



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 6QH6 / pdb_00006qh6
Title : AP2 clathrin adaptor 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 : 5.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

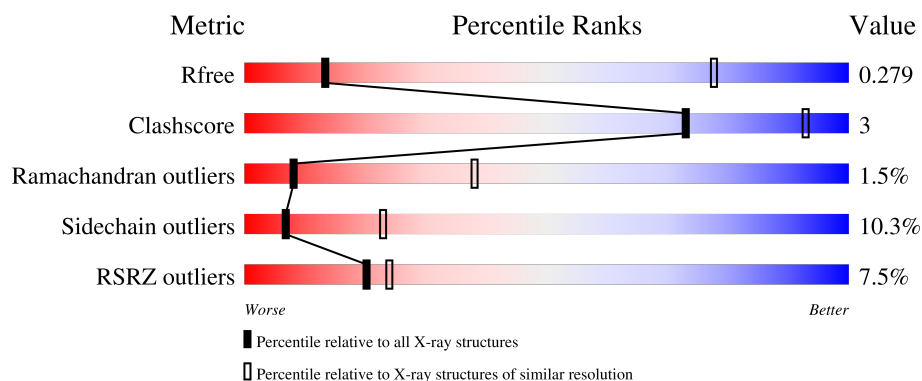
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	6% 81% 16% ..
2	B	592	8% 68% 16% • 15%
3	M	446	4% 48% 8% • 43%
4	N	446	2% 26% 7% 68%
5	P	6	100%

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Mol	Chain	Length	Quality of chain
6	Q	10	50% 30% 10% 10%
7	S	142	7% 87% 11%

2 Entry composition

There are 7 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
1	A	614	Total	C	N	O	S	0	0	0
			4844	3085	834	904	21			

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
2	B	502	Total	C	N	O	S	0	0	0
			3974	2529	661	763	21			

- Molecule 3 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	255	Total	C	N	O	S	0	0	0
			2033	1310	350	359	14			

There are 11 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
M	243	SER	-	insertion	UNP Q3ZC13
M	244	GLU	-	insertion	UNP Q3ZC13
M	245	GLU	-	insertion	UNP Q3ZC13

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Chain	Residue	Modelled	Actual	Comment	Reference
M	246	ASP	-	insertion	UNP Q3ZC13
M	247	LEU	-	insertion	UNP Q3ZC13

- Molecule 4 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	143	Total	C	N	O	S	0	0	0
			1157	742	203	207	5			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	237	MET	-	insertion	UNP P84092
N	238	GLU	-	insertion	UNP P84092
N	239	GLN	-	insertion	UNP P84092
N	240	LYS	-	insertion	UNP P84092
N	241	LEU	-	insertion	UNP P84092
N	242	ILE	-	insertion	UNP P84092
N	243	SER	-	insertion	UNP P84092
N	244	GLU	-	insertion	UNP P84092
N	245	GLU	-	insertion	UNP P84092
N	246	ASP	-	insertion	UNP P84092
N	247	LEU	-	insertion	UNP P84092

- Molecule 5 is a protein called TGN38 CARGO PEPTIDE.

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

- Molecule 6 is a protein called CD4 CARGO PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	Q	9	Total	C	N	O	P S	10	0	0
			77	46	14	15	1 1			

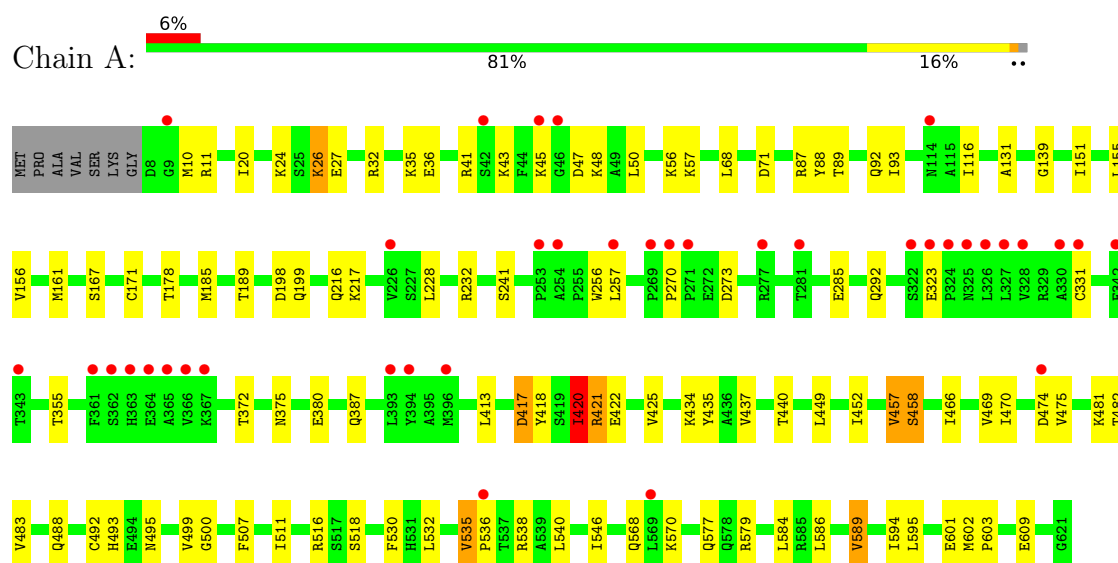
- Molecule 7 is a protein called AP-2 complex subunit sigma.

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

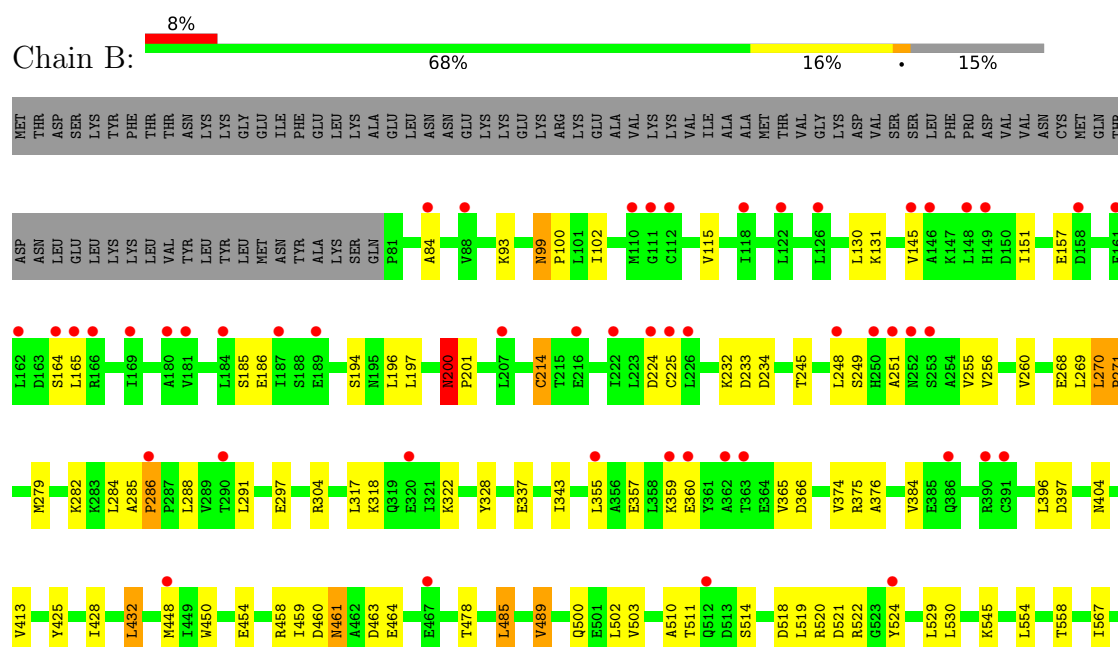
3 Residue-property plots

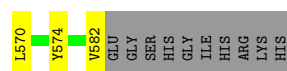
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

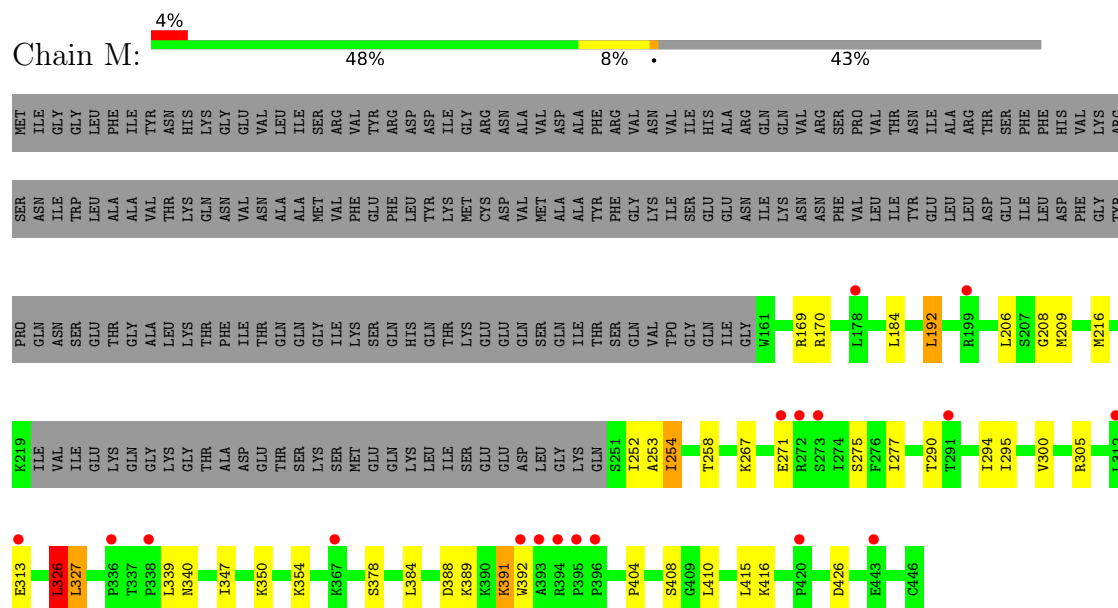


• Molecule 2: AP-2 complex subunit beta

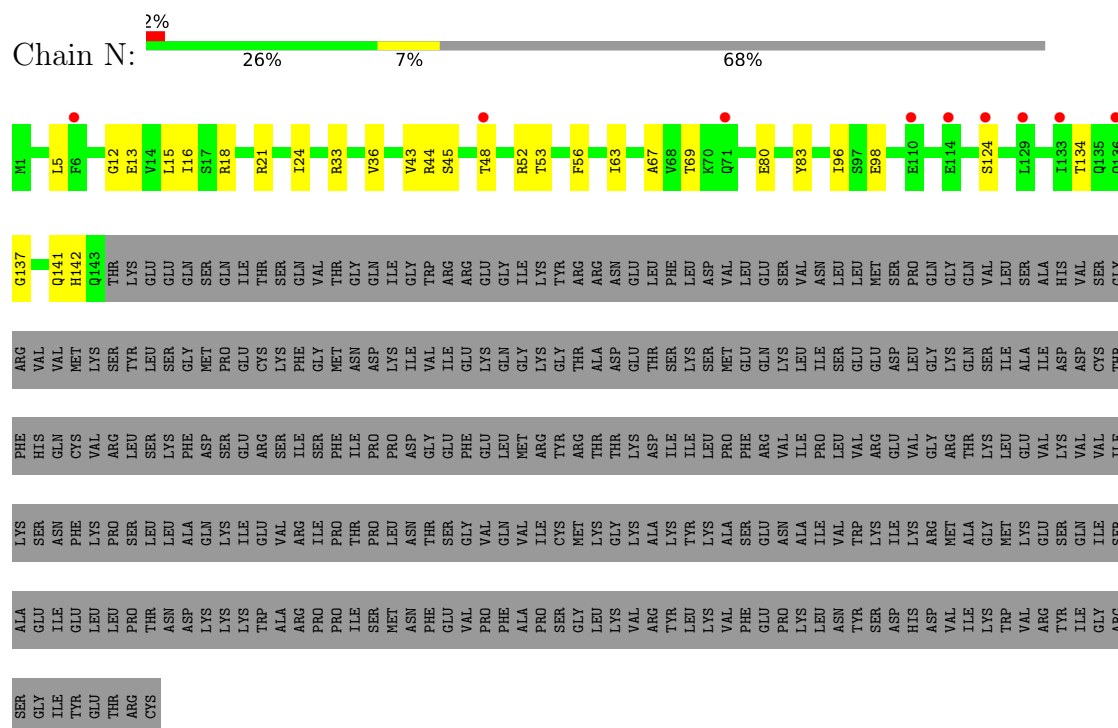




• Molecule 3: AP-2 complex subunit mu



• Molecule 4: AP-2 complex subunit mu



• Molecule 5: TGN38 CARGO PEPTIDE

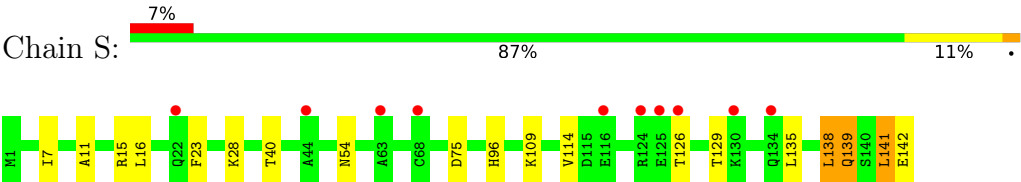


There are no outlier residues recorded for this chain.

● Molecule 6: CD4 CARGO PEPTIDE



● Molecule 7: 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, α , β , γ	180.50Å 180.50Å 210.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.00 – 5.00 91.00 – 5.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (91.00-5.00) 99.4 (91.00-5.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 5.12Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.259 , 0.285 0.244 , 0.279	Depositor DCC
R_{free} test set	743 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	256.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 559.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13342	wwPDB-VP
Average B, all atoms (Å ²)	325.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.70	2/4929 (0.0%)	1.18	7/6680 (0.1%)
2	B	0.72	0/4038	1.17	8/5488 (0.1%)
3	M	0.79	0/2076	1.00	3/2797 (0.1%)
4	N	0.79	0/1180	1.03	1/1592 (0.1%)
5	P	0.89	0/57	0.93	0/74
6	Q	0.68	0/65	1.13	1/82 (1.2%)
7	S	0.61	0/1224	1.07	3/1650 (0.2%)
All	All	0.72	2/13569 (0.0%)	1.13	23/18363 (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
2	B	0	1
3	M	0	1
6	Q	0	1
7	S	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	CA-CB	5.48	1.57	1.54
1	A	270	PRO	CA-C	5.36	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	GLU	N-CA-C	8.01	120.92	111.71
7	S	139	GLN	N-CA-C	-6.92	104.97	113.41
2	B	84	ALA	N-CA-C	6.85	118.82	111.36
2	B	286	PRO	N-CA-C	6.31	118.40	110.70
2	B	214	CYS	N-CA-C	6.28	118.41	110.24
2	B	249	SER	N-CA-C	5.70	117.89	110.53
4	N	124	SER	N-CA-C	5.57	117.12	107.93
1	A	241	SER	N-CA-C	5.49	117.98	111.33
1	A	420	ILE	N-CA-CB	5.47	117.57	110.57
2	B	234	ASP	N-CA-C	5.46	116.91	111.07
6	Q	8	LEU	N-CA-C	5.45	118.14	111.82
7	S	11	ALA	N-CA-C	5.38	117.14	111.28
3	M	388	ASP	N-CA-C	5.37	119.00	111.74
2	B	151	ILE	N-CA-C	5.34	115.55	107.75
1	A	273	ASP	CA-C-N	5.30	124.75	119.24
1	A	273	ASP	C-N-CA	5.30	124.75	119.24
3	M	326	LEU	N-CA-C	5.26	117.87	110.14
2	B	365	VAL	N-CA-C	5.20	116.28	111.45
1	A	420	ILE	CB-CA-C	-5.14	105.28	112.02
3	M	426	ASP	N-CA-C	5.08	118.74	112.54
1	A	418	TYR	N-CA-C	5.04	116.77	111.28
2	B	328	TYR	N-CA-C	5.01	116.55	111.14
7	S	40	THR	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	271	PRO	Peptide
3	M	326	LEU	Peptide
6	Q	2	MET	Mainchain
7	S	138	LEU	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	A	4844	0	4956	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3974	0	4061	35	0
3	M	2033	0	2097	6	0
4	N	1157	0	1158	10	0
5	P	57	0	53	0	0
6	Q	77	0	83	0	0
7	S	1200	0	1195	10	0
All	All	13342	0	13603	85	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 3.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLN:HE22	1:A:420:ILE:HG21	1.53	0.73
2:B:297:GLU:HB2	4:N:83:TYR:OH	1.88	0.72
2:B:200:ASN:HB3	2:B:201:PRO:HD2	1.75	0.69
2:B:343:ILE:HD11	2:B:376:ALA:HB1	1.75	0.69
2:B:200:ASN:HB3	2:B:201:PRO:CD	2.24	0.66
2:B:200:ASN:N	2:B:200:ASN:HD22	1.96	0.63
7:S:138:LEU:HA	7:S:141:LEU:HD22	1.80	0.63
1:A:198:ASP:O	1:A:232:ARG:NH2	2.33	0.61
1:A:457:VAL:HG13	1:A:458:SER:N	2.16	0.61
1:A:481:LYS:HA	1:A:511:ILE:HD12	1.84	0.60
1:A:603:PRO:O	2:B:520:ARG:NH2	2.32	0.59
1:A:116:ILE:HG23	1:A:131:ALA:HB1	1.85	0.59
1:A:425:VAL:HG11	1:A:457:VAL:HA	1.86	0.57
1:A:457:VAL:HG13	1:A:458:SER:H	1.68	0.57
2:B:459:ILE:HG22	2:B:461:ASN:HD22	1.69	0.57
1:A:10:MET:HE1	1:A:56:LYS:HE3	1.87	0.57
2:B:582:VAL:H	4:N:52:ARG:HH11	1.52	0.56
2:B:256:VAL:O	2:B:260:VAL:HG23	2.06	0.56
2:B:200:ASN:CB	2:B:201:PRO:HD2	2.37	0.55
1:A:457:VAL:CG1	1:A:458:SER:H	2.21	0.54
1:A:481:LYS:HA	1:A:511:ILE:CD1	2.37	0.54
2:B:582:VAL:H	4:N:52:ARG:HD3	1.72	0.54
2:B:251:ALA:HB3	2:B:255:VAL:HG23	1.90	0.54
3:M:290:THR:HG21	3:M:408:SER:HB2	1.89	0.53
1:A:483:VAL:HG11	1:A:500:GLY:HA2	1.92	0.51
2:B:200:ASN:CB	2:B:201:PRO:CD	2.89	0.51
3:M:327:LEU:HG	3:M:404:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:HA	1:A:47:ASP:HB3	1.93	0.50
4:N:56:PHE:HB2	4:N:67:ALA:HB3	1.93	0.50
1:A:139:GLY:O	1:A:178:THR:HG21	2.12	0.49
2:B:185:SER:OG	2:B:225:CYS:SG	2.67	0.49
2:B:194:SER:HA	2:B:197:LEU:HD11	1.95	0.49
1:A:87:ARG:HD3	7:S:142:GLU:CG	2.43	0.48
1:A:457:VAL:CG1	1:A:458:SER:N	2.76	0.48
2:B:186:GLU:OE1	4:N:21:ARG:NH2	2.47	0.48
1:A:387:GLN:NE2	1:A:420:ILE:HG21	2.27	0.47
2:B:130:LEU:HD13	2:B:164:SER:HB3	1.96	0.47
1:A:26:LYS:HE3	1:A:26:LYS:HA	1.97	0.47
4:N:63:ILE:HD11	4:N:98:GLU:HG3	1.96	0.47
3:M:184:LEU:HD22	3:M:192:LEU:HD21	1.95	0.47
1:A:32:ARG:HH12	1:A:36:GLU:HG2	1.80	0.47
1:A:493:HIS:CD2	1:A:495:ASN:H	2.34	0.46
2:B:510:ALA:O	2:B:520:ARG:HA	2.16	0.45
1:A:466:ILE:HD11	1:A:499:VAL:HA	1.98	0.45
3:M:290:THR:HG21	3:M:408:SER:CB	2.47	0.45
2:B:459:ILE:HG22	2:B:461:ASN:ND2	2.30	0.45
1:A:579:ARG:HG2	2:B:522:ARG:NH1	2.31	0.45
2:B:396:LEU:HD21	2:B:428:ILE:HG23	1.99	0.45
1:A:470:ILE:HG22	1:A:507:PHE:CE2	2.52	0.45
2:B:514:SER:HB2	2:B:519:LEU:HD23	1.98	0.45
1:A:434:LYS:HD3	1:A:435:TYR:CZ	2.52	0.44
2:B:288:LEU:HA	2:B:291:LEU:HD12	2.00	0.44
7:S:23:PHE:HB2	7:S:28:LYS:HG3	2.00	0.44
2:B:366:ASP:OD1	4:N:43:VAL:HG11	2.18	0.43
4:N:12:GLY:O	4:N:33:ARG:HD3	2.18	0.43
2:B:145:VAL:HG21	2:B:165:LEU:HD13	1.99	0.43
2:B:511:THR:HG23	2:B:524:TYR:CE2	2.53	0.43
1:A:88:TYR:N	7:S:142:GLU:OXT	2.50	0.42
3:M:254:ILE:O	3:M:254:ILE:HG23	2.19	0.42
2:B:450:TRP:CZ2	2:B:454:GLU:HG3	2.54	0.42
7:S:7:ILE:CD1	7:S:16:LEU:HD23	2.49	0.42
7:S:135:LEU:O	7:S:139:GLN:HB3	2.19	0.42
1:A:535:VAL:N	1:A:536:PRO:HD2	2.34	0.42
1:A:420:ILE:O	1:A:421:ARG:C	2.63	0.42
2:B:428:ILE:HG22	2:B:432:LEU:HD13	2.02	0.42
2:B:425:TYR:HB3	2:B:428:ILE:HD12	2.02	0.41
2:B:285:ALA:HB3	2:B:286:PRO:HD3	2.02	0.41
1:A:87:ARG:HD3	7:S:142:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ASN:HA	2:B:100:PRO:HD3	1.94	0.41
2:B:570:LEU:HG	2:B:574:TYR:CE2	2.55	0.41
2:B:485:LEU:O	2:B:489:VAL:HG13	2.20	0.41
7:S:7:ILE:HD12	7:S:16:LEU:HD23	2.02	0.41
1:A:11:ARG:HB3	1:A:57:LYS:HD3	2.03	0.41
1:A:167:SER:O	1:A:171:CYS:HB2	2.21	0.41
1:A:417:ASP:OD1	1:A:420:ILE:HG13	2.21	0.41
4:N:15:LEU:HD21	4:N:98:GLU:HG2	2.03	0.41
1:A:372:THR:O	1:A:375:ASN:HB3	2.20	0.41
1:A:185:MET:HE3	1:A:185:MET:HA	2.02	0.40
7:S:16:LEU:HD21	7:S:114:VAL:HG21	2.02	0.40
1:A:530:PHE:CE2	1:A:538:ARG:HD2	2.56	0.40
2:B:304:ARG:HD2	2:B:337:GLU:HG3	2.04	0.40
3:M:326:LEU:HD23	3:M:327:LEU:HD23	2.03	0.40
2:B:518:ASP:O	2:B:521:ASP:HB2	2.21	0.40
1:A:256:TRP:CE3	7:S:126:THR:HB	2.57	0.40
4:N:24:ILE:HD11	4:N:69:THR:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	612/621 (99%)	567 (93%)	36 (6%)	9 (2%)	8	38
2	B	500/592 (84%)	448 (90%)	46 (9%)	6 (1%)	10	42
3	M	251/446 (56%)	214 (85%)	30 (12%)	7 (3%)	4	24
4	N	141/446 (32%)	129 (92%)	11 (8%)	1 (1%)	18	55
5	P	4/6 (67%)	4 (100%)	0	0	100	100
6	Q	6/10 (60%)	4 (67%)	1 (17%)	1 (17%)	0	3
7	S	140/142 (99%)	130 (93%)	9 (6%)	1 (1%)	18	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1654/2263 (73%)	1496 (90%)	133 (8%)	25 (2%)	8	38

All (25) 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	Q	4	GLN
7	S	96	HIS
1	A	189	THR
1	A	421	ARG
1	A	589	VAL
3	M	295	ILE
3	M	391	LYS
3	M	392	TRP
1	A	602	MET
2	B	99	ASN
2	B	500	GLN
3	M	253	ALA
4	N	137	GLY
1	A	457	VAL
2	B	270	LEU
1	A	156	VAL
1	A	452	ILE
2	B	102	ILE
2	B	271	PRO
3	M	208	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	538/543 (99%)	484 (90%)	54 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	452/533 (85%)	403 (89%)	49 (11%)	6	21
3	M	227/397 (57%)	199 (88%)	28 (12%)	4	18
4	N	124/398 (31%)	110 (89%)	14 (11%)	5	20
5	P	6/6 (100%)	6 (100%)	0	100	100
6	Q	8/9 (89%)	6 (75%)	2 (25%)	0	4
7	S	131/131 (100%)	125 (95%)	6 (5%)	24	46
All	All	1486/2017 (74%)	1333 (90%)	153 (10%)	7	23

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	24	LYS
1	A	26	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	89	THR
1	A	92	GLN
1	A	93	ILE
1	A	155	LEU
1	A	161	MET
1	A	199	GLN
1	A	216	GLN
1	A	217	LYS
1	A	228	LEU
1	A	257	LEU
1	A	285	GLU
1	A	292	GLN
1	A	323	GLU
1	A	331	CYS
1	A	355	THR
1	A	413	LEU
1	A	417	ASP
1	A	420	ILE

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Mol	Chain	Res	Type
1	A	422	GLU
1	A	437	VAL
1	A	440	THR
1	A	449	LEU
1	A	469	VAL
1	A	474	ASP
1	A	475	VAL
1	A	482	THR
1	A	488	GLN
1	A	492	CYS
1	A	516	ARG
1	A	518	SER
1	A	532	LEU
1	A	535	VAL
1	A	540	LEU
1	A	546	ILE
1	A	568	GLN
1	A	570	LYS
1	A	577	GLN
1	A	584	LEU
1	A	586	LEU
1	A	589	VAL
1	A	594	ILE
1	A	595	LEU
1	A	609	GLU
2	B	93	LYS
2	B	115	VAL
2	B	131	LYS
2	B	157	GLU
2	B	196	LEU
2	B	200	ASN
2	B	214	CYS
2	B	224	ASP
2	B	232	LYS
2	B	233	ASP
2	B	245	THR
2	B	248	LEU
2	B	268	GLU
2	B	269	LEU
2	B	270	LEU
2	B	279	MET
2	B	282	LYS

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Mol	Chain	Res	Type
2	B	284	LEU
2	B	317	LEU
2	B	318	LYS
2	B	322	LYS
2	B	355	LEU
2	B	357	GLU
2	B	359	LYS
2	B	360	GLU
2	B	374	VAL
2	B	375	ARG
2	B	384	VAL
2	B	397	ASP
2	B	404	ASN
2	B	413	VAL
2	B	432	LEU
2	B	448	MET
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	529	LEU
2	B	530	LEU
2	B	545	LYS
2	B	554	LEU
2	B	558	THR
2	B	567	ILE
3	M	169	ARG
3	M	170	ARG
3	M	192	LEU
3	M	206	LEU
3	M	209	MET
3	M	216	MET
3	M	258	THR
3	M	267	LYS
3	M	271	GLU
3	M	275	SER

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Mol	Chain	Res	Type
3	M	277	ILE
3	M	294	ILE
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	347	ILE
3	M	350	LYS
3	M	354	LYS
3	M	378	SER
3	M	384	LEU
3	M	389	LYS
3	M	391	LYS
3	M	410	LEU
3	M	415	LEU
3	M	416	LYS
4	N	5	LEU
4	N	13	GLU
4	N	16	ILE
4	N	18	ARG
4	N	36	VAL
4	N	44	ARG
4	N	45	SER
4	N	48	THR
4	N	53	THR
4	N	80	GLU
4	N	96	ILE
4	N	134	THR
4	N	141	GLN
4	N	142	HIS
6	Q	2	MET
6	Q	5	ILE
7	S	15	ARG
7	S	54	ASN
7	S	75	ASP
7	S	109	LYS
7	S	129	THR
7	S	141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	70	HIS
1	A	199	GLN
1	A	292	GLN
1	A	307	ASN
1	A	336	GLN
1	A	369	HIS
1	A	403	GLN
1	A	577	GLN
2	B	154	GLN
2	B	159	GLN
2	B	179	ASN
2	B	193	ASN
2	B	200	ASN
2	B	219	GLN
2	B	250	HIS
2	B	305	ASN
2	B	461	ASN
3	M	329	GLN
4	N	38	HIS
4	N	74	ASN
4	N	122	GLN
6	Q	4	GLN
7	S	48	ASN
7	S	86	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
6	SEP	Q	3	6	8,9,10	0.74	0	7,12,14	1.03	0

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
6	SEP	Q	3	6	-	2/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Q	3	SEP	CA-CB-OG-P
6	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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	3:SEP	C	4:GLN	N	1.92

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, 95th 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	A	614/621 (98%)	0.08	38 (6%)	26	29	156, 286, 389, 516	0
2	B	502/592 (84%)	0.26	50 (9%)	12	18	157, 312, 544, 686	0
3	M	255/446 (57%)	0.12	18 (7%)	22	25	210, 355, 499, 596	0
4	N	143/446 (32%)	0.43	9 (6%)	26	28	229, 383, 529, 628	0
5	P	6/6 (100%)	0.01	0	100	100	364, 395, 431, 447	0
6	Q	8/10 (80%)	-0.57	0	100	100	286, 348, 390, 397	0
7	S	142/142 (100%)	0.07	10 (7%)	22	25	195, 282, 354, 401	0
All	All	1670/2263 (73%)	0.16	125 (7%)	20	24	156, 310, 492, 686	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	145	VAL	7.6
4	N	114	GLU	6.9
3	M	272	ARG	6.3
2	B	148	LEU	6.1
1	A	396	MET	6.0
2	B	110	MET	6.0
2	B	165	LEU	5.9
2	B	467	GLU	5.8
2	B	184	LEU	5.8
3	M	395	PRO	5.6
2	B	252	ASN	5.5
2	B	390	ARG	5.5
1	A	328	VAL	5.5
1	A	366	VAL	5.4
1	A	323	GLU	5.4
3	M	392	TRP	5.2
1	A	327	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	271	PRO	5.1
1	A	324	PRO	5.0
1	A	362	SER	5.0
1	A	331	CYS	4.9
2	B	161	PHE	4.7
7	S	44	ALA	4.6
2	B	122	LEU	4.5
2	B	386	GLN	4.5
7	S	134	GLN	4.5
1	A	342	GLU	4.3
1	A	326	LEU	4.1
7	S	22	GLN	4.1
2	B	162	LEU	4.0
2	B	189	GLU	4.0
2	B	118	ILE	4.0
4	N	129	LEU	4.0
2	B	84	ALA	3.9
3	M	396	PRO	3.9
3	M	199	ARG	3.9
2	B	253	SER	3.9
2	B	250	HIS	3.8
4	N	133	ILE	3.6
2	B	158	ASP	3.5
3	M	367	LYS	3.5
2	B	187	ILE	3.5
3	M	273	SER	3.5
7	S	63	ALA	3.5
1	A	365	ALA	3.3
1	A	367	LYS	3.3
1	A	270	PRO	3.3
3	M	271	GLU	3.3
3	M	393	ALA	3.2
1	A	253	PRO	3.2
1	A	361	PHE	3.2
7	S	116	GLU	3.2
3	M	336	PRO	3.1
7	S	125	GLU	3.1
3	M	420	PRO	3.1
2	B	207	LEU	3.0
2	B	166	ARG	3.0
4	N	124	SER	3.0
1	A	277	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	281	THR	2.9
1	A	322	SER	2.9
2	B	222	ILE	2.9
2	B	290	THR	2.9
2	B	363	THR	2.9
2	B	320	GLU	2.9
4	N	48	THR	2.9
2	B	216	GLU	2.9
2	B	226	LEU	2.8
4	N	110	GLU	2.8
3	M	338	PRO	2.8
1	A	226	VAL	2.7
1	A	45	LYS	2.7
2	B	224	ASP	2.6
2	B	181	VAL	2.6
2	B	149	HIS	2.6
2	B	251	ALA	2.6
2	B	126	LEU	2.6
1	A	269	PRO	2.6
2	B	180	ALA	2.6
1	A	114	ASN	2.6
2	B	225	CYS	2.6
2	B	391	CYS	2.6
1	A	363	HIS	2.5
2	B	359	LYS	2.5
2	B	169	ILE	2.5
1	A	474	ASP	2.5
7	S	130	LYS	2.5
2	B	88	VAL	2.5
1	A	254	ALA	2.4
3	M	394	ARG	2.4
3	M	313	GLU	2.4
1	A	394	TYR	2.4
2	B	512	GLN	2.4
2	B	286	PRO	2.4
1	A	364	GLU	2.3
4	N	6	PHE	2.3
2	B	111	GLY	2.3
7	S	68	CYS	2.3
1	A	343	THR	2.3
1	A	569	LEU	2.3
1	A	330	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	N	136	GLN	2.3
2	B	248	LEU	2.2
2	B	355	LEU	2.2
7	S	124	ARG	2.2
2	B	146	ALA	2.2
1	A	9	GLY	2.1
2	B	112	CYS	2.1
1	A	325	ASN	2.1
3	M	291	THR	2.1
2	B	448	MET	2.1
2	B	362	ALA	2.1
3	M	312	LEU	2.1
2	B	524	TYR	2.1
1	A	42	SER	2.1
2	B	164	SER	2.1
3	M	443	GLU	2.1
2	B	360	GLU	2.1
4	N	71	GLN	2.1
3	M	178	LEU	2.1
7	S	126	THR	2.0
1	A	257	LEU	2.0
1	A	393	LEU	2.0
1	A	46	GLY	2.0
1	A	536	PRO	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, 95th 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(Å ²)	Q<0.9
6	SEP	Q	3	10/11	-	-	304,379,447,489	10

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.