



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:52 AM GMT

PDB ID : 3NE5  
Title : Crystal structure of the CusBA heavy-metal efflux complex from Escherichia coli  
Authors : Su,C.-C.  
Deposited on : 2010-06-08  
Resolution : 2.90 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

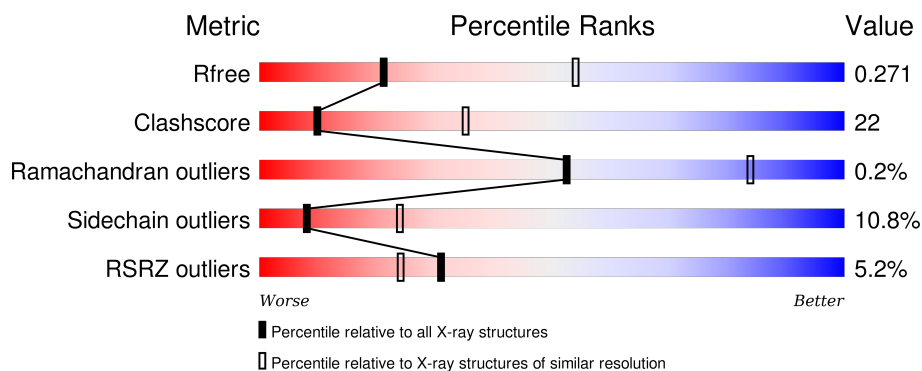
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	B	413	<div> <div>8%</div> <div>50%</div> <div>24%</div> <div>•</div> <div>22%</div> </div>
1	C	413	<div> <div>53%</div> <div>23%</div> <div>•</div> <div>22%</div> </div>
2	A	1054	<div> <div>8%</div> <div>53%</div> <div>38%</div> <div>6%</div> <div>•</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12873 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 Cation efflux system protein cusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
1	C	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239
C	408	HIS	-	EXPRESSION TAG	UNP P77239
C	409	HIS	-	EXPRESSION TAG	UNP P77239
C	410	HIS	-	EXPRESSION TAG	UNP P77239
C	411	HIS	-	EXPRESSION TAG	UNP P77239
C	412	HIS	-	EXPRESSION TAG	UNP P77239
C	413	HIS	-	EXPRESSION TAG	UNP P77239

- Molecule 2 is a protein called Cation efflux system protein cusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1028	Total	C	N	O	S	0	0	0
			7923	5124	1330	1433	36			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	EXPRESSION TAG	UNP P38054
A	-5	HIS	-	EXPRESSION TAG	UNP P38054

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P38054
A	-3	HIS	-	EXPRESSION TAG	UNP P38054
A	-2	HIS	-	EXPRESSION TAG	UNP P38054
A	-1	HIS	-	EXPRESSION TAG	UNP P38054
A	0	MET	-	EXPRESSION TAG	UNP P38054
A	1	GLY	-	EXPRESSION TAG	UNP P38054

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	O	0	0
			5	5		
3	C	10	Total	O	0	0
			10	10		
3	A	4	Total	O	0	0
			4	4		





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.27Å 160.27Å 682.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.49 – 2.90 39.50 – 2.90	Depositor EDS
% Data completeness (in resolution range)	78.9 (39.49-2.90) 88.6 (39.50-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.229 , 0.267 0.231 , 0.271	Depositor DCC
$R_{free}$ test set	3343 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 66889 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12873	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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	B	0.30	0/2498	0.49	1/3401 (0.0%)
1	C	0.23	0/2513	0.45	0/3421
2	A	0.24	0/8089	0.43	1/11015 (0.0%)
All	All	0.25	0/13100	0.44	2/17837 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	860	GLY	N-CA-C	-6.30	97.36	113.10
1	B	388	GLU	N-CA-C	5.96	127.08	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	B	2458	0	2522	99	0
1	C	2473	0	2533	75	0
2	A	7923	0	8166	427	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
All	All	12873	0	13221	577	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 22.

All (577) 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)
2:A:535:TRP:O	2:A:538:THR:HG22	1.53	1.09
1:B:280:LYS:HE3	1:B:281:TRP:H	1.17	1.06
2:A:459:LEU:HB3	2:A:882:ILE:HD11	1.38	1.05
2:A:588:MET:HE1	2:A:658:LEU:HD13	1.49	0.95
2:A:409:VAL:HB	2:A:450:LEU:HD11	1.49	0.94
2:A:964:PHE:CZ	2:A:1043:HIS:HB3	2.03	0.93
2:A:425:HIS:HB3	2:A:426:PRO:HD2	1.51	0.92
2:A:141:GLU:HG3	2:A:288:VAL:HG12	1.53	0.91
2:A:118:GLN:HE22	2:A:127:ALA:H	1.18	0.88
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.56	0.87
2:A:696:MET:HG3	2:A:854:THR:HG21	1.57	0.86
2:A:534:HIS:CD2	2:A:534:HIS:O	2.30	0.85
1:B:82:VAL:HG11	2:A:652:THR:HG23	1.56	0.84
1:B:280:LYS:HE3	1:B:281:TRP:N	1.92	0.83
2:A:493:ALA:HA	2:A:497:ILE:HB	1.58	0.83
2:A:660:ASN:ND2	2:A:660:ASN:H	1.75	0.83
2:A:534:HIS:O	2:A:535:TRP:C	2.15	0.81
2:A:534:HIS:HD2	2:A:534:HIS:O	1.62	0.81
2:A:534:HIS:C	2:A:534:HIS:CD2	2.53	0.81
1:C:254:ILE:HG22	1:C:257:LEU:HB2	1.64	0.79
2:A:364:LEU:O	2:A:368:ILE:HG12	1.82	0.79
1:B:174:THR:HB	1:B:177:GLN:HG3	1.64	0.79
1:C:271:ARG:HB3	1:C:274:LYS:HG3	1.65	0.79
2:A:574:PRO:HB2	2:A:658:LEU:HD11	1.63	0.78
2:A:68:PRO:O	2:A:72:THR:HG22	1.84	0.78
1:B:390:ASN:HD22	1:B:393:GLY:H	1.29	0.77
2:A:131:PRO:HD2	2:A:615:ALA:HB3	1.65	0.76
2:A:980:ARG:O	2:A:984:LYS:HB2	1.87	0.75
2:A:533:LEU:HA	2:A:536:PRO:HG3	1.68	0.75
2:A:964:PHE:HZ	2:A:1043:HIS:HB3	1.50	0.75
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.22	0.75
2:A:361:ARG:HB3	2:A:504:TRP:HB3	1.69	0.75
1:C:359:GLN:HG3	1:C:360:ALA:N	2.02	0.74
2:A:359:HIS:CE1	2:A:361:ARG:HB2	2.23	0.74
2:A:572:TYR:HB3	2:A:626:THR:HG23	1.70	0.74
1:C:302:ASN:HD21	1:C:307:LEU:H	1.36	0.74
1:C:242:ASP:HB3	1:C:243:PRO:HD3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:ALA:O	2:A:390:ILE:HG22	1.88	0.73
2:A:345:GLU:HG2	2:A:997:PRO:HG2	1.71	0.72
2:A:964:PHE:CE2	2:A:1043:HIS:HB3	2.24	0.72
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.70	0.72
2:A:457:ILE:HD11	2:A:936:VAL:HG22	1.70	0.72
2:A:214:ASN:H	2:A:215:GLN:NE2	1.87	0.72
2:A:878:MET:O	2:A:882:ILE:HG22	1.90	0.72
2:A:239:THR:HG22	2:A:241:ASP:H	1.54	0.71
2:A:43:SER:HB2	2:A:673:LEU:HD23	1.73	0.71
1:B:252:GLU:HG3	1:C:270:ALA:HB2	1.73	0.71
2:A:349:VAL:HG11	2:A:404:VAL:HG11	1.73	0.70
2:A:535:TRP:N	2:A:536:PRO:HD3	2.06	0.70
1:B:390:ASN:HD21	1:B:392:SER:HB2	1.57	0.70
2:A:960:ASN:HB2	2:A:961:PRO:HD3	1.74	0.69
1:B:219:THR:OG1	1:B:237:LYS:HD3	1.91	0.69
1:B:399:ARG:O	1:B:400:SER:HB2	1.93	0.69
2:A:535:TRP:N	2:A:536:PRO:CD	2.54	0.69
2:A:977:ALA:O	2:A:980:ARG:HG2	1.93	0.69
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.74	0.69
2:A:962:GLN:HG3	2:A:963:THR:N	2.07	0.69
2:A:85:PHE:HB2	2:A:92:TYR:HB2	1.75	0.69
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.75	0.69
1:C:359:GLN:HG3	1:C:360:ALA:H	1.57	0.68
2:A:641:THR:HG23	2:A:644:LYS:HD2	1.76	0.68
2:A:534:HIS:O	2:A:535:TRP:O	2.10	0.68
2:A:529:LEU:O	2:A:532:VAL:HG12	1.93	0.68
1:C:167:LEU:HD12	1:C:167:LEU:C	2.14	0.68
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.75	0.68
2:A:359:HIS:HE1	2:A:361:ARG:HE	1.42	0.68
2:A:454:LEU:O	2:A:458:THR:HG23	1.93	0.68
2:A:137:GLY:O	2:A:139:ILE:HG12	1.94	0.68
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.75	0.67
1:C:165:TYR:HE2	1:C:178:THR:HG23	1.59	0.67
1:C:106:PHE:HE2	1:C:359:GLN:HG2	1.59	0.67
2:A:574:PRO:HG2	2:A:624:VAL:HG13	1.77	0.67
1:B:123:ILE:HD13	1:B:237:LYS:HG3	1.76	0.67
1:C:353:LYS:HE2	1:C:375:GLU:OE2	1.95	0.67
2:A:684:LYS:HG2	2:A:823:TRP:CD1	2.30	0.66
2:A:453:SER:OG	2:A:939:GLU:HG2	1.95	0.66
2:A:546:SER:O	2:A:549:THR:HG22	1.96	0.66
2:A:534:HIS:HD2	2:A:535:TRP:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:955:VAL:HG12	2:A:956:PRO:HD3	1.75	0.66
2:A:604:ARG:HH21	2:A:604:ARG:CG	2.09	0.66
2:A:522:ILE:HG23	2:A:526:HIS:CD2	2.30	0.65
1:B:341:VAL:HG21	1:B:371:LEU:HD11	1.78	0.65
2:A:991:ILE:O	2:A:995:LEU:HB2	1.95	0.65
2:A:537:LYS:HD3	2:A:1037:LEU:HD11	1.77	0.65
2:A:370:LEU:HB2	2:A:371:PRO:HD3	1.77	0.65
2:A:526:HIS:HA	2:A:529:LEU:HB3	1.79	0.65
2:A:361:ARG:O	2:A:365:VAL:HG23	1.96	0.65
1:C:165:TYR:HB2	1:C:181:ILE:HG21	1.78	0.65
1:B:84:ILE:HG12	1:B:85:ASP:N	2.11	0.65
2:A:660:ASN:HD22	2:A:660:ASN:H	1.42	0.65
2:A:541:LEU:O	2:A:545:LEU:HD22	1.96	0.65
1:B:125:GLN:HE21	1:C:228:ASN:H	1.44	0.65
2:A:547:VAL:O	2:A:550:VAL:HG12	1.95	0.65
2:A:940:PHE:CE2	2:A:944:MET:HG3	2.32	0.65
2:A:572:TYR:HE1	2:A:660:ASN:HB3	1.62	0.65
2:A:136:VAL:HG22	2:A:669:ARG:HB3	1.78	0.65
2:A:620:PRO:HB2	2:A:622:GLU:HG2	1.78	0.64
1:C:384:LEU:HD21	2:A:588:MET:HE3	1.79	0.64
2:A:518:ASN:HD22	2:A:518:ASN:H	1.46	0.64
1:C:94:VAL:HG21	1:C:385:ILE:HD11	1.80	0.64
2:A:642:MET:HA	2:A:642:MET:HE3	1.80	0.64
2:A:26:TRP:HD1	2:A:379:ILE:HD13	1.63	0.63
2:A:377:ALA:O	2:A:381:MET:HG3	1.98	0.63
1:B:336:GLY:H	2:A:775:SER:HG	1.45	0.63
2:A:607:GLY:HA2	2:A:626:THR:HB	1.79	0.63
2:A:804:ILE:HG13	2:A:804:ILE:O	1.98	0.63
2:A:904:VAL:HG22	2:A:905:PRO:HD3	1.81	0.63
2:A:425:HIS:HB3	2:A:426:PRO:CD	2.25	0.63
1:B:385:ILE:HG13	2:A:272:ARG:HB2	1.80	0.63
1:B:174:THR:H	1:B:177:GLN:HE21	1.46	0.63
1:C:163:SER:HB3	1:C:204:ILE:HD11	1.79	0.62
2:A:940:PHE:HE1	2:A:984:LYS:HZ1	1.47	0.62
1:C:96:THR:OG1	1:C:376:LYS:HE3	1.98	0.62
2:A:370:LEU:HD22	2:A:400:VAL:HG23	1.81	0.62
2:A:42:LEU:H	2:A:42:LEU:HD12	1.63	0.62
2:A:891:PHE:CE1	2:A:945:LEU:HD12	2.35	0.62
2:A:436:TRP:C	2:A:436:TRP:CD1	2.73	0.62
1:B:117:ASN:HD22	1:B:119:TYR:H	1.46	0.62
2:A:422:GLN:HG2	2:A:427:ASP:OD1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:534:HIS:CD2	2:A:535:TRP:HB3	2.36	0.61
2:A:940:PHE:HE1	2:A:984:LYS:NZ	1.97	0.61
2:A:851:LYS:HB3	2:A:852:PRO:HD2	1.81	0.61
2:A:43:SER:HB2	2:A:673:LEU:CD2	2.31	0.61
1:B:384:LEU:HD23	1:B:394:ALA:HB3	1.83	0.61
2:A:707:VAL:HG21	2:A:840:LEU:HD23	1.82	0.61
2:A:991:ILE:HG21	2:A:1020:MET:SD	2.40	0.60
2:A:356:PHE:HD2	2:A:986:MET:HB3	1.65	0.60
2:A:534:HIS:HD2	2:A:534:HIS:C	2.01	0.60
1:B:387:SER:HB3	2:A:271:MET:HG3	1.83	0.60
2:A:580:ILE:HG22	2:A:622:GLU:HB2	1.84	0.60
2:A:780:PRO:O	2:A:804:ILE:HD11	2.01	0.60
1:B:336:GLY:N	2:A:775:SER:OG	2.34	0.60
1:B:117:ASN:ND2	1:B:119:TYR:H	1.99	0.60
2:A:394:GLY:O	2:A:398:ILE:HG22	2.02	0.60
2:A:897:ALA:O	2:A:901:ILE:HG22	2.02	0.60
2:A:72:THR:HG21	2:A:117:VAL:HG21	1.83	0.59
1:B:223:LEU:HD12	1:B:235:VAL:HG12	1.84	0.59
2:A:430:LEU:HB2	2:A:434:THR:HG21	1.84	0.59
1:B:342:ILE:HB	1:B:378:VAL:CG1	2.32	0.59
2:A:441:ASP:HA	2:A:444:VAL:HG23	1.83	0.59
2:A:122:PRO:HB2	2:A:125:VAL:HG13	1.83	0.59
2:A:449:ALA:O	2:A:453:SER:HB2	2.02	0.59
1:B:387:SER:HA	2:A:771:ARG:HH12	1.66	0.59
2:A:529:LEU:HD13	2:A:980:ARG:HH22	1.67	0.59
2:A:461:PHE:CZ	2:A:464:ILE:HD12	2.37	0.59
2:A:296:ASN:HB3	2:A:299:GLU:HB3	1.84	0.58
1:B:84:ILE:HD11	2:A:594:LYS:HD2	1.86	0.58
1:C:317:LEU:C	1:C:317:LEU:HD12	2.23	0.58
2:A:667:ARG:HH11	2:A:861:GLN:HE22	1.50	0.58
1:B:302:ASN:HD21	1:B:307:LEU:H	1.52	0.58
2:A:411:ILE:HA	2:A:501:MET:HE3	1.85	0.58
1:B:89:THR:H	2:A:590:GLN:HE22	1.51	0.58
2:A:893:ARG:HB3	2:A:896:GLU:HB3	1.84	0.58
1:B:340:ARG:HB3	1:B:353:LYS:O	2.04	0.58
1:B:343:THR:OG1	1:B:351:VAL:HG23	2.03	0.58
2:A:275:ILE:HB	2:A:609:THR:OG1	2.03	0.58
2:A:834:VAL:HG22	2:A:838:HIS:CD2	2.38	0.57
2:A:876:VAL:HB	2:A:877:PRO:HD3	1.86	0.57
2:A:940:PHE:CE2	2:A:1027:SER:HB2	2.39	0.57
2:A:212:ALA:C	2:A:215:GLN:HE22	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HB	1:C:227:MET:CG	2.35	0.57
1:B:388:GLU:HA	1:B:388:GLU:OE1	2.05	0.57
1:C:219:THR:OG1	1:C:237:LYS:HD2	2.04	0.57
2:A:746:PHE:O	2:A:750:ALA:HB3	2.05	0.57
2:A:189:VAL:HG22	2:A:265:VAL:HG22	1.87	0.57
2:A:391:MET:HG2	2:A:474:LEU:O	2.05	0.57
1:B:117:ASN:HD22	1:B:117:ASN:C	2.08	0.56
2:A:572:TYR:CE1	2:A:660:ASN:HB3	2.40	0.56
1:C:242:ASP:CB	1:C:243:PRO:HD3	2.35	0.56
1:B:125:GLN:NE2	1:C:228:ASN:H	2.03	0.56
1:B:387:SER:O	1:B:388:GLU:HB2	2.04	0.56
2:A:559:GLY:H	2:A:834:VAL:HG12	1.70	0.56
2:A:907:ALA:HB1	2:A:933:LEU:HD11	1.86	0.56
2:A:661:LEU:HD22	2:A:663:VAL:HG13	1.87	0.56
2:A:677:ILE:HG22	2:A:679:SER:H	1.70	0.56
2:A:837:VAL:HG21	2:A:862:PHE:CE2	2.40	0.56
2:A:984:LYS:HB3	2:A:984:LYS:NZ	2.20	0.56
1:C:242:ASP:O	1:C:302:ASN:HB3	2.06	0.56
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.06	0.56
1:B:268:VAL:CG2	1:B:271:ARG:HB2	2.36	0.56
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.34	0.56
2:A:553:PRO:HB2	2:A:912:ILE:CG2	2.36	0.56
2:A:928:THR:HG21	2:A:1012:ILE:HD11	1.86	0.56
1:B:244:VAL:HG12	1:B:300:VAL:HB	1.88	0.56
2:A:279:ASN:ND2	2:A:605:VAL:H	2.03	0.55
2:A:660:ASN:HD22	2:A:660:ASN:N	2.02	0.55
2:A:375:CYS:O	2:A:379:ILE:HG13	2.06	0.55
2:A:464:ILE:HD11	2:A:928:THR:HG23	1.89	0.55
2:A:139:ILE:HG22	2:A:301:ILE:HD11	1.87	0.55
1:B:137:PRO:O	1:B:138:LEU:HD12	2.06	0.55
2:A:578:PRO:HG2	2:A:717:ARG:HB2	1.89	0.55
2:A:950:HIS:HA	2:A:953:GLU:HB2	1.86	0.55
2:A:563:PRO:HG3	2:A:1011:ARG:HG2	1.89	0.55
2:A:1036:LYS:O	2:A:1040:LEU:HG	2.06	0.55
1:B:390:ASN:ND2	1:B:392:SER:HB2	2.21	0.55
1:B:387:SER:O	1:B:388:GLU:CB	2.50	0.55
1:B:121:TYR:OH	1:B:237:LYS:HE3	2.07	0.55
2:A:168:LEU:HB3	2:A:177:VAL:HG21	1.89	0.55
2:A:1026:LEU:O	2:A:1030:ILE:HG12	2.07	0.55
2:A:940:PHE:CE1	2:A:1024:PRO:HA	2.40	0.55
2:A:139:ILE:CG2	2:A:301:ILE:HD11	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LEU:O	1:C:317:LEU:HD12	2.07	0.55
2:A:837:VAL:HG21	2:A:862:PHE:CD2	2.41	0.55
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.89	0.54
2:A:596:ILE:HG12	2:A:653:VAL:HG21	1.89	0.54
2:A:85:PHE:HD1	2:A:812:MET:HE1	1.72	0.54
2:A:592:THR:O	2:A:596:ILE:HG13	2.06	0.54
2:A:1022:THR:O	2:A:1026:LEU:HB2	2.08	0.54
2:A:421:TRP:CE3	2:A:438:VAL:HB	2.42	0.54
2:A:246:ILE:HB	2:A:259:LEU:HB2	1.90	0.54
2:A:940:PHE:CE1	2:A:984:LYS:NZ	2.74	0.54
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.35	0.54
2:A:65:VAL:O	2:A:68:PRO:HG2	2.08	0.54
1:B:158:TRP:O	1:B:162:GLN:HG3	2.07	0.54
2:A:359:HIS:CE1	2:A:361:ARG:HE	2.25	0.54
2:A:327:ARG:O	2:A:331:ILE:HG12	2.08	0.54
2:A:696:MET:CE	2:A:850:LEU:HA	2.38	0.54
2:A:341:LYS:O	2:A:345:GLU:HG3	2.08	0.54
2:A:623:MET:HE3	2:A:625:GLU:HG3	1.90	0.54
2:A:356:PHE:HD2	2:A:986:MET:CB	2.21	0.54
2:A:536:PRO:HB3	2:A:1033:ALA:HB1	1.89	0.53
2:A:911:GLY:HA3	2:A:930:PHE:HE2	1.73	0.53
2:A:418:LEU:HD21	2:A:438:VAL:HG11	1.91	0.53
2:A:944:MET:SD	2:A:980:ARG:HD2	2.49	0.53
2:A:430:LEU:HB2	2:A:434:THR:CG2	2.38	0.53
1:B:267:THR:HG22	1:B:275:THR:HB	1.89	0.53
1:C:281:TRP:CB	1:C:298:LEU:HD23	2.38	0.53
2:A:689:VAL:HB	2:A:692:ASP:HB2	1.91	0.53
1:B:339:GLN:HG3	1:B:357:VAL:HG13	1.91	0.53
2:A:349:VAL:CG1	2:A:404:VAL:HG11	2.39	0.53
2:A:580:ILE:CG2	2:A:622:GLU:HB2	2.39	0.53
2:A:834:VAL:HG22	2:A:838:HIS:HD2	1.73	0.53
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.44	0.53
2:A:364:LEU:HD23	2:A:367:ILE:HD12	1.91	0.53
2:A:6:ILE:HD13	2:A:6:ILE:O	2.09	0.53
2:A:18:MET:HA	2:A:21:LEU:HB3	1.89	0.53
2:A:1001:GLY:HA2	2:A:1006:SER:HB2	1.91	0.53
2:A:977:ALA:HB1	2:A:980:ARG:NH2	2.24	0.53
1:C:327:ILE:HG13	1:C:328:PRO:O	2.08	0.53
2:A:482:LYS:O	2:A:486:MET:HG2	2.08	0.53
2:A:365:VAL:HG11	2:A:411:ILE:HD11	1.90	0.52
1:B:223:LEU:CD1	1:B:235:VAL:HG12	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:690:LEU:HD22	2:A:718:LEU:HD23	1.91	0.52
1:B:81:GLY:HA2	1:C:87:THR:HG21	1.91	0.52
2:A:307:LYS:O	2:A:311:LEU:HG	2.09	0.52
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.91	0.52
1:B:334:ASP:OD2	1:B:339:GLN:HB3	2.10	0.52
2:A:940:PHE:CD2	2:A:940:PHE:C	2.82	0.52
2:A:195:ARG:HD3	2:A:261:ASP:O	2.09	0.52
2:A:553:PRO:HB2	2:A:912:ILE:HG22	1.91	0.52
2:A:630:LEU:HD13	2:A:642:MET:HE1	1.92	0.52
2:A:270:GLU:HG2	2:A:271:MET:N	2.25	0.52
2:A:877:PRO:O	2:A:881:MET:HG2	2.10	0.52
2:A:973:LEU:O	2:A:977:ALA:HB2	2.10	0.52
2:A:345:GLU:O	2:A:349:VAL:HG23	2.10	0.52
2:A:168:LEU:CB	2:A:177:VAL:HG21	2.41	0.51
2:A:930:PHE:CE2	2:A:1015:PRO:HB3	2.45	0.51
1:B:280:LYS:HA	1:B:280:LYS:HE3	1.92	0.51
2:A:69:LEU:O	2:A:72:THR:HG23	2.09	0.51
2:A:933:LEU:HB2	2:A:1016:MET:HG2	1.92	0.51
2:A:552:TRP:HB3	2:A:553:PRO:HD3	1.91	0.51
2:A:842:LYS:O	2:A:846:GLU:HG2	2.11	0.51
2:A:239:THR:HG22	2:A:241:ASP:N	2.24	0.51
2:A:604:ARG:HG2	2:A:604:ARG:HH21	1.75	0.51
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.91	0.51
2:A:118:GLN:HE22	2:A:127:ALA:N	1.99	0.51
1:B:174:THR:H	1:B:177:GLN:NE2	2.08	0.51
2:A:216:GLU:HG3	2:A:236:TYR:CD1	2.45	0.51
2:A:406:ALA:HB2	2:A:454:LEU:HD11	1.93	0.51
2:A:291:LEU:HD21	2:A:295:LYS:O	2.11	0.51
1:C:183:GLU:O	1:C:187:LEU:HG	2.11	0.51
2:A:751:VAL:O	2:A:771:ARG:HD2	2.11	0.51
2:A:549:THR:HG23	2:A:913:TRP:HE1	1.77	0.50
2:A:668:ASN:O	2:A:672:MET:HG3	2.11	0.50
2:A:532:VAL:HG21	2:A:1029:PHE:HB3	1.92	0.50
1:B:387:SER:O	1:B:388:GLU:OE1	2.30	0.50
2:A:390:ILE:HD12	2:A:1005:GLY:HA3	1.94	0.50
2:A:522:ILE:HG23	2:A:526:HIS:NE2	2.27	0.50
1:B:390:ASN:HD21	1:B:392:SER:CB	2.23	0.50
2:A:906:PHE:CD1	2:A:1026:LEU:HD23	2.46	0.50
2:A:884:PHE:O	2:A:888:TYR:HB2	2.12	0.50
1:B:220:ALA:HB3	1:B:237:LYS:HB2	1.94	0.50
1:C:106:PHE:CZ	1:C:359:GLN:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:CD1	1:B:229:ILE:HB	2.42	0.50
2:A:986:MET:O	2:A:990:VAL:HG13	2.12	0.49
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.94	0.49
2:A:553:PRO:O	2:A:557:VAL:HG22	2.12	0.49
2:A:411:ILE:HG12	2:A:501:MET:HE3	1.93	0.49
1:B:342:ILE:O	1:B:378:VAL:HG12	2.12	0.49
2:A:107:ARG:NH1	2:A:130:GLY:O	2.46	0.49
2:A:529:LEU:HD22	2:A:980:ARG:NH2	2.27	0.49
2:A:420:GLU:HG3	2:A:421:TRP:N	2.27	0.49
2:A:574:PRO:HG2	2:A:624:VAL:CG1	2.43	0.49
1:B:242:ASP:O	1:B:302:ASN:HB3	2.12	0.49
2:A:525:TYR:HE2	2:A:1029:PHE:CZ	2.30	0.49
1:C:341:VAL:HG21	1:C:371:LEU:HD11	1.93	0.49
2:A:696:MET:HE1	2:A:850:LEU:HA	1.95	0.49
2:A:959:ASN:N	2:A:959:ASN:OD1	2.44	0.49
2:A:954:ALA:HB3	2:A:956:PRO:HD2	1.94	0.49
1:B:336:GLY:CA	2:A:775:SER:OG	2.61	0.49
2:A:678:LYS:HE2	2:A:825:TYR:CD2	2.48	0.49
2:A:969:LEU:HD12	2:A:969:LEU:C	2.33	0.49
1:B:385:ILE:CG1	2:A:272:ARG:H	2.25	0.49
2:A:456:ILE:HA	2:A:886:LEU:HD13	1.94	0.49
2:A:118:GLN:NE2	2:A:126:SER:HA	2.27	0.48
2:A:959:ASN:HA	2:A:962:GLN:HG2	1.95	0.48
2:A:16:VAL:HG11	2:A:495:VAL:O	2.14	0.48
2:A:536:PRO:O	2:A:539:THR:OG1	2.26	0.48
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.43	0.48
2:A:431:ASP:CG	2:A:432:ASN:H	2.17	0.48
2:A:461:PHE:CE2	2:A:932:ALA:HB2	2.49	0.48
2:A:188:GLN:HA	2:A:769:ASN:ND2	2.28	0.48
2:A:525:TYR:HE1	2:A:980:ARG:HE	1.60	0.48
1:B:280:LYS:CE	1:B:280:LYS:HA	2.43	0.48
2:A:642:MET:CE	2:A:642:MET:HA	2.44	0.48
2:A:466:THR:O	2:A:871:LYS:HE2	2.14	0.48
1:C:345:ASP:OD1	1:C:346:ALA:N	2.43	0.48
2:A:102:ASP:HB3	2:A:105:TRP:HB3	1.96	0.48
2:A:604:ARG:NH2	2:A:604:ARG:CG	2.70	0.48
1:B:360:ALA:HA	1:B:365:THR:HA	1.95	0.48
1:B:174:THR:HG22	1:B:176:THR:H	1.78	0.48
1:B:123:ILE:HB	1:C:227:MET:HG2	1.95	0.48
2:A:888:TYR:CE2	2:A:894:VAL:HG22	2.49	0.48
1:B:116:TYR:CE2	1:B:309:PRO:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:497:ILE:O	2:A:501:MET:HG2	2.13	0.48
1:C:165:TYR:CE2	1:C:178:THR:HG23	2.44	0.48
1:C:223:LEU:C	1:C:224:ARG:HD2	2.33	0.48
2:A:459:LEU:C	2:A:461:PHE:H	2.16	0.47
2:A:26:TRP:CD1	2:A:379:ILE:HD13	2.46	0.47
2:A:904:VAL:N	2:A:905:PRO:CD	2.77	0.47
2:A:769:ASN:ND2	2:A:769:ASN:C	2.68	0.47
2:A:172:PRO:O	2:A:173:ASP:HB2	2.14	0.47
1:C:166:LEU:O	1:C:170:GLU:HG2	2.14	0.47
2:A:984:LYS:CA	2:A:984:LYS:HE2	2.44	0.47
2:A:22:PHE:HA	2:A:25:ILE:HG22	1.95	0.47
2:A:868:ALA:O	2:A:872:LEU:HG	2.15	0.47
1:C:279:ARG:NH1	1:C:279:ARG:HB2	2.29	0.47
1:C:196:ARG:O	1:C:199:ILE:HG12	2.14	0.47
2:A:433:LYS:O	2:A:436:TRP:HB3	2.14	0.47
2:A:461:PHE:HE1	2:A:479:ALA:HA	1.79	0.47
2:A:6:ILE:HG13	2:A:443:SER:HB3	1.96	0.47
1:B:269:PRO:HD2	1:B:312:ASN:O	2.13	0.47
2:A:1009:MET:O	2:A:1012:ILE:HG22	2.14	0.47
2:A:957:SER:O	2:A:961:PRO:HD2	2.14	0.47
2:A:940:PHE:O	2:A:943:VAL:HG22	2.14	0.47
2:A:534:HIS:C	2:A:536:PRO:HD3	2.34	0.47
2:A:940:PHE:CZ	2:A:1024:PRO:HA	2.50	0.47
2:A:779:SER:H	2:A:782:ALA:HB3	1.79	0.47
1:B:384:LEU:N	1:B:384:LEU:HD12	2.29	0.47
1:B:223:LEU:C	1:B:224:ARG:HD2	2.35	0.47
1:B:351:VAL:HG23	1:B:351:VAL:O	2.14	0.47
2:A:689:VAL:O	2:A:693:ILE:HG23	2.15	0.47
2:A:5:ILE:HB	2:A:494:ILE:HD11	1.96	0.47
2:A:779:SER:HB2	2:A:780:PRO:HD2	1.97	0.47
1:C:281:TRP:HB2	1:C:298:LEU:HD23	1.97	0.47
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.96	0.47
1:C:151:LEU:HD12	1:C:151:LEU:C	2.35	0.47
1:B:265:THR:HB	1:B:316:GLN:HB3	1.96	0.47
2:A:397:ALA:O	2:A:400:VAL:HG12	2.14	0.47
2:A:550:VAL:HG21	2:A:909:VAL:HA	1.97	0.47
1:C:94:VAL:CG2	1:C:385:ILE:HD11	2.43	0.47
2:A:356:PHE:O	2:A:357:LEU:HD12	2.14	0.47
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.45	0.47
1:C:128:ALA:HA	1:C:231:LYS:HD3	1.97	0.47
1:B:153:LEU:HD11	1:B:155:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:596:ILE:HG21	2:A:628:ILE:HG12	1.95	0.47
2:A:955:VAL:N	2:A:956:PRO:CD	2.77	0.47
2:A:933:LEU:O	2:A:933:LEU:HD22	2.15	0.47
1:C:281:TRP:HB3	1:C:298:LEU:HD23	1.97	0.47
2:A:436:TRP:HD1	2:A:437:GLN:N	2.13	0.46
2:A:102:ASP:O	2:A:105:TRP:HB3	2.15	0.46
2:A:20:ALA:HA	2:A:23:LEU:HB3	1.97	0.46
2:A:844:ILE:HD12	2:A:858:PHE:HZ	1.80	0.46
1:C:269:PRO:HG3	1:C:314:TRP:NE1	2.30	0.46
2:A:900:ILE:O	2:A:903:SER:HB3	2.15	0.46
1:B:195:ILE:O	1:B:198:LEU:HB3	2.16	0.46
2:A:42:LEU:HD13	2:A:670:ILE:HD13	1.97	0.46
2:A:275:ILE:HD13	2:A:586:ALA:HB2	1.96	0.46
2:A:984:LYS:HE2	2:A:984:LYS:HA	1.97	0.46
1:C:383:PHE:CE1	2:A:580:ILE:HB	2.51	0.46
2:A:871:LYS:O	2:A:875:MET:HB2	2.15	0.46
2:A:995:LEU:O	2:A:1017:ILE:HD11	2.15	0.46
2:A:729:ASN:HD22	2:A:729:ASN:C	2.19	0.46
1:B:114:VAL:HG22	1:B:246:VAL:HG22	1.98	0.46
2:A:146:ASP:OD2	2:A:151:HIS:HD2	1.99	0.46
2:A:988:VAL:HG21	2:A:1024:PRO:HB3	1.97	0.46
2:A:518:ASN:ND2	2:A:518:ASN:H	2.13	0.46
2:A:572:TYR:HE1	2:A:660:ASN:CB	2.28	0.46
2:A:390:ILE:HD12	2:A:1005:GLY:CA	2.46	0.46
2:A:1020:MET:HA	2:A:1020:MET:CE	2.46	0.46
2:A:896:GLU:OE1	2:A:945:LEU:HG	2.15	0.46
2:A:270:GLU:HG2	2:A:271:MET:H	1.81	0.46
2:A:243:PHE:HB3	2:A:265:VAL:HG21	1.98	0.46
2:A:578:PRO:CG	2:A:717:ARG:HB2	2.45	0.46
2:A:769:ASN:C	2:A:769:ASN:HD22	2.18	0.46
2:A:831:ARG:NH2	2:A:839:ASP:OD1	2.43	0.46
2:A:977:ALA:HA	2:A:980:ARG:CZ	2.46	0.46
1:C:120:GLN:HE22	1:C:243:PRO:HD2	1.80	0.46
1:B:153:LEU:H	1:B:153:LEU:HD23	1.81	0.46
2:A:538:THR:O	2:A:542:VAL:HG23	2.16	0.45
2:A:947:TYR:OH	2:A:983:PRO:HG2	2.16	0.45
1:B:220:ALA:HB3	1:B:237:LYS:CB	2.46	0.45
2:A:338:LEU:HG	2:A:390:ILE:HA	1.98	0.45
1:B:336:GLY:HA3	2:A:775:SER:OG	2.16	0.45
2:A:952:ILE:HG21	2:A:1039:TRP:NE1	2.32	0.45
2:A:312:LYS:HD3	2:A:312:LYS:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:15:LEU:HA	2:A:15:LEU:HD23	1.80	0.45
2:A:370:LEU:CD2	2:A:403:MET:HG3	2.46	0.45
2:A:135:GLY:O	2:A:669:ARG:HG2	2.17	0.45
1:B:385:ILE:HG13	2:A:272:ARG:H	1.81	0.45
2:A:554:LEU:HD21	2:A:912:ILE:HG12	1.98	0.45
1:C:158:TRP:O	1:C:162:GLN:HG3	2.16	0.45
2:A:519:ARG:O	2:A:523:ARG:HG3	2.15	0.45
2:A:464:ILE:CD1	2:A:928:THR:HG23	2.47	0.45
1:C:264:PHE:HE1	1:C:281:TRP:CE2	2.35	0.45
2:A:563:PRO:HG2	2:A:1008:VAL:HA	1.98	0.45
2:A:693:ILE:HD11	2:A:718:LEU:HD22	1.99	0.45
2:A:402:ALA:HB3	2:A:486:MET:CE	2.47	0.45
2:A:729:ASN:HB3	2:A:732:LYS:HB2	1.99	0.45
2:A:984:LYS:CE	2:A:988:VAL:HG23	2.47	0.45
2:A:529:LEU:CD1	2:A:980:ARG:HH22	2.30	0.45
2:A:301:ILE:HD12	2:A:328:SER:HB3	1.99	0.45
2:A:406:ALA:CB	2:A:454:LEU:HD11	2.47	0.45
2:A:418:LEU:HA	2:A:438:VAL:HG21	1.99	0.45
2:A:564:GLN:NE2	2:A:664:PRO:HG2	2.32	0.45
2:A:237:LEU:HD12	2:A:242:ASP:HB3	1.98	0.45
2:A:532:VAL:HG23	2:A:539:THR:HG21	1.99	0.44
2:A:884:PHE:CD1	2:A:884:PHE:C	2.90	0.44
1:B:83:ARG:CZ	1:C:90:GLN:HB3	2.47	0.44
2:A:1029:PHE:N	2:A:1029:PHE:CD2	2.85	0.44
2:A:572:TYR:CD1	2:A:574:PRO:HD3	2.53	0.44
2:A:27:GLY:O	2:A:31:ILE:HG22	2.16	0.44
1:B:162:GLN:HB2	1:B:204:ILE:HG23	1.98	0.44
1:C:324:MET:HB2	1:C:366:ALA:HB1	1.99	0.44
1:B:281:TRP:HB2	1:B:296:LEU:HD21	1.99	0.44
1:B:399:ARG:O	1:B:400:SER:CB	2.64	0.44
2:A:619:ALA:HB1	2:A:623:MET:HE2	1.98	0.44
2:A:661:LEU:HD11	2:A:679:SER:HB3	1.98	0.44
2:A:445:GLU:O	2:A:448:PRO:HD2	2.17	0.44
1:B:278:ILE:HG21	1:B:298:LEU:HD13	1.99	0.44
2:A:725:ASN:O	2:A:804:ILE:HA	2.17	0.44
2:A:746:PHE:CZ	2:A:788:ILE:HG23	2.52	0.44
1:C:234:VAL:CG2	1:C:234:VAL:O	2.65	0.44
1:B:302:ASN:ND2	1:B:307:LEU:H	2.14	0.44
2:A:421:TRP:O	2:A:421:TRP:HD1	2.00	0.44
1:B:279:ARG:HB2	1:B:279:ARG:HE	1.59	0.44
1:C:302:ASN:ND2	1:C:307:LEU:H	2.10	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:619:ALA:HA	2:A:620:PRO:HD3	1.85	0.44
2:A:222:ILE:HD11	2:A:224:LEU:HD21	1.99	0.44
2:A:402:ALA:O	2:A:405:ASP:HB3	2.17	0.44
2:A:85:PHE:HD1	2:A:812:MET:CE	2.30	0.44
2:A:604:ARG:HB2	2:A:629:GLN:HE21	1.82	0.44
2:A:930:PHE:CD2	2:A:1015:PRO:HB3	2.53	0.44
1:B:292:ARG:HG3	1:C:312:ASN:HD21	1.83	0.44
2:A:940:PHE:CD1	2:A:984:LYS:HE3	2.53	0.43
1:B:256:TRP:HE1	1:B:359:GLN:NE2	2.17	0.43
2:A:315:LEU:HA	2:A:316:PRO:HD3	1.92	0.43
2:A:702:GLU:O	2:A:705:ARG:HG3	2.18	0.43
2:A:996:LEU:N	2:A:997:PRO:CD	2.81	0.43
1:C:197:ARG:HE	1:C:197:ARG:HB2	1.57	0.43
2:A:14:PHE:O	2:A:17:LEU:HB3	2.18	0.43
2:A:984:LYS:HB3	2:A:984:LYS:HZ3	1.83	0.43
2:A:836:VAL:O	2:A:840:LEU:HG	2.17	0.43
1:C:352:PRO:HB2	1:C:398:MET:SD	2.59	0.43
2:A:533:LEU:HD22	2:A:1036:LYS:HD3	2.01	0.43
2:A:961:PRO:HA	2:A:1043:HIS:HE1	1.83	0.43
2:A:28:THR:O	2:A:32:ILE:HG13	2.18	0.43
1:B:151:LEU:HD11	1:B:210:LEU:HD12	2.01	0.43
2:A:214:ASN:H	2:A:215:GLN:HE21	1.64	0.43
2:A:53:TYR:O	2:A:89:GLY:HA2	2.19	0.43
1:C:395:LEU:O	1:C:399:ARG:HG3	2.19	0.43
2:A:255:VAL:HA	2:A:256:PRO:HD3	1.83	0.43
2:A:518:ASN:O	2:A:521:LEU:HG	2.19	0.43
1:C:106:PHE:HE2	1:C:359:GLN:CG	2.29	0.43
1:B:123:ILE:CD1	1:B:237:LYS:HG3	2.45	0.43
2:A:701:GLU:O	2:A:705:ARG:HG2	2.18	0.43
2:A:927:GLY:O	2:A:931:ILE:HG12	2.18	0.43
2:A:400:VAL:HA	2:A:403:MET:CG	2.49	0.43
2:A:272:ARG:O	2:A:621:LEU:HD11	2.18	0.43
2:A:42:LEU:HD12	2:A:42:LEU:N	2.32	0.43
2:A:365:VAL:HG11	2:A:501:MET:HB3	2.01	0.43
2:A:418:LEU:CD2	2:A:438:VAL:HG11	2.49	0.43
1:B:278:ILE:HG13	1:B:298:LEU:HD13	2.01	0.43
1:B:280:LYS:CA	1:B:280:LYS:HE3	2.49	0.42
2:A:599:VAL:HA	2:A:600:PRO:HD3	1.83	0.42
1:B:128:ALA:HA	1:B:231:LYS:HD2	2.01	0.42
2:A:412:GLU:CD	2:A:982:ARG:HG2	2.39	0.42
2:A:570:LEU:HD23	2:A:628:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:599:VAL:HG21	2:A:649:LEU:CD1	2.48	0.42
2:A:739:THR:O	2:A:742:ASP:HB2	2.18	0.42
2:A:599:VAL:O	2:A:602:VAL:HG13	2.20	0.42
1:C:174:THR:HG22	1:C:176:THR:H	1.84	0.42
2:A:1021:ILE:O	2:A:1025:LEU:HB2	2.18	0.42
1:C:242:ASP:CB	1:C:243:PRO:CD	2.97	0.42
2:A:995:LEU:HD21	2:A:1016:MET:HE3	2.02	0.42
2:A:135:GLY:C	2:A:669:ARG:HG2	2.40	0.42
1:B:329:SER:HA	1:B:365:THR:HG23	2.01	0.42
2:A:982:ARG:HH21	2:A:982:ARG:HG3	1.85	0.42
2:A:353:CYS:O	2:A:357:LEU:HB2	2.19	0.42
2:A:115:ASN:C	2:A:115:ASN:ND2	2.73	0.42
2:A:980:ARG:O	2:A:983:PRO:HD2	2.20	0.42
2:A:37:ASP:HA	2:A:331:ILE:HD12	2.01	0.42
2:A:790:THR:OG1	2:A:794:GLN:HB2	2.20	0.42
2:A:518:ASN:OD1	2:A:982:ARG:NH2	2.52	0.42
2:A:525:TYR:CE1	2:A:980:ARG:NH2	2.87	0.42
2:A:975:HIS:C	2:A:977:ALA:H	2.23	0.42
1:C:360:ALA:HB2	1:C:365:THR:HB	2.02	0.42
2:A:771:ARG:HG3	2:A:772:TYR:N	2.35	0.42
2:A:21:LEU:O	2:A:21:LEU:HD22	2.20	0.42
1:C:341:VAL:HB	1:C:377:VAL:CG2	2.50	0.42
2:A:191:ILE:HG21	2:A:196:LEU:HD11	2.01	0.42
2:A:340:GLY:O	2:A:344:GLU:HG3	2.19	0.42
2:A:940:PHE:CZ	2:A:944:MET:HG3	2.54	0.42
2:A:455:LEU:HD13	2:A:459:LEU:HD13	2.01	0.42
2:A:338:LEU:HD21	2:A:390:ILE:HG13	2.01	0.42
2:A:436:TRP:CD1	2:A:437:GLN:N	2.88	0.42
1:C:342:ILE:O	1:C:378:VAL:HG12	2.19	0.42
2:A:191:ILE:HA	2:A:263:ALA:HB2	2.02	0.42
2:A:67:TYR:N	2:A:68:PRO:HD2	2.34	0.42
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.80	0.42
2:A:883:ILE:O	2:A:887:LEU:HG	2.19	0.42
1:C:134:LYS:HG3	1:C:135:VAL:N	2.34	0.42
2:A:365:VAL:CG1	2:A:411:ILE:HD11	2.50	0.42
2:A:715:ALA:HB2	2:A:824:ILE:HG23	2.02	0.41
2:A:412:GLU:OE1	2:A:983:PRO:HG3	2.20	0.41
2:A:932:ALA:O	2:A:936:VAL:HG23	2.20	0.41
2:A:660:ASN:ND2	2:A:660:ASN:N	2.46	0.41
1:B:302:ASN:HD21	1:B:306:ALA:N	2.18	0.41
2:A:705:ARG:NH1	2:A:713:ALA:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:984:LYS:CB	2:A:984:LYS:NZ	2.84	0.41
2:A:952:ILE:HG22	2:A:952:ILE:O	2.20	0.41
2:A:463:PRO:HG2	2:A:879:THR:OG1	2.19	0.41
1:C:88:GLN:HG2	2:A:654:ARG:O	2.20	0.41
2:A:707:VAL:HA	2:A:708:PRO:HD3	1.88	0.41
1:C:223:LEU:O	1:C:224:ARG:HD2	2.21	0.41
2:A:38:ALA:HB2	2:A:331:ILE:HD13	2.03	0.41
2:A:1035:TYR:O	2:A:1039:TRP:HB2	2.21	0.41
2:A:998:ILE:CD1	2:A:1013:ALA:HB2	2.51	0.41
1:C:284:LEU:HD12	1:C:295:GLN:HB2	2.03	0.41
2:A:425:HIS:CB	2:A:426:PRO:HD2	2.34	0.41
2:A:962:GLN:CG	2:A:963:THR:N	2.81	0.41
1:C:161:ALA:HB3	1:C:185:LEU:HD11	2.01	0.41
2:A:636:TRP:CD1	2:A:636:TRP:N	2.89	0.41
2:A:439:ILE:HG23	2:A:501:MET:HE2	2.03	0.41
2:A:390:ILE:HD11	2:A:1008:VAL:CG1	2.50	0.41
2:A:700:ILE:HA	2:A:703:VAL:HG22	2.03	0.41
2:A:984:LYS:CE	2:A:984:LYS:CA	2.99	0.41
2:A:526:HIS:N	2:A:527:PRO:CD	2.84	0.41
2:A:569:ASP:OD2	2:A:629:GLN:HG2	2.20	0.41
2:A:27:GLY:HA3	2:A:375:CYS:HB3	2.02	0.41
1:B:124:VAL:HB	1:B:235:VAL:HG22	2.03	0.41
2:A:530:LEU:HD12	2:A:530:LEU:C	2.41	0.41
2:A:786:LEU:HB3	2:A:798:LEU:HB2	2.02	0.41
2:A:114:LEU:HA	2:A:114:LEU:HD12	1.86	0.41
1:B:335:THR:HG22	1:B:391:ILE:HD12	2.02	0.41
2:A:975:HIS:HA	2:A:978:VAL:HG12	2.03	0.41
2:A:411:ILE:HA	2:A:501:MET:CE	2.49	0.41
1:C:257:LEU:HD12	1:C:257:LEU:HA	1.92	0.41
2:A:403:MET:H	2:A:403:MET:HG2	1.52	0.41
2:A:141:GLU:HB3	2:A:325:TYR:HB3	2.01	0.40
1:B:242:ASP:O	1:B:302:ASN:N	2.54	0.40
2:A:497:ILE:HB	2:A:498:PRO:HD3	2.03	0.40
2:A:589:LEU:HD22	2:A:609:THR:HG23	2.03	0.40
1:C:219:THR:HG21	1:C:239:GLN:OE1	2.21	0.40
2:A:914:LEU:HD23	2:A:1014:ALA:O	2.20	0.40
2:A:376:ILE:HG21	2:A:488:GLY:HA3	2.03	0.40
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.80	0.40
2:A:637:ARG:HH11	2:A:637:ARG:HB2	1.86	0.40
1:B:350:PHE:HB3	1:B:398:MET:HE3	2.03	0.40
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:ALA:O	2:A:390:ILE:CG2	2.66	0.40
2:A:608:LYS:HE2	2:A:625:GLU:HB2	2.02	0.40
2:A:1028:LEU:O	2:A:1032:PRO:HG2	2.22	0.40
2:A:898:LEU:O	2:A:898:LEU:HD23	2.21	0.40
2:A:554:LEU:HD23	2:A:912:ILE:HG21	2.03	0.40
1:C:174:THR:H	1:C:177:GLN:HE21	1.68	0.40
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.38	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	B	320/413 (78%)	304 (95%)	15 (5%)	1 (0%)	46	79
1	C	322/413 (78%)	312 (97%)	9 (3%)	1 (0%)	46	79
2	A	1024/1054 (97%)	969 (95%)	54 (5%)	1 (0%)	56	87
All	All	1666/1880 (89%)	1585 (95%)	78 (5%)	3 (0%)	52	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	852	PRO
1	C	137	PRO
1	B	137	PRO

### 5.3.2 Protein sidechains [i](#)

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	B	263/338 (78%)	229 (87%)	34 (13%)	5	16
1	C	265/338 (78%)	237 (89%)	28 (11%)	8	25
2	A	847/871 (97%)	761 (90%)	86 (10%)	9	27
All	All	1375/1547 (89%)	1227 (89%)	148 (11%)	8	24

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ILE
1	B	105	THR
1	B	117	ASN
1	B	121	TYR
1	B	134	LYS
1	B	140	VAL
1	B	159	VAL
1	B	182	LEU
1	B	185	LEU
1	B	199	ILE
1	B	203	LYS
1	B	207	ARG
1	B	234	VAL
1	B	235	VAL
1	B	241	MET
1	B	244	VAL
1	B	252	GLU
1	B	268	VAL
1	B	275	THR
1	B	280	LYS
1	B	282	THR
1	B	298	LEU
1	B	299	GLU
1	B	322	GLU
1	B	330	GLN
1	B	340	ARG
1	B	349	ARG
1	B	364	VAL
1	B	365	THR
1	B	367	LEU
1	B	379	SER

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Mol	Chain	Res	Type
1	B	385	ILE
1	B	388	GLU
1	B	396	GLU
1	C	96	THR
1	C	98	THR
1	C	104	LEU
1	C	105	THR
1	C	121	TYR
1	C	138	LEU
1	C	140	VAL
1	C	150	LEU
1	C	167	LEU
1	C	182	LEU
1	C	185	LEU
1	C	206	THR
1	C	235	VAL
1	C	258	VAL
1	C	276	LEU
1	C	283	LEU
1	C	292	ARG
1	C	317	LEU
1	C	330	GLN
1	C	339	GLN
1	C	343	THR
1	C	351	VAL
1	C	354	ARG
1	C	364	VAL
1	C	365	THR
1	C	373	GLU
1	C	377	VAL
1	C	378	VAL
2	A	6	ILE
2	A	8	ARG
2	A	12	ASN
2	A	18	MET
2	A	21	LEU
2	A	37	ASP
2	A	42	LEU
2	A	59	GLN
2	A	69	LEU
2	A	72	THR
2	A	109	ARG

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Mol	Chain	Res	Type
2	A	115	ASN
2	A	117	VAL
2	A	125	VAL
2	A	144	LEU
2	A	145	VAL
2	A	157	ARG
2	A	168	LEU
2	A	188	GLN
2	A	190	VAL
2	A	203	LEU
2	A	210	LEU
2	A	211	ASP
2	A	215	GLN
2	A	222	ILE
2	A	259	LEU
2	A	273	ARG
2	A	298	ARG
2	A	322	VAL
2	A	358	TRP
2	A	390	ILE
2	A	398	ILE
2	A	403	MET
2	A	412	GLU
2	A	432	ASN
2	A	434	THR
2	A	436	TRP
2	A	445	GLU
2	A	455	LEU
2	A	464	ILE
2	A	492	LEU
2	A	521	LEU
2	A	531	LYS
2	A	532	VAL
2	A	534	HIS
2	A	545	LEU
2	A	548	LEU
2	A	549	THR
2	A	554	LEU
2	A	569	ASP
2	A	592	THR
2	A	602	VAL
2	A	624	VAL

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Mol	Chain	Res	Type
2	A	626	THR
2	A	634	GLU
2	A	637	ARG
2	A	641	THR
2	A	642	MET
2	A	643	ASP
2	A	649	LEU
2	A	660	ASN
2	A	661	LEU
2	A	693	ILE
2	A	705	ARG
2	A	729	ASN
2	A	769	ASN
2	A	775	SER
2	A	781	GLN
2	A	783	LEU
2	A	789	LEU
2	A	812	MET
2	A	813	LEU
2	A	815	THR
2	A	879	THR
2	A	882	ILE
2	A	884	PHE
2	A	901	ILE
2	A	904	VAL
2	A	945	LEU
2	A	946	MET
2	A	959	ASN
2	A	969	LEU
2	A	984	LYS
2	A	1020	MET
2	A	1026	LEU
2	A	1039	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	125	GLN
1	B	177	GLN
1	B	295	GLN
1	B	302	ASN

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Mol	Chain	Res	Type
1	B	359	GLN
1	B	390	ASN
1	C	120	GLN
1	C	125	GLN
1	C	177	GLN
1	C	295	GLN
1	C	302	ASN
2	A	115	ASN
2	A	118	GLN
2	A	151	HIS
2	A	194	GLN
2	A	215	GLN
2	A	238	GLN
2	A	279	ASN
2	A	329	GLN
2	A	337	ASN
2	A	359	HIS
2	A	423	HIS
2	A	432	ASN
2	A	470	GLN
2	A	526	HIS
2	A	534	HIS
2	A	564	GLN
2	A	629	GLN
2	A	633	GLN
2	A	651	ASN
2	A	660	ASN
2	A	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
2	A	838	HIS
2	A	869	ASN
2	A	1043	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	322/413 (77%)	-0.28	6 (1%) 70 66	20, 42, 81, 134	0
1	C	324/413 (78%)	-0.37	0 100 100	20, 43, 81, 131	0
2	A	1028/1054 (97%)	0.11	81 (7%) 15 10	20, 67, 181, 263	0
All	All	1674/1880 (89%)	-0.06	87 (5%) 31 24	20, 54, 155, 263	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	428	ALA	8.3
2	A	7	ARG	7.4
2	A	429	THR	7.2
2	A	427	ASP	6.6
2	A	520	PHE	6.4
2	A	530	LEU	5.6
2	A	421	TRP	5.2
1	B	79	ALA	4.8
2	A	960	ASN	4.6
2	A	430	LEU	4.6
2	A	426	PRO	4.6
2	A	1036	LYS	4.5
2	A	1037	LEU	4.4
2	A	405	ASP	4.3
2	A	29	TRP	4.1
2	A	418	LEU	4.1
2	A	964	PHE	4.1
2	A	1038	MET	4.0
1	B	386	ASP	3.9
2	A	424	GLN	3.8
2	A	432	ASN	3.8
2	A	504	TRP	3.8
2	A	958	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	444	VAL	3.6
2	A	425	HIS	3.6
2	A	873	LYS	3.6
2	A	896	GLU	3.6
2	A	519	ARG	3.6
2	A	528	LEU	3.5
2	A	1001	GLY	3.4
2	A	422	GLN	3.3
2	A	435	ARG	3.3
2	A	889	LEU	3.3
2	A	436	TRP	3.2
2	A	971	GLU	3.2
1	B	80	SER	3.2
2	A	433	LYS	3.1
2	A	523	ARG	3.0
2	A	970	ASP	3.0
2	A	538	THR	3.0
2	A	26	TRP	3.0
2	A	1039	TRP	3.0
1	B	388	GLU	3.0
1	B	387	SER	2.9
2	A	874	LEU	2.9
2	A	14	PHE	2.8
2	A	15	LEU	2.8
2	A	17	LEU	2.8
2	A	895	GLY	2.7
2	A	437	GLN	2.7
2	A	524	VAL	2.7
2	A	431	ASP	2.7
2	A	954	ALA	2.7
2	A	434	THR	2.7
2	A	962	GLN	2.6
2	A	423	HIS	2.6
2	A	401	GLY	2.6
1	B	242	ASP	2.6
2	A	406	ALA	2.5
2	A	888	TYR	2.5
2	A	33	ASN	2.5
2	A	10	VAL	2.5
2	A	955	VAL	2.5
2	A	974	TYR	2.4
2	A	462	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	966	GLU	2.4
2	A	1041	HIS	2.4
2	A	30	THR	2.3
2	A	358	TRP	2.3
2	A	521	LEU	2.3
2	A	32	ILE	2.3
2	A	383	PHE	2.3
2	A	409	VAL	2.3
2	A	495	VAL	2.3
2	A	527	PRO	2.3
2	A	446	VAL	2.2
2	A	556	LYS	2.2
2	A	956	PRO	2.2
2	A	407	ALA	2.2
2	A	13	ARG	2.1
2	A	975	HIS	2.1
2	A	12	ASN	2.1
2	A	1035	TYR	2.1
2	A	552	TRP	2.1
2	A	980	ARG	2.1
2	A	1040	LEU	2.0
2	A	1002	THR	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.