



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 AM GMT

PDB ID : 2XPI  
Title : Crystal structure of APC/C hetero-tetramer Cut9-Hcn1  
Authors : Zhang, Z.; Kulkarni, K.A.; Barford, D.  
Deposited on : 2010-08-26  
Resolution : 2.60 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

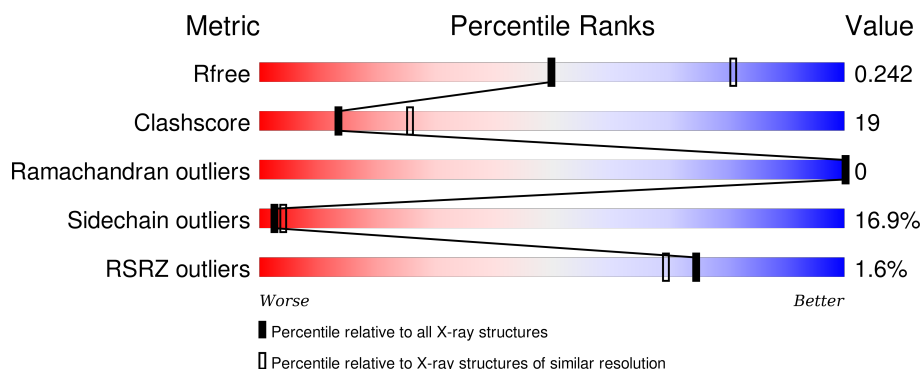
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	597	<div> <div></div> <div>52% 26% 8% 13%</div> </div>
1	D	597	<div> <div>2%</div> <div>54% 27% 5% 13%</div> </div>
2	B	81	<div> <div></div> <div>20% 7% • 70%</div> </div>
2	E	81	<div> <div></div> <div>15% 12% • 70%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8679 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 ANAPHASE-PROMOTING COMPLEX SUBUNIT CUT9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	21	0	0
			4140	2650	691	776	23			
1	D	518	Total	C	N	O	S	64	0	0
			4134	2648	693	771	22			

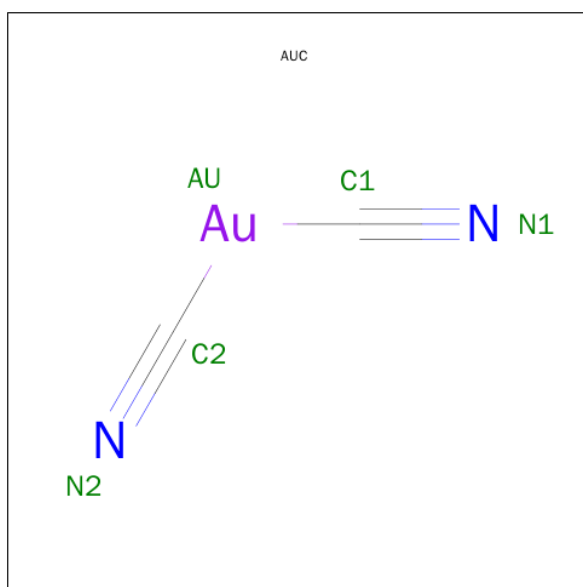
- Molecule 2 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT HCN1 HCN1/CDC26,20S CYCLOSOME/APC COMPLEX PROTEIN HCN1, CHAPERONE-LIKE PROTEIN HCN1, HIGH COPY SUPPRESSOR OF CUT9 PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	S	0	0	0
			176	111	31	33	1			
2	E	24	Total	C	N	O	S	0	0	0
			176	111	31	33	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ACE	-	EXPRESSION TAG	UNP O13916
E	1	ACE	-	EXPRESSION TAG	UNP O13916

- Molecule 3 is GOLD (I) CYANIDE ION (three-letter code: AUC) (formula: C<sub>2</sub>AuN<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Au 1 1	0	0
3	A	1	Total Au 1 1	0	0
3	D	1	Total Au 1 1	0	0
3	D	1	Total Au 1 1	0	0

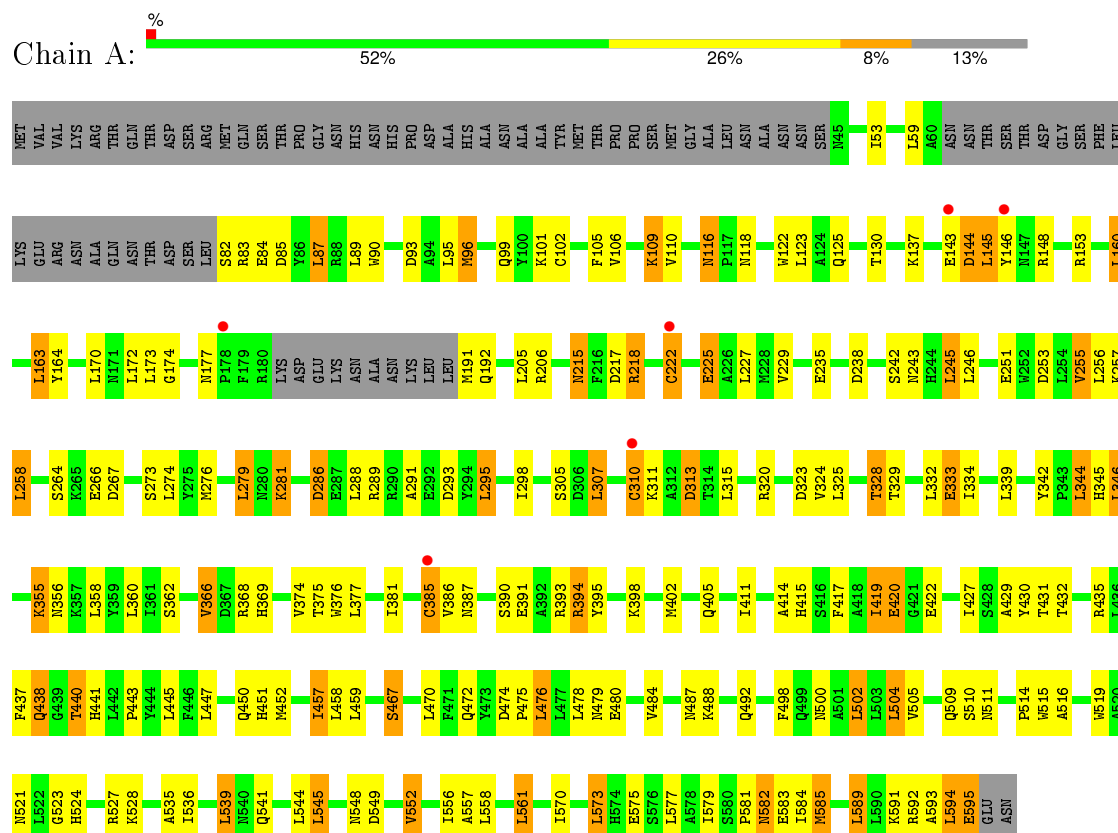
- Molecule 4 is water.

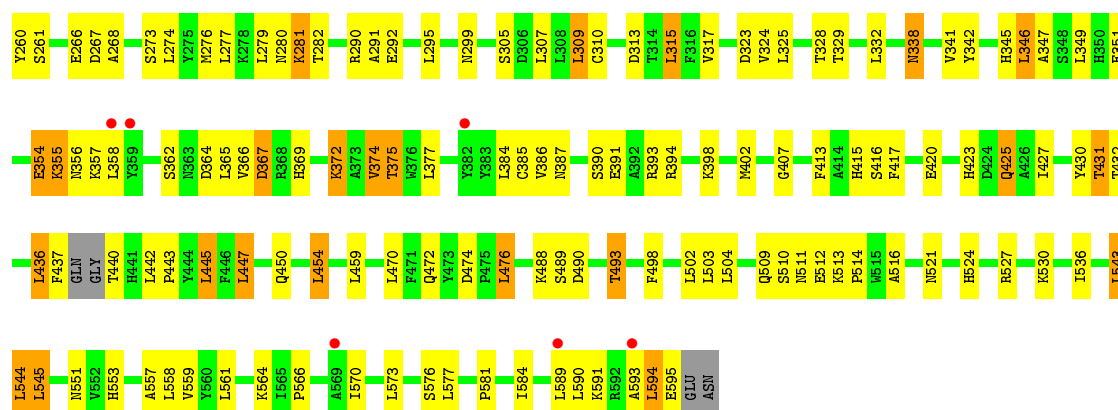
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	2	Total O 2 2	0	0
4	D	18	Total O 18 18	0	0

### 3 Residue-property plots

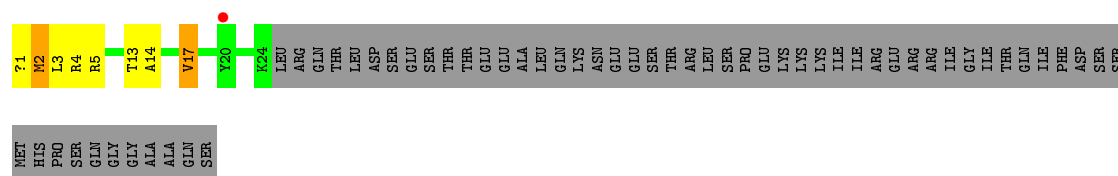
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ANAPHASE-PROMOTING COMPLEX SUBUNIT CUT9





- Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT HCN1 HCN1/CDC26,20S CYCLOSOME/APC COMPLEX PROTEIN HCN1, CHAPERONE-LIKE PROTEIN HCN1, HIGH COPY SUPPRESSOR OF CUT9 PROTEIN 1



- Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT HCN1 HCN1/CDC26,20S CYCLOSOME/APC COMPLEX PROTEIN HCN1, CHAPERONE-LIKE PROTEIN HCN1, HIGH COPY SUPPRESSOR OF CUT9 PROTEIN 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.40Å 151.92Å 91.87Å 90.00° 90.84° 90.00°	Depositor
Resolution (Å)	54.39 – 2.60 54.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (54.39-2.60) 99.1 (54.39-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.189 , 0.245 0.189 , 0.242	Depositor DCC
$R_{free}$ test set	1577 reflections (3.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.8	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 45388 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

Bond lengths and bond angles in the following residue types are not validated in this section: AUC, ACE

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	0.54	3/4230 (0.1%)	0.64	1/5739 (0.0%)
1	D	0.47	1/4223 (0.0%)	0.59	1/5727 (0.0%)
2	B	0.49	0/175	0.77	0/238
2	E	0.43	0/175	0.68	0/238
All	All	0.50	4/8803 (0.0%)	0.62	2/11942 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	CYS	CB-SG	13.42	2.05	1.82
1	D	222	CYS	CB-SG	11.92	2.02	1.82
1	A	385	CYS	CB-SG	7.13	1.94	1.82
1	A	310	CYS	CB-SG	6.83	1.93	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	CYS	CB-CA-C	6.64	123.68	110.40
1	D	377	LEU	CA-CB-CG	6.28	129.75	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4140	0	4063	177	0
1	D	4134	0	4077	158	0
2	B	176	0	172	15	0
2	E	176	0	172	10	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	29	0	0	0	0
4	B	2	0	0	0	0
4	D	18	0	0	0	0
All	All	8679	0	8484	316	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 19.

All (316) 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:222:CYS:CB	1:D:222:CYS:SG	2.02	1.45
1:A:222:CYS:CB	1:A:222:CYS:SG	2.05	1.41
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.09	1.07
1:A:385:CYS:SG	1:A:385:CYS:O	2.19	1.00
1:D:385:CYS:SG	1:D:385:CYS:O	2.21	0.97
1:D:45:ASN:N	1:D:45:ASN:HD22	1.67	0.92
1:D:354:GLU:HG2	1:D:357:LYS:HG3	1.52	0.91
1:D:415:HIS:HD2	1:D:430:TYR:OH	1.52	0.90
1:D:96:MET:HE2	1:D:96:MET:HA	1.57	0.86
1:D:323:ASP:H	1:D:509:GLN:HE22	1.20	0.86
1:A:328:THR:HG23	1:A:345:HIS:CD2	2.12	0.85
1:A:53:ILE:HG22	1:A:122:TRP:HE1	1.42	0.84
1:A:328:THR:CG2	1:A:345:HIS:HD2	1.88	0.84
1:A:276:MET:HA	1:A:279:LEU:HD22	1.60	0.83
1:D:524:HIS:HD2	1:D:527:ARG:HH21	1.27	0.82
1:D:328:THR:CG2	1:D:345:HIS:HD2	1.95	0.79
1:A:437:PHE:O	1:A:440:THR:HG23	1.83	0.79
1:D:527:ARG:HG3	1:D:559:VAL:HG22	1.65	0.77
1:A:394:ARG:NH1	1:A:394:ARG:HG3	1.84	0.76
1:D:259:ASN:HD21	1:D:261:SER:HB3	1.51	0.75
1:D:415:HIS:CD2	1:D:430:TYR:OH	2.39	0.75
1:A:362:SER:O	1:A:366:VAL:HG13	1.87	0.75
1:D:524:HIS:CD2	1:D:527:ARG:HH21	2.05	0.75
1:A:96:MET:HB3	1:D:50:THR:HG21	1.68	0.75
1:D:427:ILE:O	1:D:431:THR:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:SER:HB3	1:A:85:ASP:HB2	1.70	0.74
1:A:328:THR:HG23	1:A:345:HIS:HD2	1.45	0.74
1:D:369:HIS:O	1:D:375:THR:HG21	1.87	0.74
1:D:365:LEU:HB3	1:D:375:THR:HB	1.69	0.74
1:A:116:ASN:HD22	1:A:118:ASN:H	1.36	0.74
1:A:143:GLU:HB3	1:A:145:LEU:HD22	1.69	0.73
1:A:323:ASP:H	1:A:509:GLN:HE22	1.36	0.73
1:A:174:GLY:O	1:A:206:ARG:HD3	1.87	0.73
1:A:415:HIS:HD2	1:A:430:TYR:OH	1.72	0.72
1:A:398:LYS:HE3	1:A:402:MET:HE1	1.70	0.72
1:A:594:LEU:HD22	1:A:595:GLU:OE2	1.89	0.72
1:D:490:ASP:HB3	1:D:493:THR:HG23	1.69	0.72
1:D:325:LEU:HA	1:D:328:THR:HG22	1.72	0.71
1:A:96:MET:HA	1:A:96:MET:HE2	1.74	0.70
1:A:53:ILE:HG22	1:A:53:ILE:O	1.92	0.70
1:A:376:TRP:CD1	1:A:402:MET:HE1	2.27	0.70
1:A:191:MET:HG2	1:A:192:GLN:H	1.55	0.70
2:B:14:ALA:O	2:B:17:VAL:HG13	1.92	0.69
1:D:328:THR:HG23	1:D:345:HIS:HD2	1.56	0.69
1:D:407:GLY:HA2	1:D:436:LEU:HD12	1.74	0.69
1:D:553:HIS:HB2	1:D:576:SER:HB3	1.74	0.69
1:A:549:ASP:HB3	1:A:552:VAL:HG13	1.75	0.68
1:A:478:LEU:HD12	1:A:504:LEU:HD23	1.75	0.68
1:A:457:ILE:HD12	1:A:457:ILE:H	1.59	0.68
1:A:376:TRP:CD1	1:A:402:MET:CE	2.76	0.67
1:D:281:LYS:HD3	1:D:313:ASP:HB3	1.76	0.67
1:A:476:LEU:O	1:A:480:GLU:HG2	1.95	0.66
1:A:585:MET:HE1	2:B:13:THR:C	2.15	0.66
1:A:438:GLN:HA	1:A:438:GLN:HE21	1.61	0.66
1:A:101:LYS:HB2	1:D:235:GLU:OE2	1.96	0.65
1:A:398:LYS:HG2	1:A:402:MET:HE2	1.78	0.65
1:D:220:LYS:HE2	1:D:246:LEU:HD23	1.77	0.65
1:A:328:THR:CG2	1:A:345:HIS:CD2	2.74	0.65
1:A:116:ASN:ND2	1:A:118:ASN:H	1.94	0.65
1:D:430:TYR:HB3	1:D:447:LEU:HD22	1.78	0.65
1:D:573:LEU:HD13	1:D:590:LEU:HA	1.78	0.65
2:E:13:THR:O	2:E:16:ASP:HB2	1.96	0.64
1:A:475:PRO:HB2	1:A:515:TRP:CH2	2.32	0.64
1:D:328:THR:CG2	1:D:345:HIS:CD2	2.81	0.64
1:A:594:LEU:H	1:A:594:LEU:HD13	1.63	0.64
1:A:344:LEU:HD13	2:B:1:ACE:CH3	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:MET:CB	1:D:50:THR:HG21	2.29	0.63
1:D:325:LEU:HA	1:D:328:THR:CG2	2.29	0.63
1:A:355:LYS:HG2	1:A:385:CYS:SG	2.38	0.63
1:A:267:ASP:OD1	1:D:83:ARG:HD3	1.99	0.63
1:D:354:GLU:CG	1:D:357:LYS:HG3	2.28	0.63
1:A:276:MET:CE	1:A:291:ALA:HB2	2.29	0.63
1:D:415:HIS:HE1	2:E:3:LEU:O	1.81	0.62
1:D:436:LEU:O	1:D:437:PHE:HB2	1.98	0.62
1:A:320:ARG:C	1:A:509:GLN:HE21	2.03	0.62
1:A:87:LEU:HB3	1:A:110:VAL:HG22	1.82	0.62
1:D:328:THR:HG23	1:D:329:THR:N	2.15	0.62
1:A:368:ARG:HG3	1:A:369:HIS:CD2	2.35	0.61
1:D:440:THR:HG22	1:D:442:LEU:H	1.66	0.61
1:D:328:THR:HG23	1:D:345:HIS:CD2	2.36	0.61
1:A:443:PRO:HD3	2:B:2:MET:HE1	1.83	0.61
1:D:543:LEU:HD12	1:D:544:LEU:N	2.16	0.60
1:A:478:LEU:CD1	1:A:504:LEU:HD23	2.31	0.60
1:A:479:ASN:HD21	1:A:521:ASN:HD22	1.50	0.60
1:A:438:GLN:HA	1:A:438:GLN:NE2	2.16	0.60
1:D:177:ASN:HD22	1:D:178:PRO:CD	2.15	0.59
1:A:405:GLN:NE2	1:A:435:ARG:HH12	2.00	0.59
1:D:247:THR:HB	1:D:250:GLU:H	1.67	0.59
1:D:593:ALA:O	1:D:595:GLU:HG2	2.03	0.58
1:A:96:MET:HG2	1:D:50:THR:HG21	1.85	0.58
1:D:551:ASN:HD21	2:E:12:ILE:H	1.50	0.58
1:D:450:GLN:NE2	2:E:5:ARG:HH12	2.01	0.58
1:A:325:LEU:HA	1:A:328:THR:HG22	1.85	0.58
1:D:177:ASN:ND2	1:D:179:PHE:H	2.03	0.57
1:A:519:TRP:CE2	1:A:541:GLN:HG2	2.38	0.57
1:A:243:ASN:HA	1:A:405:GLN:HG2	1.86	0.57
1:A:116:ASN:HD22	1:A:118:ASN:N	2.01	0.57
1:A:235:GLU:CG	1:D:99:GLN:HB3	2.34	0.56
1:A:591:LYS:O	1:A:594:LEU:HD12	2.05	0.56
1:A:99:GLN:HB3	1:D:235:GLU:CG	2.36	0.56
1:A:344:LEU:HD13	2:B:1:ACE:H1	1.87	0.56
1:A:441:HIS:O	1:A:467:SER:HB3	2.06	0.56
1:D:391:GLU:O	1:D:394:ARG:HB3	2.07	0.55
1:A:191:MET:HG2	1:A:192:GLN:N	2.22	0.55
1:A:130:THR:O	1:A:130:THR:HG22	2.06	0.55
1:D:240:LEU:HD23	1:D:245:LEU:HD23	1.87	0.55
1:D:45:ASN:N	1:D:45:ASN:ND2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:O	1:A:110:VAL:HG23	2.07	0.55
1:D:84:GLU:O	1:D:88:ARG:HG3	2.06	0.55
1:D:170:LEU:HD13	1:D:175:GLU:HG2	1.88	0.54
1:A:398:LYS:HG2	1:A:402:MET:CE	2.37	0.54
1:D:239:GLN:O	1:D:243:ASN:HB2	2.08	0.54
1:A:143:GLU:O	1:A:144:ASP:OD1	2.26	0.54
1:A:516:ALA:HB2	1:A:545:LEU:HB2	1.90	0.54
1:D:315:LEU:HB3	1:D:324:VAL:HG23	1.88	0.54
1:D:276:MET:HE3	1:D:291:ALA:HB2	1.90	0.53
1:D:248:ALA:HB1	1:D:280:ASN:ND2	2.23	0.53
1:A:427:ILE:O	1:A:431:THR:HG23	2.08	0.53
1:A:235:GLU:OE2	1:D:101:LYS:N	2.41	0.53
1:D:474:ASP:OD2	2:E:4:ARG:NH2	2.40	0.53
1:A:267:ASP:OD2	1:D:83:ARG:NH1	2.42	0.53
1:D:177:ASN:HD22	1:D:178:PRO:HD2	1.73	0.53
1:D:445:LEU:HD11	1:D:476:LEU:HD13	1.91	0.53
1:D:332:LEU:HD11	1:D:341:VAL:HG11	1.91	0.52
1:A:346:LEU:HB3	1:A:381:ILE:CD1	2.39	0.52
1:D:305:SER:O	1:D:309:LEU:HB2	2.09	0.52
1:A:524:HIS:HD2	1:A:527:ARG:HH11	1.56	0.52
1:A:143:GLU:HG2	1:A:148:ARG:HH12	1.75	0.52
1:A:511:ASN:O	1:A:514:PRO:HD2	2.09	0.52
1:A:298:ILE:HD12	1:D:83:ARG:NH2	2.25	0.52
1:A:474:ASP:CG	2:B:4:ARG:HH22	2.13	0.52
1:A:53:ILE:HG22	1:A:122:TRP:NE1	2.19	0.52
1:D:345:HIS:CE1	1:D:349:LEU:HD11	2.45	0.52
1:A:235:GLU:OE2	1:D:101:LYS:HB2	2.10	0.52
1:A:313:ASP:CG	1:A:344:LEU:HD21	2.30	0.51
1:A:90:TRP:CE2	1:D:232:LYS:HB3	2.45	0.51
1:D:513:LYS:HG2	1:D:545:LEU:O	2.10	0.51
1:A:53:ILE:CG2	1:A:122:TRP:HE1	2.18	0.51
1:D:259:ASN:HD22	1:D:259:ASN:C	2.12	0.51
1:D:543:LEU:HD12	1:D:544:LEU:H	1.76	0.51
1:D:254:LEU:O	1:D:258:LEU:HD13	2.09	0.51
1:D:561:LEU:HD21	1:D:593:ALA:HB2	1.91	0.51
1:A:450:GLN:NE2	2:B:5:ARG:HH12	2.09	0.51
1:A:96:MET:HG2	1:D:50:THR:CG2	2.41	0.51
1:A:96:MET:CG	1:D:50:THR:HG21	2.41	0.51
1:A:575:GLU:O	1:A:579:ILE:HD12	2.11	0.51
1:A:474:ASP:OD2	2:B:4:ARG:NH2	2.44	0.51
1:A:146:TYR:O	1:A:153:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ASN:O	1:A:548:ASN:CG	2.49	0.51
1:A:457:ILE:HD12	1:A:457:ILE:N	2.24	0.50
1:D:423:HIS:HB3	1:D:454:LEU:CD1	2.41	0.50
1:A:276:MET:HE1	1:A:291:ALA:HB2	1.91	0.50
1:A:102:CYS:N	1:D:235:GLU:OE2	2.44	0.50
1:D:223:TYR:HB2	1:D:240:LEU:HD21	1.94	0.50
1:A:475:PRO:HB3	1:A:505:VAL:HG23	1.94	0.50
1:A:479:ASN:HD21	1:A:521:ASN:ND2	2.09	0.50
1:A:346:LEU:HB3	1:A:381:ILE:HD13	1.93	0.50
1:A:391:GLU:O	1:A:395:TYR:HD2	1.95	0.50
1:D:87:LEU:HB3	1:D:110:VAL:HG22	1.93	0.50
1:D:443:PRO:HG3	2:E:2:MET:HE3	1.94	0.50
1:D:498:PHE:CZ	1:D:521:ASN:HB3	2.47	0.50
1:A:328:THR:HG21	1:A:345:HIS:HD2	1.74	0.49
1:A:393:ARG:HD2	1:A:417:PHE:CZ	2.47	0.49
1:D:96:MET:HE2	1:D:96:MET:CA	2.36	0.49
1:A:84:GLU:H	1:A:84:GLU:CD	2.16	0.49
1:D:372:LYS:HB3	1:D:374:VAL:HG23	1.94	0.49
1:A:570:ILE:HD11	1:A:593:ALA:O	2.13	0.49
1:D:393:ARG:NH2	1:D:420:GLU:HB2	2.27	0.49
1:A:59:LEU:CD1	1:D:57:THR:HA	2.43	0.49
1:A:276:MET:HE2	1:A:291:ALA:HB2	1.95	0.49
1:A:235:GLU:HG3	1:D:99:GLN:HB3	1.95	0.49
1:D:281:LYS:NZ	1:D:310:CYS:SG	2.86	0.48
1:A:411:ILE:HG13	2:B:2:MET:CG	2.43	0.48
1:D:558:LEU:HB2	1:D:589:LEU:HD21	1.95	0.48
1:A:594:LEU:HD22	1:A:595:GLU:N	2.28	0.48
1:D:553:HIS:CB	1:D:576:SER:HB3	2.42	0.48
1:A:524:HIS:HD2	1:A:527:ARG:NH1	2.11	0.48
1:A:419:ILE:HG22	1:A:420:GLU:OE1	2.14	0.48
1:D:325:LEU:CA	1:D:328:THR:HG22	2.42	0.48
1:A:516:ALA:HB2	1:A:545:LEU:CB	2.44	0.48
1:A:83:ARG:NH1	1:D:267:ASP:OD2	2.47	0.48
1:D:243:ASN:HB3	1:D:245:LEU:HD13	1.94	0.47
1:D:425:GLN:HB2	1:D:425:GLN:HE21	1.52	0.47
1:A:492:GLN:HA	1:A:492:GLN:OE1	2.14	0.47
1:A:163:LEU:O	1:A:164:TYR:HB2	2.14	0.47
1:D:427:ILE:O	1:D:431:THR:CG2	2.60	0.47
1:D:259:ASN:ND2	1:D:261:SER:HB3	2.25	0.47
1:A:594:LEU:CD1	1:A:594:LEU:H	2.27	0.47
1:A:405:GLN:HE21	1:A:435:ARG:HH12	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:OD2	1:D:50:THR:HB	2.15	0.47
1:D:488:LYS:O	1:D:489:SER:HB2	2.15	0.47
1:D:328:THR:CG2	1:D:329:THR:N	2.77	0.47
1:A:99:GLN:HB3	1:D:235:GLU:HG2	1.95	0.47
1:A:329:THR:O	1:A:333:GLU:HG2	2.14	0.47
1:D:417:PHE:CZ	1:D:425:GLN:HG2	2.50	0.47
1:A:487:ASN:C	1:A:488:LYS:O	2.53	0.47
1:A:215:ASN:OD1	1:A:215:ASN:N	2.48	0.47
1:D:362:SER:O	1:D:366:VAL:HG13	2.14	0.47
1:D:431:THR:HG22	1:D:447:LEU:HD11	1.97	0.47
1:D:227:LEU:HD11	1:D:237:PHE:HB2	1.96	0.47
1:A:527:ARG:NH2	1:A:528:LYS:HZ1	2.13	0.46
1:D:259:ASN:ND2	1:D:261:SER:H	2.13	0.46
1:D:423:HIS:HB3	1:D:454:LEU:HD12	1.98	0.46
1:D:106:VAL:O	1:D:110:VAL:HG23	2.16	0.46
1:D:116:ASN:HB3	1:D:119:ASP:OD2	2.15	0.46
1:A:535:ALA:O	1:A:539:LEU:HD23	2.16	0.46
1:A:83:ARG:HD3	1:D:267:ASP:OD1	2.15	0.46
1:D:260:TYR:HB2	1:D:268:ALA:HB1	1.98	0.46
1:D:328:THR:HG23	1:D:329:THR:H	1.79	0.46
1:D:143:GLU:O	1:D:144:ASP:HB3	2.15	0.46
1:D:445:LEU:CD1	1:D:476:LEU:HD13	2.45	0.46
1:D:364:ASP:HA	1:D:367:ASP:HB3	1.97	0.46
1:D:277:LEU:HD13	1:D:307:LEU:HA	1.98	0.46
1:A:227:LEU:HB3	1:A:258:LEU:HD11	1.97	0.46
1:D:369:HIS:HB3	1:D:372:LYS:HG2	1.99	0.46
1:A:320:ARG:CA	1:A:509:GLN:HE21	2.29	0.46
1:A:415:HIS:CD2	1:A:430:TYR:OH	2.60	0.46
1:A:238:ASP:O	1:A:242:SER:HB2	2.17	0.45
1:D:474:ASP:CG	2:E:4:ARG:HH22	2.20	0.45
1:A:535:ALA:O	1:A:539:LEU:CD2	2.64	0.45
1:A:125:GLN:HE21	1:A:125:GLN:HA	1.80	0.45
1:D:338:ASN:O	1:D:338:ASN:OD1	2.34	0.45
1:D:174:GLY:O	1:D:206:ARG:HD3	2.17	0.45
1:A:443:PRO:CD	2:B:2:MET:HE1	2.47	0.45
1:D:255:VAL:HA	1:D:258:LEU:HD22	1.98	0.45
1:D:332:LEU:CD1	1:D:341:VAL:HG11	2.47	0.45
1:D:246:LEU:HA	1:D:250:GLU:OE1	2.17	0.45
1:D:282:THR:HG21	1:D:317:VAL:HG11	1.99	0.45
1:A:457:ILE:H	1:A:457:ILE:CD1	2.14	0.45
1:D:566:PRO:O	1:D:570:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:590:LEU:HD12	1:D:590:LEU:O	2.17	0.44
1:D:332:LEU:N	1:D:332:LEU:HD12	2.32	0.44
1:A:177:ASN:HB2	1:A:225:GLU:OE2	2.17	0.44
1:D:577:LEU:O	1:D:581:PRO:HA	2.16	0.44
1:D:591:LYS:HA	1:D:594:LEU:HD23	1.99	0.44
1:D:255:VAL:HG11	1:D:279:LEU:HD11	2.00	0.44
1:A:414:ALA:HB2	1:A:429:ALA:HB3	1.98	0.44
1:A:523:GLY:HA3	1:A:539:LEU:HD22	1.99	0.44
1:A:286:ASP:O	1:A:289:ARG:HG2	2.16	0.44
1:A:585:MET:HE1	2:B:13:THR:CA	2.46	0.44
1:A:235:GLU:HG2	1:D:99:GLN:HB3	1.98	0.44
1:A:307:LEU:HD13	1:A:311:LYS:HE2	1.98	0.44
1:A:558:LEU:O	1:A:561:LEU:CD2	2.65	0.44
1:D:281:LYS:HD3	1:D:313:ASP:CB	2.47	0.44
1:A:225:GLU:O	1:A:229:VAL:HG23	2.16	0.44
2:E:17:VAL:CG2	2:E:18:LEU:N	2.81	0.44
1:A:519:TRP:CD2	1:A:541:GLN:HG2	2.53	0.44
1:D:516:ALA:HB2	1:D:545:LEU:HB3	1.98	0.43
1:A:391:GLU:O	1:A:395:TYR:CD2	2.71	0.43
1:D:87:LEU:CB	1:D:110:VAL:HG22	2.48	0.43
1:A:376:TRP:CD1	1:A:402:MET:HE3	2.52	0.43
1:A:577:LEU:O	1:A:581:PRO:HA	2.18	0.43
1:A:160:LEU:HA	1:A:160:LEU:HD12	1.79	0.43
1:D:527:ARG:HG3	1:D:559:VAL:CG2	2.43	0.43
1:D:259:ASN:C	1:D:259:ASN:ND2	2.71	0.43
1:A:59:LEU:HD13	1:D:57:THR:HA	1.99	0.43
1:A:105:PHE:O	1:A:109:LYS:HD2	2.19	0.43
1:A:573:LEU:HD21	1:A:589:LEU:HB3	1.99	0.43
1:D:511:ASN:O	1:D:514:PRO:HD2	2.19	0.43
1:A:218:ARG:O	1:A:222:CYS:SG	2.77	0.43
1:D:595:GLU:OE2	1:D:595:GLU:HA	2.17	0.43
1:A:130:THR:O	1:A:130:THR:CG2	2.66	0.43
1:A:420:GLU:OE1	1:A:420:GLU:HA	2.18	0.43
1:A:205:LEU:HA	1:A:205:LEU:HD12	1.91	0.43
1:A:90:TRP:NE1	1:D:232:LYS:HB3	2.33	0.43
1:D:173:LEU:O	1:D:206:ARG:NH1	2.52	0.42
1:D:347:ALA:O	1:D:351:GLU:HG2	2.20	0.42
1:D:398:LYS:O	1:D:402:MET:HG3	2.19	0.42
1:A:405:GLN:NE2	1:A:435:ARG:NH1	2.67	0.42
1:A:366:VAL:HA	1:A:375:THR:HG21	2.01	0.42
1:A:324:VAL:O	1:A:328:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:THR:CG2	1:D:329:THR:H	2.31	0.42
1:A:405:GLN:HE21	1:A:435:ARG:NH1	2.17	0.42
1:D:332:LEU:HD11	1:D:341:VAL:CG1	2.49	0.42
1:D:342:TYR:O	1:D:346:LEU:HD22	2.19	0.42
1:D:144:ASP:OD1	1:D:147:ASN:HB2	2.20	0.42
1:A:557:ALA:O	1:A:561:LEU:HD22	2.20	0.42
1:D:356:ASN:ND2	1:D:356:ASN:H	2.16	0.42
1:D:355:LYS:HB2	1:D:355:LYS:HE3	1.62	0.42
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.81	0.42
1:A:585:MET:CE	2:B:13:THR:C	2.86	0.42
1:D:49:SER:OG	1:D:195:GLY:HA3	2.20	0.41
1:D:516:ALA:HB2	1:D:545:LEU:CB	2.50	0.41
1:D:154:TYR:CE1	1:D:201:SER:HB3	2.56	0.41
1:D:524:HIS:HD2	1:D:527:ARG:NH2	2.07	0.41
1:A:90:TRP:CD2	1:A:106:VAL:HG21	2.55	0.41
1:A:451:HIS:CE1	1:A:459:LEU:HD23	2.55	0.41
1:A:356:ASN:O	1:A:360:LEU:HG	2.20	0.41
1:A:443:PRO:HG3	2:B:2:MET:HE3	2.01	0.41
1:A:281:LYS:HD3	1:A:288:LEU:HD21	2.03	0.41
1:A:536:ILE:HA	1:A:536:ILE:HD13	1.91	0.41
1:A:246:LEU:HB2	1:A:251:GLU:HG3	2.01	0.41
1:A:411:ILE:HG13	2:B:2:MET:HG2	2.02	0.41
1:D:177:ASN:HA	1:D:178:PRO:HD3	1.84	0.41
1:A:561:LEU:H	1:A:561:LEU:HD22	1.85	0.41
1:D:273:SER:HA	1:D:276:MET:CE	2.51	0.41
1:A:251:GLU:O	1:A:255:VAL:HG13	2.21	0.41
1:A:276:MET:HE2	1:A:291:ALA:CB	2.51	0.41
1:A:484:VAL:O	1:A:488:LYS:HG3	2.21	0.41
1:A:498:PHE:O	1:A:502:LEU:HD22	2.21	0.41
1:D:122:TRP:O	1:D:125:GLN:HB2	2.21	0.41
2:E:21:ASP:C	2:E:23:GLU:H	2.23	0.41
1:D:384:LEU:C	1:D:386:VAL:H	2.24	0.41
1:D:328:THR:HG21	1:D:345:HIS:CD2	2.55	0.41
1:A:552:VAL:O	1:A:556:ILE:HG13	2.21	0.41
1:A:452:MET:HE1	1:A:480:GLU:HB3	2.03	0.41
1:A:342:TYR:HB3	1:A:346:LEU:HD22	2.03	0.40
1:A:245:LEU:O	1:A:246:LEU:HD23	2.21	0.40
1:A:450:GLN:HE21	2:B:5:ARG:HH12	1.67	0.40
1:D:536:ILE:HD13	1:D:536:ILE:HA	1.93	0.40
2:E:14:ALA:O	2:E:18:LEU:HD13	2.21	0.40
1:D:557:ALA:CB	1:D:573:LEU:HG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASN:O	1:A:583:GLU:C	2.59	0.40
1:A:53:ILE:CG2	1:A:53:ILE:O	2.63	0.40
1:D:564:LYS:C	1:D:566:PRO:HD3	2.42	0.40
1:A:273:SER:HB3	1:A:295:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/597 (86%)	498 (97%)	16 (3%)	0	100	100
1	D	510/597 (85%)	493 (97%)	17 (3%)	0	100	100
2	B	22/81 (27%)	20 (91%)	2 (9%)	0	100	100
2	E	22/81 (27%)	20 (91%)	2 (9%)	0	100	100
All	All	1068/1356 (79%)	1031 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	441/512 (86%)	357 (81%)	84 (19%)	2	3
1	D	442/512 (86%)	376 (85%)	66 (15%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	16/71 (22%)	13 (81%)	3 (19%)	2	3
2	E	16/71 (22%)	14 (88%)	2 (12%)	6	10
All	All	915/1166 (78%)	760 (83%)	155 (17%)	2	4

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LEU
1	A	89	LEU
1	A	95	LEU
1	A	96	MET
1	A	109	LYS
1	A	116	ASN
1	A	123	LEU
1	A	137	LYS
1	A	144	ASP
1	A	145	LEU
1	A	160	LEU
1	A	163	LEU
1	A	170	LEU
1	A	173	LEU
1	A	215	ASN
1	A	217	ASP
1	A	218	ARG
1	A	225	GLU
1	A	245	LEU
1	A	253	ASP
1	A	255	VAL
1	A	256	LEU
1	A	257	LYS
1	A	258	LEU
1	A	264	SER
1	A	266	GLU
1	A	274	LEU
1	A	279	LEU
1	A	281	LYS
1	A	286	ASP
1	A	293	ASP
1	A	295	LEU
1	A	305	SER
1	A	307	LEU

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Mol	Chain	Res	Type
1	A	310	CYS
1	A	313	ASP
1	A	315	LEU
1	A	328	THR
1	A	332	LEU
1	A	333	GLU
1	A	334	ILE
1	A	339	LEU
1	A	344	LEU
1	A	346	LEU
1	A	355	LYS
1	A	358	LEU
1	A	366	VAL
1	A	374	VAL
1	A	377	LEU
1	A	386	VAL
1	A	387	ASN
1	A	390	SER
1	A	394	ARG
1	A	419	ILE
1	A	420	GLU
1	A	422	GLU
1	A	432	THR
1	A	438	GLN
1	A	440	THR
1	A	445	LEU
1	A	447	LEU
1	A	457	ILE
1	A	458	LEU
1	A	467	SER
1	A	470	LEU
1	A	472	GLN
1	A	476	LEU
1	A	500	ASN
1	A	502	LEU
1	A	504	LEU
1	A	510	SER
1	A	539	LEU
1	A	544	LEU
1	A	545	LEU
1	A	552	VAL
1	A	561	LEU

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Mol	Chain	Res	Type
1	A	573	LEU
1	A	582	ASN
1	A	584	ILE
1	A	585	MET
1	A	589	LEU
1	A	592	ARG
1	A	594	LEU
1	A	595	GLU
2	B	2	MET
2	B	3	LEU
2	B	17	VAL
1	D	45	ASN
1	D	50	THR
1	D	89	LEU
1	D	91	ARG
1	D	96	MET
1	D	109	LYS
1	D	123	LEU
1	D	126	VAL
1	D	137	LYS
1	D	143	GLU
1	D	160	LEU
1	D	163	LEU
1	D	176	THR
1	D	205	LEU
1	D	221	GLU
1	D	225	GLU
1	D	245	LEU
1	D	255	VAL
1	D	256	LEU
1	D	258	LEU
1	D	259	ASN
1	D	266	GLU
1	D	274	LEU
1	D	281	LYS
1	D	290	ARG
1	D	292	GLU
1	D	295	LEU
1	D	299	ASN
1	D	309	LEU
1	D	315	LEU
1	D	338	ASN

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Mol	Chain	Res	Type
1	D	346	LEU
1	D	354	GLU
1	D	355	LYS
1	D	358	LEU
1	D	367	ASP
1	D	372	LYS
1	D	374	VAL
1	D	375	THR
1	D	387	ASN
1	D	390	SER
1	D	413	PHE
1	D	416	SER
1	D	425	GLN
1	D	431	THR
1	D	432	THR
1	D	436	LEU
1	D	445	LEU
1	D	447	LEU
1	D	454	LEU
1	D	459	LEU
1	D	470	LEU
1	D	472	GLN
1	D	476	LEU
1	D	493	THR
1	D	502	LEU
1	D	503	LEU
1	D	504	LEU
1	D	510	SER
1	D	512	GLU
1	D	530	LYS
1	D	543	LEU
1	D	544	LEU
1	D	545	LEU
1	D	584	ILE
1	D	594	LEU
2	E	3	LEU
2	E	17	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	116	ASN
1	A	118	ASN
1	A	125	GLN
1	A	284	HIS
1	A	345	HIS
1	A	363	ASN
1	A	369	HIS
1	A	405	GLN
1	A	415	HIS
1	A	438	GLN
1	A	450	GLN
1	A	479	ASN
1	A	496	ASN
1	A	499	GLN
1	A	509	GLN
1	A	511	ASN
1	A	524	HIS
2	B	6	ASN
1	D	98	GLN
1	D	99	GLN
1	D	118	ASN
1	D	125	GLN
1	D	167	GLN
1	D	177	ASN
1	D	259	ASN
1	D	280	ASN
1	D	284	HIS
1	D	345	HIS
1	D	356	ASN
1	D	363	ASN
1	D	405	GLN
1	D	415	HIS
1	D	425	GLN
1	D	450	GLN
1	D	453	GLN
1	D	472	GLN
1	D	509	GLN
1	D	511	ASN
1	D	524	HIS
1	D	551	ASN
2	E	6	ASN

### 5.3.3 RNA [i](#)

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](#)

Of 4 ligands modelled in this entry, 4 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	520/597 (87%)	0.03	6 (1%) 81 77	35, 54, 88, 119	6 (1%)
1	D	518/597 (86%)	0.08	9 (1%) 73 68	33, 60, 91, 118	16 (3%)
2	B	23/81 (28%)	0.01	1 (4%) 39 31	40, 67, 82, 87	0
2	E	23/81 (28%)	0.06	1 (4%) 39 31	44, 78, 98, 101	0
All	All	1084/1356 (79%)	0.05	17 (1%) 74 69	33, 57, 92, 119	22 (2%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	144	ASP	5.3
1	D	359	TYR	4.6
1	D	143	GLU	3.3
1	D	382	TYR	3.0
1	D	593	ALA	2.8
1	A	222	CYS	2.7
2	E	13	THR	2.7
1	D	175	GLU	2.5
1	A	143	GLU	2.4
1	D	589	LEU	2.3
1	A	310	CYS	2.3
2	B	20	TYR	2.3
1	A	385	CYS	2.1
1	A	178	PRO	2.1
1	A	146	TYR	2.1
1	D	358	LEU	2.1
1	D	569	ALA	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AUC	A	1597	1/5	0.87	0.15	-0.98	250,250,250,250	0
3	AUC	D	1597	1/5	0.98	0.11	-2.19	113,113,113,113	0
3	AUC	A	1596	1/5	0.94	0.09	-2.46	144,144,144,144	0
3	AUC	D	1596	1/5	0.95	0.08	-2.68	135,135,135,135	0

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

There are no such residues in this entry.