



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:05 am BST

PDB ID : 6QH7  
Title : AP2 clathrin adaptor mu2T156-phosphorylated core with two cargo peptides  
in open+ conformation  
Authors : Wrobel, A.G.; Owen, D.J.; McCoy, A.J.; Evans, P.R.  
Deposited on : 2019-01-15  
Resolution : 3.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

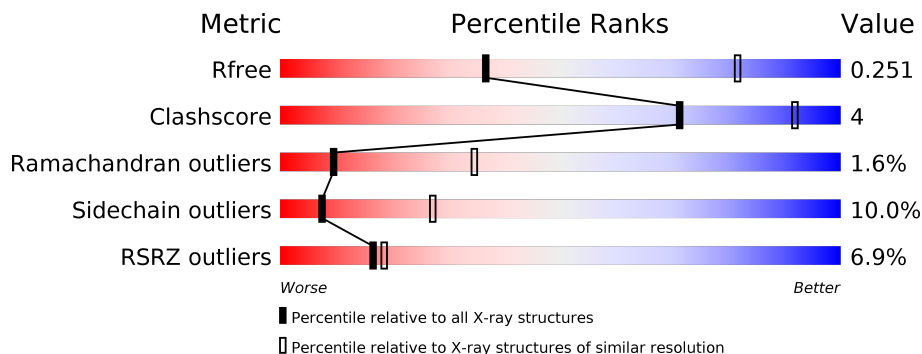
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.



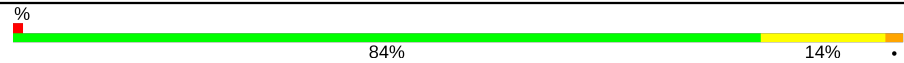
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 respectively. 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	621	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 81% 15% ..</p>
2	B	592	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7% 68% 15% • 15%</p>
3	M	446	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 47% 9% • 43%</p>
3	N	446	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">13% 27% 5% 68%</p>
4	P	6	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <p style="font-size: small; margin-top: 5px;">100%</p>
5	Q	10	<div style="display: flex; align-items: center;"> <div style="width: 20%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">20% 60% 30% 10%</p>

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Mol	Chain	Length	Quality of chain
6	S	142	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left labeled '84%' and a yellow segment on the right labeled '14%'. A small red square is at the beginning of the bar, and a small black dot is at the end. A '%' symbol is positioned above the bar on the left side.</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13342 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 AP-2 complex subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	614	4844	3085	834	904	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	GLU	conflict	UNP Q66HM2

- Molecule 2 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	502	3974	2529	661	763	21	0	0	0

- Molecule 3 is a protein called ADAPTOR-RELATED PROTEIN COMPLEX 2, MU 2 SUB-UNIT, C-TERMINAL DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	255	2033	1310	350	359	14	0	0	0
3	N	143	1157	742	203	207	5	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	237	MET	-	insertion	UNP Q3ZC13
M	238	GLU	-	insertion	UNP Q3ZC13
M	239	GLN	-	insertion	UNP Q3ZC13
M	240	LYS	-	insertion	UNP Q3ZC13
M	241	LEU	-	insertion	UNP Q3ZC13
M	242	ILE	-	insertion	UNP Q3ZC13

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Chain	Residue	Modelled	Actual	Comment	Reference
M	243	SER	-	insertion	UNP Q3ZC13
M	244	GLU	-	insertion	UNP Q3ZC13
M	245	GLU	-	insertion	UNP Q3ZC13
M	246	ASP	-	insertion	UNP Q3ZC13
M	247	LEU	-	insertion	UNP Q3ZC13
N	237	MET	-	insertion	UNP Q3ZC13
N	238	GLU	-	insertion	UNP Q3ZC13
N	239	GLN	-	insertion	UNP Q3ZC13
N	240	LYS	-	insertion	UNP Q3ZC13
N	241	LEU	-	insertion	UNP Q3ZC13
N	242	ILE	-	insertion	UNP Q3ZC13
N	243	SER	-	insertion	UNP Q3ZC13
N	244	GLU	-	insertion	UNP Q3ZC13
N	245	GLU	-	insertion	UNP Q3ZC13
N	246	ASP	-	insertion	UNP Q3ZC13
N	247	LEU	-	insertion	UNP Q3ZC13

- Molecule 4 is a protein called TGN38 CARGO PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	P	6	57	34	11	12	0	0	0

- Molecule 5 is a protein called CD4 CARGO PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
5	Q	9	77	46	14	15	1	1	0	0	0

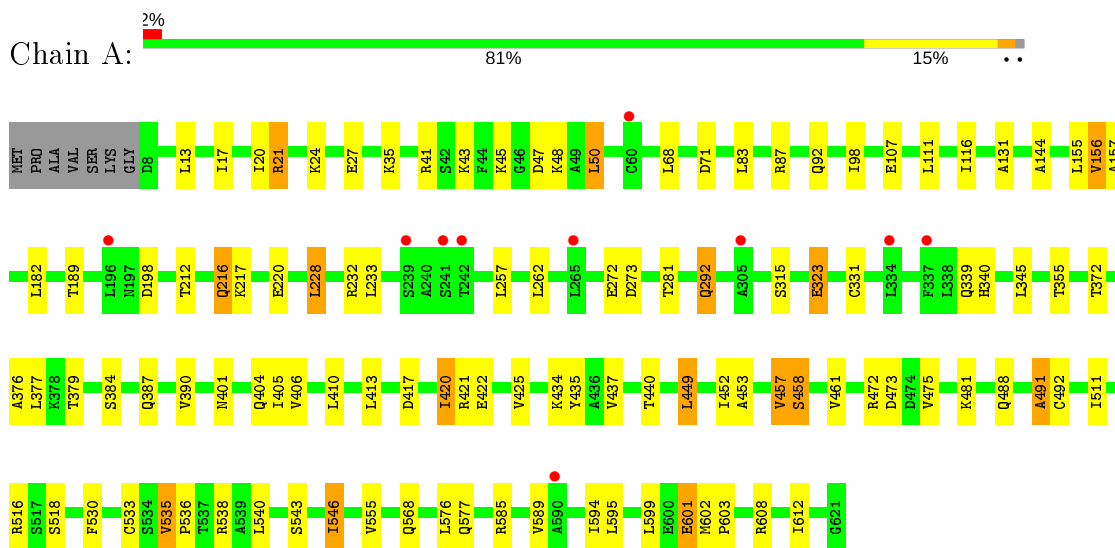
- Molecule 6 is a protein called AP-2 complex subunit sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	S	142	1200	778	200	215	7	0	0	0

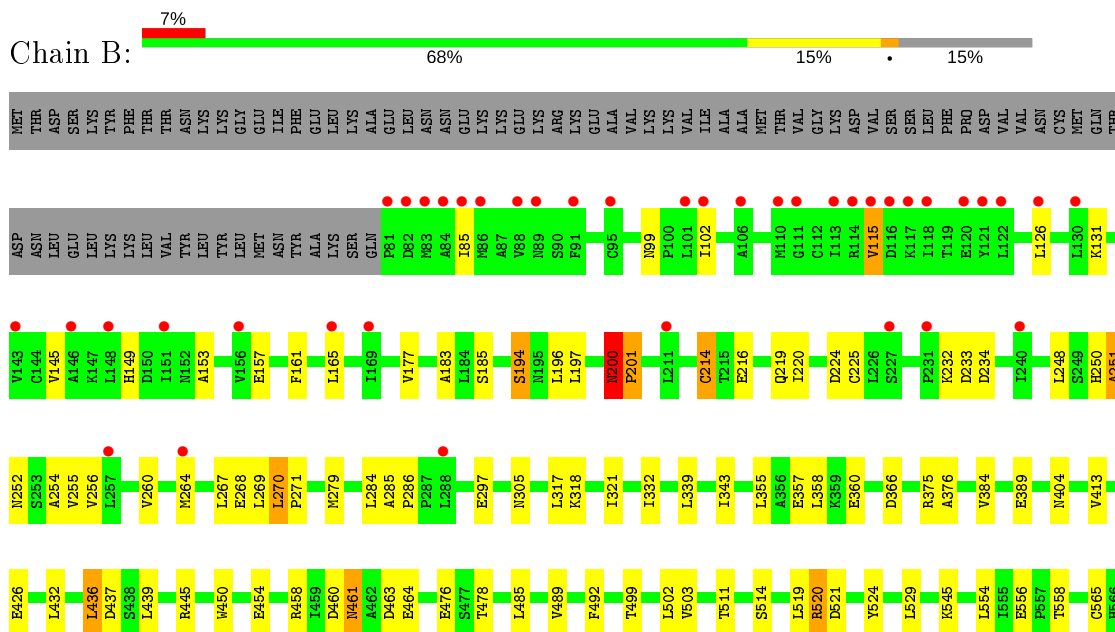
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: AP-2 complex subunit alpha



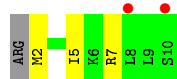
- Molecule 2: AP-2 complex subunit beta



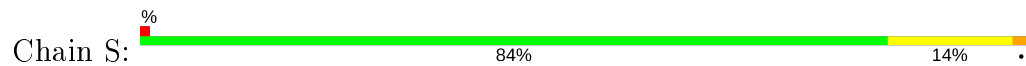


There are no outlier residues recorded for this chain.

- Molecule 5: CD4 CARGO PEPTIDE



- Molecule 6: AP-2 complex subunit sigma





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.18Å 182.18Å 211.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.00 – 3.40 110.03 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (110.00-3.40) 99.7 (110.03-3.40)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 3.41Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.208 , 0.248 0.211 , 0.251	Depositor DCC
$R_{free}$ test set	2526 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.9	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 103.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, 0.333 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: SEP

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	0/4929	0.77	4/6680 (0.1%)
2	B	0.55	0/4038	0.74	1/5488 (0.0%)
3	M	0.55	0/2076	0.77	2/2797 (0.1%)
3	N	0.57	0/1180	0.70	1/1592 (0.1%)
4	P	0.51	0/57	0.63	0/74
5	Q	0.67	0/65	0.99	0/82
6	S	0.56	0/1224	0.77	0/1650
All	All	0.55	0/13569	0.76	8/18363 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
3	M	0	1
6	S	0	1
All	All	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	21	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	B	520	ARG	NE-CZ-NH2	-5.55	117.52	120.30
3	M	192	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	601	GLU	N-CA-C	5.24	125.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	206	LEU	CA-CB-CG	5.19	127.24	115.30
3	N	52	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	472	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	491	ALA	Peptide
2	B	251	ALA	Peptide
2	B	271	PRO	Peptide
3	M	293	ASP	Peptide
6	S	138	LEU	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4844	0	4956	36	0
2	B	3974	0	4061	39	0
3	M	2033	0	2097	11	0
3	N	1157	0	1158	8	0
4	P	57	0	53	0	0
5	Q	77	0	83	0	0
6	S	1200	0	1195	7	0
All	All	13342	0	13603	95	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 4.

All (95) 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:B:251:ALA:HB3	2:B:255:VAL:HG23	1.62	0.80
1:A:198:ASP:O	1:A:232:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLN:HE22	1:A:420:ILE:HG21	1.62	0.64
2:B:200:ASN:HD22	2:B:200:ASN:N	1.97	0.61
2:B:332:ILE:HG21	3:N:43:VAL:HG13	1.84	0.60
3:M:300:VAL:CG1	3:M:444:THR:HG21	2.34	0.56
2:B:194:SER:HA	2:B:197:LEU:HD11	1.88	0.56
2:B:149:HIS:HD1	2:B:153:ALA:HB1	1.69	0.56
2:B:256:VAL:O	2:B:260:VAL:HG23	2.06	0.56
2:B:200:ASN:HB3	2:B:201:PRO:CD	2.37	0.55
1:A:603:PRO:O	2:B:520:ARG:NH2	2.41	0.54
1:A:116:ILE:HG23	1:A:131:ALA:HB1	1.88	0.54
1:A:481:LYS:HA	1:A:511:ILE:CD1	2.39	0.53
1:A:533:CYS:O	1:A:538:ARG:NH1	2.42	0.53
2:B:251:ALA:HB3	2:B:255:VAL:CG2	2.37	0.53
1:A:144:ALA:HB1	1:A:182:LEU:HD12	1.91	0.53
3:N:9:ASN:HD21	3:N:13:GLU:HB2	1.75	0.52
2:B:511:THR:HG23	2:B:524:TYR:CE2	2.45	0.51
1:A:425:VAL:HG11	1:A:457:VAL:HA	1.92	0.51
1:A:292:GLN:HE21	1:A:292:GLN:HA	1.76	0.50
1:A:457:VAL:O	1:A:458:SER:CB	2.60	0.50
2:B:285:ALA:HB3	2:B:286:PRO:HD3	1.94	0.49
2:B:343:ILE:HD11	2:B:376:ALA:HB1	1.93	0.49
2:B:185:SER:OG	2:B:225:CYS:SG	2.70	0.49
1:A:43:LYS:HA	1:A:47:ASP:HB3	1.94	0.49
2:B:514:SER:HB2	2:B:519:LEU:HD23	1.95	0.49
2:B:216:GLU:HG3	2:B:251:ALA:HB2	1.94	0.48
2:B:436:LEU:HA	2:B:439:LEU:HG	1.94	0.48
2:B:511:THR:HG23	2:B:524:TYR:CZ	2.49	0.48
2:B:297:GLU:HB2	3:N:83:TYR:OH	2.13	0.48
2:B:126:LEU:HD23	2:B:161:PHE:CE2	2.47	0.48
1:A:546:ILE:HG23	1:A:599:LEU:HD11	1.96	0.48
2:B:461:ASN:C	2:B:461:ASN:HD22	2.17	0.48
6:S:138:LEU:HA	6:S:141:LEU:HD22	1.95	0.48
6:S:8:GLN:HE21	6:S:32:ILE:HG23	1.79	0.47
6:S:65:LEU:HD21	6:S:100:GLU:HG3	1.96	0.47
2:B:85:ILE:HD11	2:B:115:VAL:HG21	1.96	0.47
1:A:410:LEU:HD21	1:A:449:LEU:HD13	1.96	0.47
2:B:250:HIS:O	2:B:252:ASN:N	2.47	0.47
2:B:339:LEU:HD11	2:B:358:LEU:CD2	2.45	0.47
1:A:376:ALA:HA	1:A:379:THR:HG22	1.98	0.46
3:N:43:VAL:O	3:N:43:VAL:HG12	2.16	0.46
3:M:265:LEU:HG	3:M:271:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:THR:HG21	1:A:323:GLU:HG3	1.97	0.46
3:M:290:THR:HG21	3:M:408:SER:HB2	1.96	0.46
1:A:17:ILE:HB	6:S:105:PHE:CE1	2.51	0.45
1:A:212:THR:O	1:A:216:GLN:NE2	2.50	0.45
2:B:445:ARG:NH1	2:B:476:GLU:OE2	2.49	0.45
2:B:196:LEU:O	2:B:196:LEU:HD13	2.17	0.45
3:M:300:VAL:HG11	3:M:444:THR:HG21	1.98	0.45
1:A:457:VAL:HG13	1:A:458:SER:N	2.31	0.45
3:N:59:LYS:O	3:N:60:ARG:NH1	2.50	0.45
1:A:377:LEU:CD1	1:A:390:VAL:HG22	2.46	0.45
2:B:200:ASN:CB	2:B:201:PRO:CD	2.95	0.45
1:A:530:PHE:CE2	1:A:538:ARG:HD2	2.52	0.45
3:M:387:ASN:HD21	3:M:390:LYS:HB3	1.82	0.45
2:B:450:TRP:CZ2	2:B:454:GLU:HG3	2.51	0.44
3:M:397:ILE:HB	3:M:444:THR:HG23	2.00	0.44
1:A:156:VAL:HG23	1:A:157:ALA:N	2.32	0.44
2:B:177:VAL:HG23	2:B:214:CYS:SG	2.58	0.44
2:B:200:ASN:ND2	2:B:200:ASN:N	2.65	0.43
1:A:377:LEU:HD12	1:A:390:VAL:HG22	2.00	0.43
1:A:13:LEU:HD11	1:A:17:ILE:HD11	2.01	0.43
1:A:406:VAL:HG12	1:A:410:LEU:HD12	2.01	0.42
2:B:165:LEU:HD21	2:B:183:ALA:HB3	2.01	0.42
3:M:171:ASN:O	3:M:429:VAL:HA	2.19	0.42
3:N:56:PHE:HB2	3:N:67:ALA:HB3	2.01	0.42
2:B:570:LEU:HG	2:B:574:TYR:CE2	2.53	0.42
3:M:214:PHE:CZ	3:M:216:MET:HE3	2.54	0.42
1:A:50:LEU:HD23	1:A:50:LEU:N	2.34	0.42
2:B:220:ILE:HG12	2:B:254:ALA:HB1	2.01	0.42
3:M:346:VAL:HG22	3:M:379:ALA:HB2	2.02	0.42
3:M:290:THR:HG21	3:M:408:SER:CB	2.50	0.42
3:N:20:TYR:CE2	3:N:116:LEU:HD23	2.55	0.42
2:B:219:GLN:HE22	2:B:250:HIS:CE1	2.38	0.41
1:A:434:LYS:HD3	1:A:435:TYR:CZ	2.55	0.41
1:A:228:LEU:N	1:A:228:LEU:HD23	2.36	0.41
1:A:340:HIS:CE1	1:A:345:LEU:HD12	2.56	0.41
1:A:535:VAL:N	1:A:536:PRO:HD2	2.35	0.41
2:B:145:VAL:HG11	2:B:165:LEU:HD22	2.01	0.41
3:M:254:ILE:O	3:M:254:ILE:HG23	2.20	0.41
1:A:233:LEU:HD21	1:A:262:LEU:HD21	2.03	0.41
1:A:401:ASN:HB3	1:A:405:ILE:HD12	2.02	0.41
2:B:267:LEU:HA	2:B:267:LEU:HD12	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:135:LEU:O	6:S:139:GLN:HB3	2.20	0.41
1:A:339:GLN:HE21	1:A:372:THR:HG21	1.86	0.41
2:B:366:ASP:OD1	3:N:43:VAL:HG11	2.20	0.41
6:S:140:SER:OG	6:S:141:LEU:N	2.54	0.41
1:A:461:VAL:HA	1:A:612:ILE:HD11	2.03	0.41
2:B:492:PHE:HA	2:B:499:THR:HG21	2.02	0.41
1:A:107:GLU:O	1:A:111:LEU:HG	2.21	0.40
1:A:83:LEU:HD11	1:A:98:ILE:HD13	2.03	0.40
1:A:87:ARG:HD3	6:S:142:GLU:CG	2.50	0.40
2:B:149:HIS:HA	2:B:153:ALA:HB2	2.03	0.40
2:B:305:ASN:OD1	2:B:567:ILE:O	2.39	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	612/621 (99%)	563 (92%)	35 (6%)	14 (2%)	6	28
2	B	500/592 (84%)	449 (90%)	44 (9%)	7 (1%)	11	37
3	M	251/446 (56%)	211 (84%)	35 (14%)	5 (2%)	7	30
3	N	141/446 (32%)	123 (87%)	18 (13%)	0	100	100
4	P	4/6 (67%)	4 (100%)	0	0	100	100
5	Q	6/10 (60%)	4 (67%)	2 (33%)	0	100	100
6	S	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	22	55
All	All	1654/2263 (73%)	1482 (90%)	145 (9%)	27 (2%)	9	34

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	SER
1	A	601	GLU
2	B	200	ASN
3	M	252	ILE
3	M	254	ILE
6	S	96	HIS
1	A	189	THR
1	A	384	SER
1	A	421	ARG
1	A	491	ALA
2	B	321	ILE
1	A	272	GLU
1	A	453	ALA
1	A	473	ASP
1	A	589	VAL
1	A	602	MET
2	B	99	ASN
2	B	194	SER
3	M	208	GLY
2	B	426	GLU
3	M	191	VAL
3	M	295	ILE
1	A	457	VAL
2	B	270	LEU
1	A	156	VAL
2	B	102	ILE
1	A	452	ILE

### 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	538/543 (99%)	490 (91%)	48 (9%)	9	33
2	B	452/533 (85%)	404 (89%)	48 (11%)	6	24
3	M	227/398 (57%)	200 (88%)	27 (12%)	5	19
3	N	124/398 (31%)	114 (92%)	10 (8%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P	6/6 (100%)	6 (100%)	0	100	100
5	Q	8/9 (89%)	5 (62%)	3 (38%)	0	0
6	S	131/131 (100%)	118 (90%)	13 (10%)	8	27
All	All	1486/2018 (74%)	1337 (90%)	149 (10%)	7	27

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	21	ARG
1	A	24	LYS
1	A	27	GLU
1	A	35	LYS
1	A	41	ARG
1	A	45	LYS
1	A	48	LYS
1	A	50	LEU
1	A	68	LEU
1	A	71	ASP
1	A	92	GLN
1	A	155	LEU
1	A	216	GLN
1	A	217	LYS
1	A	220	GLU
1	A	228	LEU
1	A	257	LEU
1	A	273	ASP
1	A	292	GLN
1	A	315	SER
1	A	323	GLU
1	A	331	CYS
1	A	355	THR
1	A	404	GLN
1	A	413	LEU
1	A	417	ASP
1	A	420	ILE
1	A	422	GLU
1	A	437	VAL
1	A	440	THR
1	A	449	LEU
1	A	475	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	488	GLN
1	A	492	CYS
1	A	516	ARG
1	A	518	SER
1	A	535	VAL
1	A	540	LEU
1	A	543	SER
1	A	546	ILE
1	A	555	VAL
1	A	568	GLN
1	A	576	LEU
1	A	577	GLN
1	A	594	ILE
1	A	595	LEU
1	A	608	ARG
2	B	115	VAL
2	B	131	LYS
2	B	157	GLU
2	B	200	ASN
2	B	201	PRO
2	B	214	CYS
2	B	224	ASP
2	B	232	LYS
2	B	233	ASP
2	B	234	ASP
2	B	248	LEU
2	B	264	MET
2	B	268	GLU
2	B	269	LEU
2	B	270	LEU
2	B	279	MET
2	B	284	LEU
2	B	317	LEU
2	B	318	LYS
2	B	355	LEU
2	B	357	GLU
2	B	360	GLU
2	B	375	ARG
2	B	384	VAL
2	B	389	GLU
2	B	404	ASN
2	B	413	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	432	LEU
2	B	436	LEU
2	B	437	ASP
2	B	458	ARG
2	B	460	ASP
2	B	461	ASN
2	B	463	ASP
2	B	464	GLU
2	B	478	THR
2	B	485	LEU
2	B	489	VAL
2	B	502	LEU
2	B	503	VAL
2	B	521	ASP
2	B	529	LEU
2	B	545	LYS
2	B	554	LEU
2	B	556	GLU
2	B	558	THR
2	B	565	CYS
2	B	567	ILE
3	M	169	ARG
3	M	170	ARG
3	M	190	GLN
3	M	192	LEU
3	M	206	LEU
3	M	209	MET
3	M	219	LYS
3	M	258	THR
3	M	267	LYS
3	M	272	ARG
3	M	275	SER
3	M	294	ILE
3	M	299	ARG
3	M	300	VAL
3	M	305	ARG
3	M	313	GLU
3	M	327	LEU
3	M	339	LEU
3	M	340	ASN
3	M	350	LYS
3	M	354	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	M	378	SER
3	M	384	LEU
3	M	390	LYS
3	M	391	LYS
3	M	415	LEU
3	M	416	LYS
3	N	15	LEU
3	N	16	ILE
3	N	18	ARG
3	N	36	VAL
3	N	44	ARG
3	N	48	THR
3	N	80	GLU
3	N	93	PHE
3	N	96	ILE
3	N	134	THR
5	Q	2	MET
5	Q	5	ILE
5	Q	7	ARG
6	S	3	ARG
6	S	15	ARG
6	S	18	LYS
6	S	21	MET
6	S	54	ASN
6	S	75	ASP
6	S	93	GLU
6	S	109	LYS
6	S	116	GLU
6	S	126	THR
6	S	129	THR
6	S	141	LEU
6	S	142	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	216	GLN
1	A	292	GLN
1	A	339	GLN
1	A	401	ASN
2	B	173	ASN
2	B	200	ASN

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Mol	Chain	Res	Type
2	B	219	GLN
2	B	305	ASN
2	B	319	GLN
2	B	461	ASN
3	N	62	ASN
3	N	123	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](#)

1 non-standard protein/DNA/RNA residue is 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
5	SEP	Q	3	5	8,9,10	0.71	0	8,12,14	1.20	1 (12%)

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
5	SEP	Q	3	5	-	2/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	3	SEP	P-OG-CB	2.00	123.81	118.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	3	SEP	CA-CB-OG-P
5	Q	3	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

## 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 i

### 6.1 Protein, DNA and RNA chains i

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	614/621 (98%)	0.32	10 (1%) 72 70	79, 121, 176, 229	0
2	B	502/592 (84%)	0.52	40 (7%) 12 13	81, 137, 260, 311	0
3	M	255/446 (57%)	0.04	5 (1%) 65 64	104, 162, 224, 270	0
3	N	143/446 (32%)	1.72	56 (39%) 0 0	121, 190, 237, 280	0
4	P	6/6 (100%)	0.10	0 100 100	158, 182, 208, 215	0
5	Q	8/10 (80%)	1.25	2 (25%) 0 0	142, 169, 190, 193	0
6	S	142/142 (100%)	0.39	2 (1%) 75 74	84, 117, 160, 185	0
All	All	1670/2263 (73%)	0.47	115 (6%) 16 18	79, 136, 236, 311	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	143	GLN	9.4
3	N	124	SER	7.2
2	B	85	ILE	6.8
3	N	65	LEU	6.4
3	N	138	ILE	6.0
2	B	91	PHE	5.6
3	N	126	THR	5.5
2	B	110	MET	5.2
2	B	122	LEU	5.2
5	Q	10	SER	5.0
3	N	137	GLY	5.0
3	N	133	ILE	4.7
3	N	125	GLU	4.5
3	N	16	ILE	4.4
3	N	136	GLN	4.4
3	N	127	GLY	4.3
3	N	141	GLN	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	N	111	LEU	4.1
3	M	268	PHE	4.1
2	B	121	TYR	4.1
3	M	392	TRP	4.1
2	B	84	ALA	4.0
3	N	122	GLN	3.9
3	N	101	ILE	3.9
3	N	123	ASN	3.9
3	N	92	TYR	3.9
3	N	88	VAL	3.9
2	B	117	LYS	3.8
3	N	131	THR	3.8
2	B	86	MET	3.8
2	B	89	ASN	3.8
2	B	126	LEU	3.7
2	B	106	ALA	3.6
3	N	85	MET	3.6
3	N	128	ALA	3.6
3	N	89	MET	3.4
1	A	590	ALA	3.4
1	A	242	THR	3.4
3	N	121	PRO	3.4
3	N	66	ALA	3.3
2	B	81	PRO	3.3
2	B	88	VAL	3.2
2	B	130	LEU	3.2
3	M	446	CYS	3.2
1	A	265	LEU	3.2
3	N	106	VAL	3.1
1	A	305	ALA	3.0
3	N	116	LEU	3.0
5	Q	8	LEU	3.0
2	B	113	ILE	3.0
2	B	95	CYS	3.0
1	A	196	LEU	3.0
3	N	129	LEU	3.0
3	N	64	TRP	3.0
2	B	114	ARG	3.0
2	B	115	VAL	3.0
2	B	146	ALA	2.9
2	B	227	SER	2.9
2	B	101	LEU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	N	5	LEU	2.9
3	N	81	PHE	2.9
2	B	156	VAL	2.8
3	N	6	PHE	2.8
3	N	115	ILE	2.8
3	N	139	LYS	2.8
3	N	103	ASN	2.7
3	M	269	ASP	2.7
3	N	140	SER	2.7
2	B	118	ILE	2.7
6	S	67	PHE	2.6
3	N	142	HIS	2.6
2	B	231	PRO	2.6
3	N	1	MET	2.6
3	N	104	ASN	2.5
2	B	211	LEU	2.5
2	B	169	ILE	2.5
2	B	257	LEU	2.5
1	A	337	PHE	2.5
3	N	8	TYR	2.4
1	A	239	SER	2.4
3	N	43	VAL	2.4
2	B	143	VAL	2.4
3	N	118	PHE	2.4
2	B	288	LEU	2.3
3	N	15	LEU	2.3
3	N	24	ILE	2.3
3	N	112	LEU	2.3
3	M	417	VAL	2.3
3	N	91	ALA	2.3
3	N	4	GLY	2.3
3	N	110	GLU	2.3
2	B	120	GLU	2.2
2	B	264	MET	2.2
1	A	60	CYS	2.2
3	N	120	TYR	2.2
3	N	87	ASP	2.2
2	B	83	MET	2.2
2	B	102	ILE	2.2
3	N	96	ILE	2.2
3	N	107	LEU	2.1
2	B	111	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	165	LEU	2.1
2	B	151	ILE	2.1
1	A	241	SER	2.1
2	B	116	ASP	2.1
6	S	60	ARG	2.1
2	B	240	ILE	2.1
2	B	82	ASP	2.1
3	N	82	LEU	2.1
3	N	114	GLU	2.1
3	N	108	ILE	2.1
3	N	20	TYR	2.0
3	N	105	PHE	2.0
1	A	334	LEU	2.0
2	B	148	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SEP	Q	3	10/11	0.90	0.14	149,224,292,333	0

## 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.