Full wwPDB X-ray Structure Validation Report (i)

Jul 5, 2016 – 09:10 AM EDT

PDB ID	:	5KKN
Title	:	Crystal structure of human ACC2 BC domain in complex with ND-646, the primary amide of ND-630
Authors	:	Wang, R.; Paul, D.; Tong, L.
Deposited on	:	2016-06-22
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

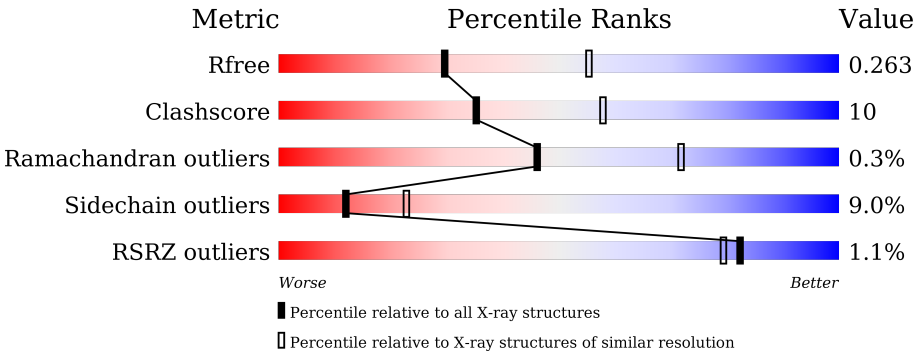
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

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 >=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 <=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	540	70% 16% • 11%
1	C	540	68% 17% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7586 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 Acetyl-CoA carboxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	482	Total	C	N	O	S	0	0	0
			3789	2425	653	693	18			
1	C	470	Total	C	N	O	S	0	0	0
			3691	2365	629	679	18			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	221	MET	-	initiating methionine	UNP O00763
B	222	GLY	-	expression tag	UNP O00763
B	223	SER	-	expression tag	UNP O00763
B	224	SER	-	expression tag	UNP O00763
B	225	HIS	-	expression tag	UNP O00763
B	226	HIS	-	expression tag	UNP O00763
B	227	HIS	-	expression tag	UNP O00763
B	228	HIS	-	expression tag	UNP O00763
B	229	HIS	-	expression tag	UNP O00763
B	230	HIS	-	expression tag	UNP O00763
B	231	GLU	-	expression tag	UNP O00763
B	232	ASN	-	expression tag	UNP O00763
B	233	LEU	-	expression tag	UNP O00763
B	234	TYR	-	expression tag	UNP O00763
B	235	PHE	-	expression tag	UNP O00763
B	236	GLN	-	expression tag	UNP O00763
B	237	GLY	-	expression tag	UNP O00763
C	221	MET	-	initiating methionine	UNP O00763
C	222	GLY	-	expression tag	UNP O00763
C	223	SER	-	expression tag	UNP O00763
C	224	SER	-	expression tag	UNP O00763
C	225	HIS	-	expression tag	UNP O00763
C	226	HIS	-	expression tag	UNP O00763
C	227	HIS	-	expression tag	UNP O00763
C	228	HIS	-	expression tag	UNP O00763

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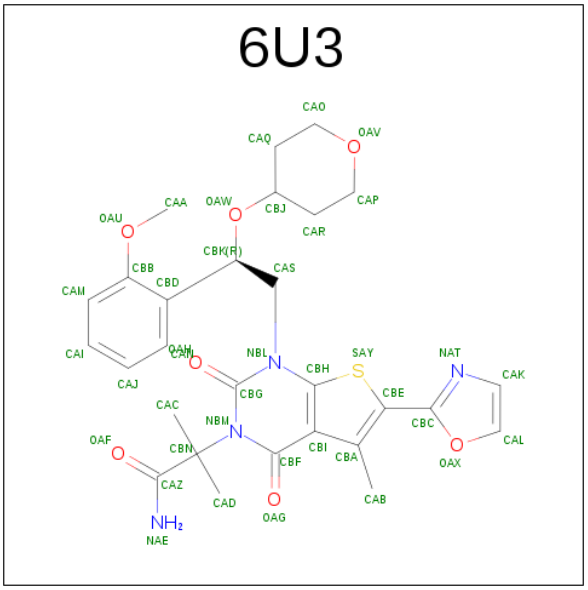
Chain	Residue	Modelled	Actual	Comment	Reference
C	229	HIS	-	expression tag	UNP O00763
C	230	HIS	-	expression tag	UNP O00763
C	231	GLU	-	expression tag	UNP O00763
C	232	ASN	-	expression tag	UNP O00763
C	233	LEU	-	expression tag	UNP O00763
C	234	TYR	-	expression tag	UNP O00763
C	235	PHE	-	expression tag	UNP O00763
C	236	GLN	-	expression tag	UNP O00763
C	237	GLY	-	expression tag	UNP O00763

- Molecule 2 is 2-[1-[(2 {R})-2-(2-methoxyphenyl)-2-(oxan-4-yloxy)ethyl]-5-methyl-6-(1,3-oxazol-2-yl)-2,4-bis(oxidanylidene)thieno[2,3-d]pyrimidin-3-yl]-2-methyl-propanamide (three-letter code: 6U3) (formula: $C_{28}H_{32}N_4O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			40	28	4	7	1		
2	C	1	Total	C	N	O	S	0	0
			40	28	4	7	1		

- Molecule 3 is water.

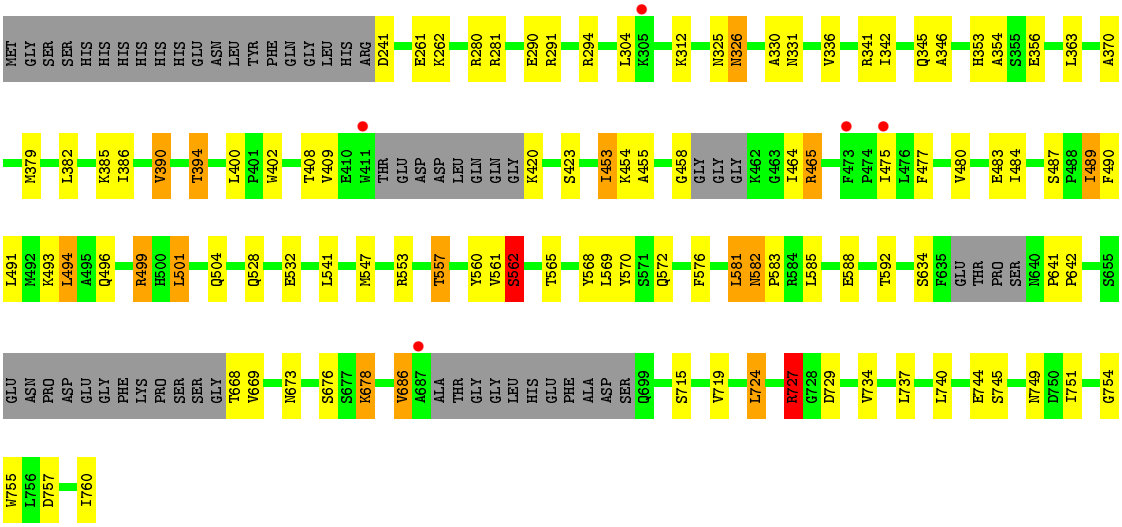
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	15	Total	O	0	0
			15	15		
3	C	11	Total	O	0	0
			11	11		

3 Residue-property plots (i)

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.

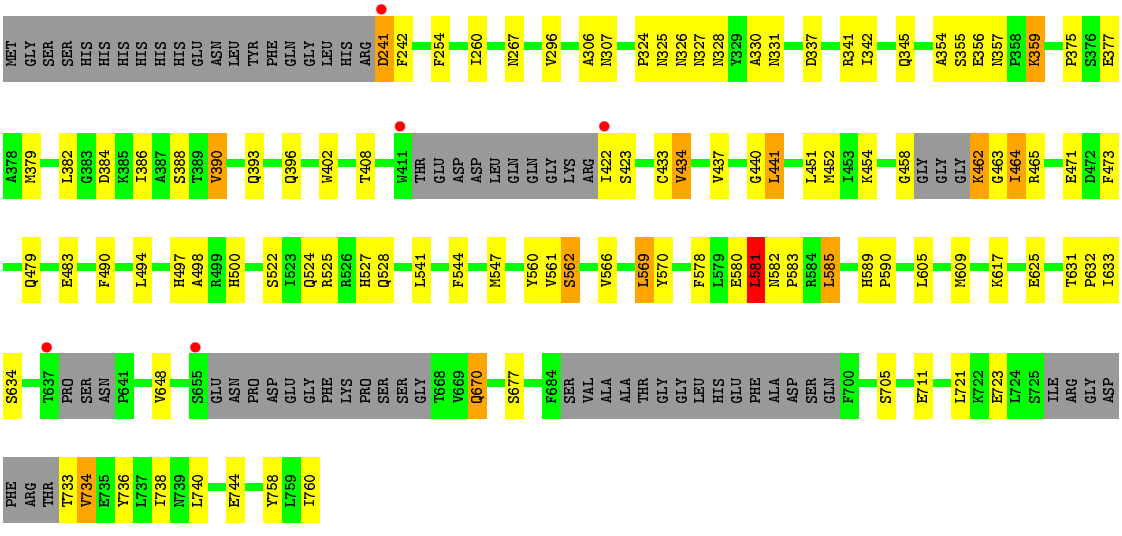
- Molecule 1: Acetyl-CoA carboxylase 2

Chain B:



- Molecule 1: Acetyl-CoA carboxylase 2

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.67Å 141.67Å 163.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 45.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.60) 92.3 (45.36-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.220 , 0.266 0.223 , 0.263	Depositor DCC
R_{free} test set	2440 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 6U3

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	0.78	1/3875 (0.0%)	0.75	2/5259 (0.0%)
1	C	0.78	1/3775 (0.0%)	0.77	4/5124 (0.1%)
All	All	0.78	2/7650 (0.0%)	0.76	6/10383 (0.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	560	TYR	CE2-CZ	-6.22	1.30	1.38
1	B	560	TYR	CE1-CZ	-5.27	1.31	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	581	LEU	CA-CB-CG	6.86	131.07	115.30
1	B	727	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	727	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	434	VAL	CB-CA-C	5.37	121.61	111.40
1	C	569	LEU	CA-CB-CG	-5.13	103.49	115.30
1	C	585	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	668	THR	Peptide

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	3789	0	3758	78	0
1	C	3691	0	3655	66	0
2	B	40	0	0	3	0
2	C	40	0	0	2	0
3	B	15	0	0	0	0
3	C	11	0	0	0	0
All	All	7586	0	7413	147	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 10.

All (147) 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:C:734:VAL:O	1:C:738:ILE:HD12	1.38	1.22
1:C:458:GLY:O	1:C:462:LYS:NZ	1.73	1.21
1:B:678:LYS:H	1:B:678:LYS:HD2	1.26	1.00
1:B:294:ARG:HG2	1:B:294:ARG:HH11	1.26	0.98
1:B:453:ILE:HD12	1:B:489:ILE:HD13	1.43	0.98
1:C:528:GLN:NE2	1:C:760:ILE:HD11	1.82	0.94
1:B:496:GLN:O	1:B:754:GLY:O	1.86	0.92
1:B:454:LYS:HD3	1:B:464:ILE:HG12	1.50	0.90
1:C:500:HIS:HD2	1:C:524:GLN:HE22	1.20	0.89
1:B:294:ARG:HG2	1:B:294:ARG:NH1	1.90	0.85
1:B:326:ASN:O	1:B:331:ASN:HB2	1.78	0.82
1:C:528:GLN:HE22	1:C:760:ILE:HD11	1.41	0.82
1:B:724:LEU:HD13	1:B:734:VAL:HG21	1.62	0.80
2:B:801:6U3:OAG	2:B:801:6U3:CAD	2.29	0.80
1:C:462:LYS:O	1:C:483:GLU:OE1	2.00	0.79
1:B:499:ARG:NH2	1:B:749:ASN:OD1	2.16	0.79
1:C:500:HIS:CD2	1:C:524:GLN:HE22	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:GLY:HA2	1:C:483:GLU:OE1	1.86	0.76
1:C:734:VAL:O	1:C:738:ILE:CD1	2.30	0.75
1:C:760:ILE:HD12	1:C:760:ILE:O	1.87	0.74
1:B:390:VAL:O	1:B:394:THR:HG22	1.90	0.72
2:C:801:6U3:CAZ	2:C:801:6U3:OAG	2.40	0.69
1:C:465:ARG:HE	1:C:479:GLN:HE21	1.40	0.69
1:B:394:THR:HG21	1:B:409:VAL:HG22	1.75	0.69
1:B:678:LYS:CD	1:B:678:LYS:H	2.04	0.68
1:B:464:ILE:O	1:B:465:ARG:HD3	1.94	0.68
1:B:291:ARG:HB3	1:B:294:ARG:HH12	1.59	0.67
1:B:261:GLU:H	1:B:345:GLN:HE21	1.41	0.67
1:B:454:LYS:HD2	1:B:455:ALA:H	1.60	0.67
1:B:727:ARG:HH11	1:B:727:ARG:HG3	1.60	0.66
1:C:386:ILE:HD12	1:C:433:CYS:SG	2.36	0.65
1:C:465:ARG:HE	1:C:479:GLN:NE2	1.95	0.65
1:C:544:PHE:HA	1:C:547:MET:HE2	1.78	0.65
1:C:670:GLN:HE21	1:C:670:GLN:HA	1.63	0.64
1:B:553:ARG:O	1:B:557:THR:HG23	1.97	0.64
1:C:527:HIS:O	1:C:760:ILE:HG13	1.98	0.63
1:C:242:PHE:CZ	1:C:254:PHE:HZ	2.17	0.62
1:C:296:VAL:HG11	1:C:342:ILE:HD13	1.82	0.61
1:C:721:LEU:HB3	1:C:734:VAL:HG11	1.80	0.61
1:C:357:ASN:OD1	1:C:359:LYS:HB2	2.01	0.61
1:C:296:VAL:HG11	1:C:342:ILE:CD1	2.32	0.59
1:C:464:ILE:HD13	1:C:758:TYR:CG	2.38	0.58
1:B:454:LYS:HD2	1:B:455:ALA:N	2.18	0.57
1:C:441:LEU:HD13	1:C:473:PHE:CD1	2.40	0.57
1:C:375:PRO:HD3	1:C:561:VAL:HB	1.85	0.57
1:C:544:PHE:CD1	1:C:547:MET:HE3	2.39	0.57
1:B:382:LEU:HD13	1:B:581:LEU:HG	1.87	0.57
1:C:382:LEU:HA	1:C:388:SER:HB2	1.86	0.57
1:B:453:ILE:HD11	1:B:480:VAL:HB	1.87	0.56
1:B:400:LEU:HD11	1:B:569:LEU:HD12	1.86	0.56
1:B:582:ASN:HD22	1:B:583:PRO:HD2	1.69	0.56
1:C:260:ILE:HD12	1:C:609:MET:HG2	1.88	0.55
1:B:496:GLN:HG3	1:B:755:TRP:CZ3	2.42	0.55
1:C:393:GLN:OE1	1:C:402:TRP:NE1	2.26	0.55
1:B:676:SER:HB2	1:B:719:VAL:HG12	1.91	0.53
1:B:532:GLU:HG3	1:B:588:GLU:HG2	1.90	0.53
1:C:355:SER:O	1:C:379:MET:HE1	2.09	0.53
1:C:464:ILE:CD1	1:C:758:TYR:CG	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ARG:CG	1:B:727:ARG:HH11	2.22	0.53
1:B:483:GLU:HG2	1:B:484:ILE:HG13	1.92	0.52
1:C:452:MET:HG2	1:C:494:LEU:CD2	2.39	0.52
1:C:544:PHE:HD1	1:C:547:MET:HE3	1.72	0.52
1:C:325:ASN:O	1:C:327:ASN:O	2.28	0.52
1:B:453:ILE:HG13	1:B:453:ILE:O	2.10	0.52
1:B:453:ILE:HG13	1:B:480:VAL:HG21	1.91	0.51
1:B:501:LEU:HD11	1:B:570:TYR:HB2	1.91	0.51
1:C:721:LEU:HB3	1:C:734:VAL:CG1	2.40	0.51
1:B:261:GLU:H	1:B:345:GLN:NE2	2.07	0.51
2:C:801:6U3:OAH	2:C:801:6U3:CAC	2.57	0.51
1:B:281:ARG:NH2	2:B:801:6U3:NAE	2.59	0.51
1:B:458:GLY:HA3	1:B:484:ILE:CD1	2.41	0.51
1:C:337:ASP:OD1	1:C:341:ARG:HD2	2.10	0.51
1:B:325:ASN:OD1	1:B:353:HIS:CE1	2.63	0.51
1:B:356:GLU:HA	1:B:379:MET:CE	2.41	0.50
1:B:386:ILE:O	1:B:390:VAL:HG13	2.11	0.50
1:B:678:LYS:N	1:B:678:LYS:HD2	2.07	0.50
1:B:346:ALA:HB2	1:B:370:ALA:HB3	1.93	0.50
1:B:494:LEU:HD12	1:B:755:TRP:HB3	1.95	0.49
1:B:729:ASP:OD1	1:B:729:ASP:N	2.42	0.49
1:C:544:PHE:HA	1:C:547:MET:CE	2.42	0.49
1:C:306:ALA:O	1:C:307:ASN:HB2	2.13	0.49
1:C:326:ASN:O	1:C:331:ASN:HB2	2.12	0.49
1:B:727:ARG:HB2	1:B:729:ASP:OD1	2.13	0.48
1:B:325:ASN:ND2	1:B:353:HIS:ND1	2.61	0.48
1:B:569:LEU:O	1:B:576:PHE:HA	2.13	0.48
1:B:356:GLU:HA	1:B:379:MET:HE3	1.95	0.48
1:B:501:LEU:N	1:B:501:LEU:HD12	2.28	0.48
1:B:727:ARG:HG3	1:B:727:ARG:NH1	2.24	0.48
1:C:324:PRO:HB2	1:C:326:ASN:OD1	2.13	0.48
1:C:625:GLU:HG3	1:C:633:ILE:HG12	1.96	0.48
1:C:242:PHE:CZ	1:C:254:PHE:CZ	2.99	0.48
1:C:434:VAL:HG11	1:C:440:GLY:HA2	1.96	0.48
1:C:566:VAL:HG22	1:C:581:LEU:HD22	1.96	0.48
1:C:561:VAL:O	1:C:562:SER:CB	2.60	0.47
1:B:501:LEU:H	1:B:501:LEU:HD12	1.80	0.47
1:B:582:ASN:HD22	1:B:583:PRO:CD	2.27	0.47
1:B:678:LYS:CD	1:B:678:LYS:N	2.72	0.47
1:B:458:GLY:HA3	1:B:484:ILE:HD13	1.96	0.47
1:B:561:VAL:O	1:B:562:SER:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:LYS:CD	1:B:464:ILE:HG12	2.35	0.47
1:B:572:GLN:HB2	1:B:751:ILE:HD12	1.97	0.47
1:B:477:PHE:CE1	1:B:489:ILE:HG12	2.51	0.46
1:B:330:ALA:HA	1:B:354:ALA:HB2	1.97	0.46
1:B:453:ILE:CD1	1:B:489:ILE:HD13	2.30	0.46
1:B:489:ILE:HD12	1:B:490:PHE:N	2.31	0.45
1:B:356:GLU:C	1:B:379:MET:HE2	2.36	0.45
1:C:242:PHE:O	1:C:242:PHE:CD1	2.70	0.45
1:C:578:PHE:CZ	1:C:580:GLU:HA	2.52	0.45
1:C:325:ASN:HA	1:C:328:ASN:OD1	2.16	0.45
1:B:363:LEU:HD12	1:B:363:LEU:HA	1.79	0.45
1:B:496:GLN:NE2	1:C:241:ASP:O	2.50	0.45
1:B:342:ILE:HA	1:B:342:ILE:HD13	1.86	0.45
1:B:390:VAL:O	1:B:394:THR:CG2	2.64	0.45
1:B:294:ARG:CG	1:B:294:ARG:NH1	2.69	0.44
1:B:325:ASN:HB3	1:B:330:ALA:HB3	1.99	0.44
1:C:465:ARG:NE	1:C:479:GLN:HE21	2.11	0.44
1:B:402:TRP:HB2	1:B:491:LEU:O	2.17	0.44
1:B:280:ARG:HG2	1:B:290:GLU:O	2.18	0.44
1:B:262:LYS:H	1:B:345:GLN:NE2	2.15	0.44
1:B:382:LEU:HD22	1:B:581:LEU:HB3	1.99	0.44
1:C:589:HIS:N	1:C:590:PRO:CD	2.81	0.44
1:C:648:VAL:HA	1:C:705:SER:O	2.18	0.44
1:C:330:ALA:HA	1:C:354:ALA:HB2	1.99	0.43
1:C:736:TYR:O	1:C:740:LEU:HB2	2.17	0.43
1:C:454:LYS:HD3	1:C:490:PHE:CZ	2.53	0.43
1:C:605:LEU:O	1:C:609:MET:HG3	2.18	0.43
1:C:356:GLU:HA	1:C:379:MET:HE1	2.00	0.43
1:B:336:VAL:HG21	1:B:363:LEU:HB3	2.01	0.43
1:B:641:PRO:HA	1:B:642:PRO:HD3	1.94	0.43
1:B:493:LYS:HG3	1:B:494:LEU:N	2.33	0.43
1:B:568:TYR:O	1:B:569:LEU:HD23	2.18	0.42
1:C:582:ASN:HA	1:C:583:PRO:HD3	1.89	0.42
1:C:631:THR:HG22	1:C:632:PRO:O	2.19	0.42
1:B:547:MET:HE1	1:B:570:TYR:HD2	1.85	0.42
1:C:386:ILE:O	1:C:390:VAL:HG13	2.19	0.42
1:C:451:LEU:HD12	1:C:451:LEU:C	2.40	0.42
1:B:504:GLN:HG2	1:B:592:THR:HG21	2.01	0.42
1:C:498:ALA:HA	1:C:570:TYR:O	2.20	0.42
1:C:325:ASN:C	1:C:327:ASN:O	2.59	0.41
1:B:453:ILE:HD12	1:B:489:ILE:CD1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:GLN:HA	1:C:528:GLN:NE2	2.35	0.41
1:C:462:LYS:HE2	1:C:462:LYS:N	2.36	0.41
1:C:589:HIS:CG	1:C:590:PRO:HD3	2.56	0.41
1:B:453:ILE:HD13	1:B:477:PHE:CD1	2.56	0.40
1:B:484:ILE:HG22	1:B:487:SER:HB2	2.02	0.40
2:B:801:6U3:OAG	2:B:801:6U3:CAB	2.69	0.40
1:C:528:GLN:HA	1:C:528:GLN:HE21	1.87	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	470/540 (87%)	453 (96%)	15 (3%)	2 (0%)	39 65
1	C	456/540 (84%)	439 (96%)	16 (4%)	1 (0%)	52 77
All	All	926/1080 (86%)	892 (96%)	31 (3%)	3 (0%)	46 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	562	SER
1	C	562	SER
1	B	686	VAL

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	403/450 (90%)	363 (90%)	40 (10%)	10 18
1	C	394/450 (88%)	362 (92%)	32 (8%)	15 28
All	All	797/900 (89%)	725 (91%)	72 (9%)	12 23

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	ASP
1	B	304	LEU
1	B	312	LYS
1	B	326	ASN
1	B	341	ARG
1	B	385	LYS
1	B	390	VAL
1	B	394	THR
1	B	408	THR
1	B	420	LYS
1	B	423	SER
1	B	453	ILE
1	B	465	ARG
1	B	475	ILE
1	B	489	ILE
1	B	494	LEU
1	B	499	ARG
1	B	501	LEU
1	B	528	GLN
1	B	541	LEU
1	B	557	THR
1	B	562	SER
1	B	565	THR
1	B	581	LEU
1	B	582	ASN
1	B	585	LEU
1	B	634	SER
1	B	669	VAL
1	B	673	ASN
1	B	678	LYS
1	B	686	VAL
1	B	715	SER
1	B	724	LEU
1	B	727	ARG

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Mol	Chain	Res	Type
1	B	737	LEU
1	B	740	LEU
1	B	744	GLU
1	B	745	SER
1	B	757	ASP
1	B	760	ILE
1	C	241	ASP
1	C	267	ASN
1	C	345	GLN
1	C	359	LYS
1	C	377	GLU
1	C	384	ASP
1	C	390	VAL
1	C	396	GLN
1	C	408	THR
1	C	422	ILE
1	C	423	SER
1	C	437	VAL
1	C	441	LEU
1	C	462	LYS
1	C	464	ILE
1	C	471	GLU
1	C	497	HIS
1	C	522	SER
1	C	525	ARG
1	C	541	LEU
1	C	569	LEU
1	C	581	LEU
1	C	585	LEU
1	C	617	LYS
1	C	634	SER
1	C	670	GLN
1	C	677	SER
1	C	711	GLU
1	C	723	GLU
1	C	733	THR
1	C	734	VAL
1	C	744	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	345	GLN
1	B	496	GLN
1	B	497	HIS
1	B	524	GLN
1	B	572	GLN
1	B	582	ASN
1	B	739	ASN
1	C	316	HIS
1	C	479	GLN
1	C	500	HIS
1	C	528	GLN
1	C	572	GLN
1	C	670	GLN
1	C	679	ASN
1	C	716	ASN
1	C	739	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	6U3	B	801	-	32,44,44	2.85	9 (28%)	28,65,65	2.10	6 (21%)
2	6U3	C	801	-	32,44,44	2.25	8 (25%)	28,65,65	1.49	6 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6U3	B	801	-	-	0/19/38/38	0/4/5/5
2	6U3	C	801	-	-	0/19/38/38	0/4/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	6U3	CBH-SAY	-11.10	1.60	1.74
2	C	801	6U3	CBH-SAY	-9.37	1.62	1.74
2	B	801	6U3	CBN-CAZ	-5.48	1.49	1.54
2	B	801	6U3	CBA-CBI	-5.13	1.35	1.40
2	C	801	6U3	CBH-NBL	-3.88	1.34	1.40
2	B	801	6U3	CBD-CBK	-3.74	1.41	1.52
2	B	801	6U3	CBF-CBI	-3.72	1.35	1.41
2	C	801	6U3	CBA-CBI	-3.67	1.37	1.40
2	B	801	6U3	CBH-NBL	-3.56	1.35	1.40
2	C	801	6U3	CBD-CBK	-3.31	1.42	1.52
2	B	801	6U3	CBF-NBM	-3.03	1.33	1.38
2	C	801	6U3	CBF-CBI	-2.95	1.36	1.41
2	C	801	6U3	CBE-SAY	-2.87	1.62	1.74
2	C	801	6U3	CBF-NBM	-2.06	1.35	1.38
2	B	801	6U3	CAD-CBN	2.15	1.56	1.53
2	C	801	6U3	CBN-CAZ	2.21	1.56	1.54
2	B	801	6U3	CAZ-NAE	2.22	1.37	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	6U3	CAA-OAU-CBB	-3.18	112.89	117.53
2	B	801	6U3	CAD-CBN-CAZ	-3.02	98.33	108.67
2	C	801	6U3	CAA-OAU-CBB	-2.58	113.76	117.53
2	C	801	6U3	OAU-CBB-CAM	-2.40	120.32	124.35
2	C	801	6U3	CAQ-CBJ-CAR	-2.08	108.13	111.56
2	C	801	6U3	OAU-CBB-CBD	2.10	117.93	115.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	6U3	OAU-CBB-CBD	2.13	117.96	115.79
2	C	801	6U3	CAD-CBN-NBM	2.42	111.50	108.96
2	B	801	6U3	OAF-CAZ-NAE	2.95	129.70	123.24
2	C	801	6U3	CAC-CBN-NBM	4.57	113.76	108.96
2	B	801	6U3	CAC-CBN-NBM	4.84	114.04	108.96
2	B	801	6U3	CAD-CBN-NBM	6.77	116.08	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	6U3	3	0
2	C	801	6U3	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	B	482/540 (89%)	-0.35	5 (1%)	84	81	23, 35, 57, 72	0
1	C	470/540 (87%)	-0.39	5 (1%)	82	79	20, 35, 65, 93	0
All	All	952/1080 (88%)	-0.37	10 (1%)	82	79	20, 35, 61, 93	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	687	ALA	3.6
1	C	637	THR	3.5
1	C	241	ASP	2.9
1	B	305	LYS	2.9
1	C	655	SER	2.6
1	B	475	ILE	2.5
1	C	411	TRP	2.4
1	B	411	TRP	2.3
1	B	473	PHE	2.3
1	C	422	ILE	2.3

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

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^{th} 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(Å^2)	Q<0.9
2	6U3	B	801	40/40	0.95	0.17	1.67	31,44,51,52	0
2	6U3	C	801	40/40	0.96	0.19	1.20	46,68,72,76	0

6.5 Other polymers

There are no such residues in this entry.