59	0.43
1:B:38:ASP:HB2	1:B:39:ARG:H	1.66	0.43
1:B:363:THR:HG23	1:B:389:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLY:O	1:B:75:HIS:N	2.49	0.43
1:B:337:VAL:H	1:B:337:VAL:HG13	1.56	0.43
1:A:54:THR:HG21	1:A:209:VAL:HG21	1.99	0.43
1:A:31:VAL:HG12	1:A:32:GLU:O	2.18	0.43
1:B:384:TRP:O	1:B:386:ASP:N	2.52	0.42
1:A:94:TRP:O	1:A:95:HIS:HB2	2.19	0.42
1:B:118:MET:O	1:B:121:ALA:HB3	2.18	0.42
1:A:444:LYS:HB2	1:A:444:LYS:HE3	1.80	0.42
1:B:22:LEU:HD13	1:B:45:ALA:HB3	2.01	0.42
1:A:235:PRO:HG3	1:A:242:TYR:CD2	2.54	0.42
1:A:365:GLY:C	1:A:367:ALA:H	2.22	0.42
1:A:151:MET:HG2	1:A:155:SER:OG	2.20	0.42
1:B:358:LEU:HD21	1:B:384:TRP:CZ2	2.54	0.42
1:B:229:ASP:HA	1:B:448:ALA:HA	2.01	0.42
1:B:244:VAL:O	1:B:247:ILE:HG13	2.19	0.42
1:B:395:LYS:CE	1:B:419:ASP:HA	2.48	0.42
1:B:35:HIS:CE1	1:B:43:LEU:HD12	2.55	0.42
1:B:76:ILE:O	1:B:79:ALA:HB3	2.20	0.42
1:B:316:PRO:HB3	1:B:354:PRO:HB2	2.00	0.42
1:B:305:ARG:NH1	1:B:305:ARG:HB2	2.29	0.42
1:A:339:ARG:O	1:A:341:GLY:N	2.52	0.42
1:B:353:VAL:O	1:B:355:ARG:HD3	2.19	0.42
1:B:228:THR:OG1	1:B:230:ILE:HG12	2.19	0.42
1:B:151:MET:HE3	1:B:157:VAL:N	2.21	0.42
1:B:398:VAL:HG13	1:B:425:HIS:HE2	1.83	0.42
1:B:224:GLU:N	1:B:224:GLU:OE1	2.53	0.42
1:A:70:VAL:HA	1:A:110:ALA:CB	2.50	0.42
1:A:282:GLY:HA3	1:A:317:LEU:HD23	2.01	0.42
1:A:262:GLN:OE1	1:A:302:LYS:HE3	2.19	0.42
1:A:115:PHE:CD2	1:B:345:LEU:HD13	2.54	0.42
1:A:16:ARG:HA	1:A:21:ARG:CZ	2.50	0.42
1:B:27:ASP:OD1	1:B:49:VAL:HA	2.20	0.42
1:A:319:VAL:HB	1:A:357:THR:HG23	2.01	0.42
1:A:454:LEU:HD22	1:A:454:LEU:H	1.85	0.42
1:A:80:TYR:HA	1:A:90:ILE:HD13	2.02	0.42
1:B:70:VAL:HG21	1:B:106:ARG:HB3	2.02	0.42
1:A:220:ARG:HG3	1:A:221:SER:N	2.34	0.41
1:A:207:ARG:O	1:A:211:LEU:HG	2.20	0.41
1:A:261:PHE:N	1:A:261:PHE:CD1	2.87	0.41
1:A:258:PHE:HA	1:A:259:ASP:C	2.41	0.41
1:B:379:THR:HB	1:B:380:LYS:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:HIS:HA	1:A:384:TRP:CH2	2.55	0.41
1:B:16:ARG:HD3	1:B:95:HIS:CE1	2.56	0.41
1:A:141:TYR:HE1	1:B:338:VAL:HA	1.85	0.41
1:A:287:ASN:HA	1:A:288:PRO:HD3	1.77	0.41
1:B:222:LYS:HB3	1:B:277:SER:HA	2.02	0.41
1:A:349:GLY:HA3	1:B:119:ILE:HD13	2.00	0.41
1:B:291:LEU:O	1:B:327:LEU:HD11	2.20	0.41
1:A:156:ARG:O	1:A:157:VAL:HG23	2.20	0.41
1:A:35:HIS:HE1	1:A:42:VAL:O	2.04	0.41
1:A:67:ALA:CB	1:A:100:ARG:HG3	2.51	0.41
1:B:26:PHE:CE1	1:B:54:THR:HG22	2.56	0.41
1:B:39:ARG:O	1:B:63:VAL:HG11	2.19	0.41
1:B:185:HIS:CD2	1:B:185:HIS:O	2.73	0.41
1:B:324:PRO:HA	1:B:364:TYR:CD2	2.56	0.41
1:B:308:ARG:NH2	1:B:350:GLU:OE1	2.52	0.41
1:A:339:ARG:HH11	1:A:340:ARG:HE	1.68	0.41
1:B:261:PHE:CD1	1:B:261:PHE:N	2.88	0.41
1:A:392:MET:HB2	1:A:397:ALA:HB1	2.01	0.41
1:A:155:SER:H	1:A:155:SER:HG	1.61	0.41
1:A:296:ASN:H	1:A:299:SER:HG	1.60	0.41
1:A:103:GLU:HB2	1:A:107:ALA:HB2	2.01	0.41
1:A:132:VAL:HA	1:A:152:ALA:CB	2.51	0.41
1:B:227:ASP:HB3	1:B:451:ARG:HB3	2.03	0.41
1:A:324:PRO:CA	1:A:362:LYS:HD2	2.51	0.41
1:A:230:ILE:HG12	1:A:447:PRO:O	2.21	0.41
1:A:282:GLY:O	1:A:317:LEU:HA	2.21	0.41
1:B:405:LYS:C	1:B:407:ALA:H	2.22	0.41
1:B:445:ILE:CG2	1:B:453:LYS:HG2	2.50	0.40
1:A:319:VAL:O	1:A:358:LEU:HD23	2.22	0.40
1:A:99:ALA:HB2	1:A:111:VAL:HG21	2.03	0.40
1:A:131:VAL:HG11	1:A:135:ALA:HB2	2.04	0.40
1:B:107:ALA:O	1:B:110:ALA:HB3	2.21	0.40
1:B:297:SER:O	1:B:301:GLU:HG3	2.21	0.40
1:A:57:PHE:CD2	1:A:76:ILE:HG12	2.55	0.40
1:A:284:LEU:HD21	1:A:307:VAL:HG23	2.03	0.40
1:B:185:HIS:CD2	1:B:264:ASN:H	2.40	0.40
1:A:438:ILE:HG21	1:B:106:ARG:HG2	2.02	0.40
1:B:289:LEU:HB3	1:B:290:ARG:H	1.62	0.40
1:B:311:ASP:CG	1:B:352:THR:H	2.22	0.40
1:A:410:PRO:HB2	1:A:412:HIS:H	1.86	0.40
1:A:48:THR:HA	1:A:53:ARG:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ASP:HA	1:B:353:VAL:CG1	2.51	0.40
1:A:86:ASP:O	1:A:88:SER:N	2.55	0.40
1:B:99:ALA:O	1:B:100:ARG:C	2.60	0.40
1:B:242:TYR:CG	1:B:243:ASP:N	2.89	0.40
1:A:28:ASP:HB2	1:A:29:GLY:H	1.71	0.40

All (1) 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:102:ALA:O	1:A:405:LYS:NZ[2_555]	2.06	0.14

## 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	427/473 (90%)	321 (75%)	76 (18%)	30 (7%)	1	7
1	B	419/473 (89%)	309 (74%)	84 (20%)	26 (6%)	2	10
All	All	846/946 (89%)	630 (74%)	160 (19%)	56 (7%)	1	8

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	87	GLN
1	A	95	HIS
1	A	122	SER
1	A	253	ASP
1	A	257	PRO
1	A	258	PHE
1	A	332	GLN

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Mol	Chain	Res	Type
1	A	337	VAL
1	A	406	LEU
1	A	410	PRO
1	A	419	ASP
1	A	430	GLY
1	A	432	VAL
1	B	263	ALA
1	B	289	LEU
1	B	328	PRO
1	B	400	ILE
1	B	403	LYS
1	A	39	ARG
1	A	238	SER
1	A	239	ARG
1	A	262	GLN
1	A	363	THR
1	A	418	HIS
1	A	468	HIS
1	B	30	SER
1	B	35	HIS
1	B	100	ARG
1	B	242	TYR
1	B	322	ASP
1	B	412	HIS
1	B	435	ALA
1	A	27	ASP
1	B	62	THR
1	B	97	GLY
1	B	155	SER
1	B	225	ALA
1	B	406	LEU
1	B	426	GLU
1	A	146	THR
1	A	236	GLU
1	A	322	ASP
1	A	340	ARG
1	A	429	ALA
1	B	63	VAL
1	B	147	ASP
1	B	224	GLU
1	A	405	LYS
1	B	153	PRO

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Mol	Chain	Res	Type
1	B	226	GLY
1	B	385	PRO
1	B	425	HIS
1	A	324	PRO
1	A	338	VAL
1	B	288	PRO

### 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	301/362 (83%)	237 (79%)	64 (21%)	1	6
1	B	296/362 (82%)	227 (77%)	69 (23%)	1	4
All	All	597/724 (82%)	464 (78%)	133 (22%)	1	5

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	19	LEU
1	A	24	ASN
1	A	27	ASP
1	A	30	SER
1	A	32	GLU
1	A	33	LEU
1	A	35	HIS
1	A	37	ARG
1	A	42	VAL
1	A	48	THR
1	A	54	THR
1	A	58	CYS
1	A	62	THR
1	A	68	MET
1	A	71	GLU
1	A	75	HIS

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Mol	Chain	Res	Type
1	A	86	ASP
1	A	88	SER
1	A	108	LEU
1	A	122	SER
1	A	129	SER
1	A	158	PHE
1	A	191	CYS
1	A	197	ASP
1	A	212	PHE
1	A	215	GLN
1	A	219	ASP
1	A	221	SER
1	A	230	ILE
1	A	236	GLU
1	A	242	TYR
1	A	245	ARG
1	A	253	ASP
1	A	258	PHE
1	A	262	GLN
1	A	265	TRP
1	A	273	LEU
1	A	281	VAL
1	A	286	ASN
1	A	301	GLU
1	A	305	ARG
1	A	322	ASP
1	A	327	LEU
1	A	337	VAL
1	A	340	ARG
1	A	350	GLU
1	A	351	CYS
1	A	358	LEU
1	A	359	VAL
1	A	363	THR
1	A	368	TYR
1	A	400	ILE
1	A	404	LYS
1	A	425	HIS
1	A	426	GLU
1	A	427	ARG
1	A	434	SER
1	A	436	LEU

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Mol	Chain	Res	Type
1	A	437	ASP
1	A	438	ILE
1	A	452	SER
1	A	456	GLU
1	A	464	ARG
1	B	21	ARG
1	B	22	LEU
1	B	34	LEU
1	B	38	ASP
1	B	55	ILE
1	B	58	CYS
1	B	63	VAL
1	B	64	MET
1	B	75	HIS
1	B	82	THR
1	B	87	GLN
1	B	90	ILE
1	B	100	ARG
1	B	101	LEU
1	B	111	VAL
1	B	130	VAL
1	B	141	TYR
1	B	156	ARG
1	B	157	VAL
1	B	158	PHE
1	B	160	THR
1	B	183	THR
1	B	193	ILE
1	B	194	VAL
1	B	196	ASP
1	B	200	ASP
1	B	208	LEU
1	B	221	SER
1	B	224	GLU
1	B	227	ASP
1	B	229	ASP
1	B	245	ARG
1	B	251	ILE
1	B	255	ASP
1	B	259	ASP
1	B	271	VAL
1	B	277	SER

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Mol	Chain	Res	Type
1	B	279	ARG
1	B	281	VAL
1	B	284	LEU
1	B	289	LEU
1	B	291	LEU
1	B	295	LEU
1	B	305	ARG
1	B	320	VAL
1	B	321	VAL
1	B	338	VAL
1	B	339	ARG
1	B	343	LYS
1	B	346	HIS
1	B	350	GLU
1	B	351	CYS
1	B	355	ARG
1	B	368	TYR
1	B	391	VAL
1	B	398	VAL
1	B	418	HIS
1	B	420	GLN
1	B	421	LEU
1	B	424	GLU
1	B	425	HIS
1	B	432	VAL
1	B	436	LEU
1	B	437	ASP
1	B	438	ILE
1	B	442	ASP
1	B	443	GLU
1	B	453	LYS
1	B	464	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no 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, 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	435/473 (91%)	0.65	51 (11%) 6 2	13, 50, 87, 139	0
1	B	427/473 (90%)	0.52	36 (8%) 14 5	6, 44, 89, 123	0
All	All	862/946 (91%)	0.59	87 (10%) 9 3	6, 47, 88, 139	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	GLU	8.5
1	A	428	ILE	7.3
1	A	398	VAL	6.3
1	A	72	GLY	5.6
1	B	429	ALA	5.2
1	B	222	LYS	5.0
1	A	390	ALA	4.9
1	B	428	ILE	4.9
1	A	228	THR	4.8
1	A	235	PRO	4.8
1	A	391	VAL	4.7
1	B	410	PRO	4.2
1	A	413	GLU	4.2
1	B	327	LEU	4.0
1	A	410	PRO	4.0
1	B	415	GLU	3.9
1	B	294	CYS	3.8
1	A	314	GLY	3.8
1	A	426	GLU	3.8
1	A	59	THR	3.6
1	A	201	ALA	3.6
1	A	29	GLY	3.6
1	B	63	VAL	3.4
1	A	405	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	427	ARG	3.3
1	B	404	LYS	3.3
1	B	227	ASP	3.3
1	B	231	HIS	3.3
1	B	409	ALA	3.3
1	B	399	GLY	3.2
1	B	407	ALA	3.2
1	A	54	THR	3.1
1	A	420	GLN	3.1
1	B	400	ILE	3.0
1	A	371	MET	3.0
1	B	376	LEU	3.0
1	A	387	ALA	2.9
1	B	387	ALA	2.9
1	A	25	PHE	2.9
1	A	97	GLY	2.9
1	B	401	LEU	2.9
1	B	413	GLU	2.9
1	A	202	TYR	2.9
1	B	443	GLU	2.9
1	A	14	ASP	2.9
1	B	360	THR	2.8
1	A	69	GLY	2.8
1	A	221	SER	2.7
1	A	303	ALA	2.7
1	A	392	MET	2.7
1	A	417	LEU	2.7
1	B	418	HIS	2.7
1	B	202	TYR	2.7
1	A	452	SER	2.5
1	B	158	PHE	2.5
1	A	236	GLU	2.5
1	A	61	GLY	2.5
1	A	213	CYS	2.4
1	A	406	LEU	2.4
1	A	103	GLU	2.4
1	B	384	TRP	2.4
1	A	36	GLU	2.3
1	A	17	ASP	2.3
1	A	28	ASP	2.3
1	A	15	PRO	2.3
1	A	403	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	197	ASP	2.3
1	B	342	ALA	2.3
1	A	30	SER	2.3
1	A	41	GLY	2.2
1	A	96	SER	2.2
1	B	405	LYS	2.2
1	B	284	LEU	2.2
1	B	403	LYS	2.1
1	B	106	ARG	2.1
1	A	383	ALA	2.1
1	B	220	ARG	2.1
1	B	217	HIS	2.1
1	B	223	ALA	2.1
1	A	419	ASP	2.1
1	B	139	ALA	2.1
1	A	141	TYR	2.0
1	B	414	ARG	2.0
1	A	35	HIS	2.0
1	A	60	ASP	2.0
1	A	301	GLU	2.0
1	A	283	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.