Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 08:36 PM EDT

PDB ID	:	6W8S
Title	:	Crystal structure of metacaspase 4 from Arabidopsis
Authors	:	Zhu, P.; Yu, X.H.; Wang, C.; Zhang, Q.; Liu, W.; McSweeney, S.; Shanklin, J.; Lam, E.; Liu, Q.
Deposited on	:	2020-03-21
Resolution	:	3.48 Å(reported)

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

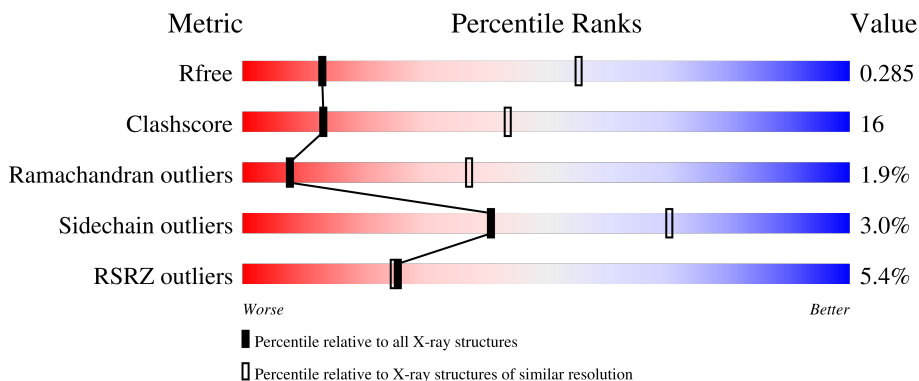|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.48 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	Percentile Ranks	Value
Rfree		0.285
Clashscore		16
Ramachandran outliers		1.9%
Sidechain outliers		3.0%
RSRZ outliers		5.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 <=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	426	4% 56% 27% • 15%
1	B	426	5% 55% 27% • 16%
1	C	426	3% 54% 29% • 15%
1	D	426	6% 54% 28% • 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	503	-	-	-	X

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 10908 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 Metacaspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2728	1684	465	561	18			
1	B	357	Total	C	N	O	S	0	0	0
			2698	1666	461	553	18			
1	C	361	Total	C	N	O	S	0	0	0
			2732	1688	465	561	18			
1	D	358	Total	C	N	O	S	0	0	0
			2710	1674	462	556	18			

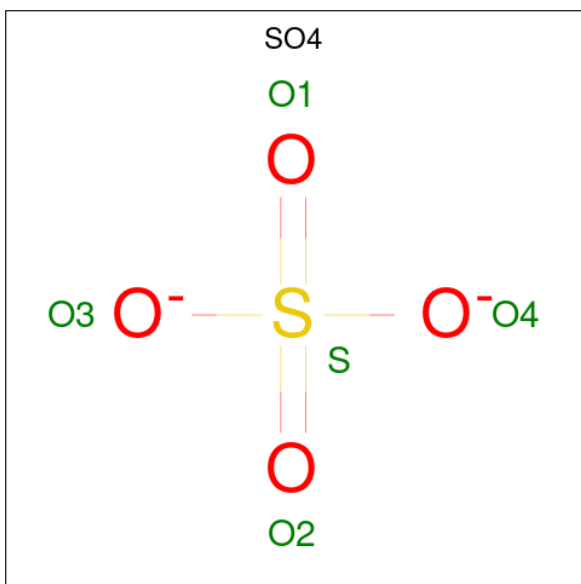There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	VAL	-	expression tag	UNP O64517
A	420	GLU	-	expression tag	UNP O64517
A	421	HIS	-	expression tag	UNP O64517
A	422	HIS	-	expression tag	UNP O64517
A	423	HIS	-	expression tag	UNP O64517
A	424	HIS	-	expression tag	UNP O64517
A	425	HIS	-	expression tag	UNP O64517
A	426	HIS	-	expression tag	UNP O64517
B	419	VAL	-	expression tag	UNP O64517
B	420	GLU	-	expression tag	UNP O64517
B	421	HIS	-	expression tag	UNP O64517
B	422	HIS	-	expression tag	UNP O64517
B	423	HIS	-	expression tag	UNP O64517
B	424	HIS	-	expression tag	UNP O64517
B	425	HIS	-	expression tag	UNP O64517
B	426	HIS	-	expression tag	UNP O64517
C	419	VAL	-	expression tag	UNP O64517
C	420	GLU	-	expression tag	UNP O64517
C	421	HIS	-	expression tag	UNP O64517
C	422	HIS	-	expression tag	UNP O64517
C	423	HIS	-	expression tag	UNP O64517

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Chain	Residue	Modelled	Actual	Comment	Reference
C	424	HIS	-	expression tag	UNP O64517
C	425	HIS	-	expression tag	UNP O64517
C	426	HIS	-	expression tag	UNP O64517
D	419	VAL	-	expression tag	UNP O64517
D	420	GLU	-	expression tag	UNP O64517
D	421	HIS	-	expression tag	UNP O64517
D	422	HIS	-	expression tag	UNP O64517
D	423	HIS	-	expression tag	UNP O64517
D	424	HIS	-	expression tag	UNP O64517
D	425	HIS	-	expression tag	UNP O64517
D	426	HIS	-	expression tag	UNP O64517

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

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: Metacaspase-4

Chain A:

- Molecule 1: Metacaspase-4

Chain B:

• Molecule 1: Metacaspase-4

Chain C:

• Molecule 1: Metacaspase-4

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	125.91Å 284.44Å 57.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.80 – 3.48 38.80 – 3.48	Depositor EDS
% Data completeness (in resolution range)	88.9 (38.80-3.48) 88.9 (38.80-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.250 , 0.284 0.252 , 0.285	Depositor DCC
R_{free} test set	1242 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	89.7	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.5	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10908	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: SO4

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	0.39	0/2766	0.74	1/3732 (0.0%)
1	B	0.34	0/2735	0.74	3/3688 (0.1%)
1	C	0.34	0/2769	0.73	2/3734 (0.1%)
1	D	0.41	1/2747 (0.0%)	0.77	1/3704 (0.0%)
All	All	0.37	1/11017 (0.0%)	0.74	7/14858 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	215	GLU	CB-CG	5.95	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	217	GLY	N-CA-C	6.00	128.10	113.10
1	B	334	LEU	CA-CB-CG	5.79	128.63	115.30
1	B	338	GLY	N-CA-C	-5.47	99.42	113.10
1	B	329	ARG	C-N-CA	5.23	133.28	122.30
1	C	338	GLY	N-CA-C	-5.20	100.09	113.10
1	A	338	GLY	N-CA-C	-5.12	100.31	113.10
1	D	294	LEU	CA-CB-CG	-5.03	103.73	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	2728	0	2672	86	0
1	B	2698	0	2645	80	0
1	C	2732	0	2679	96	0
1	D	2710	0	2660	91	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	15	0	0	1	0
2	D	5	0	0	1	0
All	All	10908	0	10656	349	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 16.

All (349) 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:B:20:ARG:HD3	1:B:359:PRO:HB3	1.39	1.04
1:C:20:ARG:HD3	1:C:359:PRO:HB3	1.44	0.98
1:D:66:LEU:HD11	1:D:122:LEU:HD13	1.51	0.91
1:C:145:ILE:HG23	1:C:334:LEU:HD12	1.61	0.81
1:D:145:ILE:HG23	1:D:334:LEU:HD12	1.65	0.79
1:A:348:GLN:NE2	1:A:402:GLN:H	1.83	0.76
1:A:145:ILE:HG21	1:A:406:TYR:HB3	1.66	0.76
1:C:348:GLN:NE2	1:C:402:GLN:H	1.83	0.76
1:D:348:GLN:NE2	1:D:402:GLN:H	1.85	0.75
1:C:145:ILE:HG21	1:C:406:TYR:HB3	1.69	0.75
1:B:348:GLN:NE2	1:B:402:GLN:H	1.84	0.74
1:D:145:ILE:HG21	1:D:406:TYR:HB3	1.68	0.74
1:B:37:TYR:HD1	1:B:418:CYS:HG	1.35	0.73
1:D:49:ASP:OD1	1:D:50:THR:N	2.22	0.72
1:B:345:GLN:H	1:B:348:GLN:NE2	1.88	0.71
1:D:13:PRO:HD3	1:D:49:ASP:OD2	1.90	0.71
1:A:145:ILE:HG23	1:A:334:LEU:HD12	1.73	0.70
1:D:345:GLN:H	1:D:348:GLN:NE2	1.90	0.70
1:D:3:LYS:HG2	1:D:78:VAL:HB	1.74	0.70
1:C:345:GLN:H	1:C:348:GLN:NE2	1.90	0.69
1:A:37:TYR:HD1	1:A:418:CYS:HG	1.37	0.69
1:C:70:VAL:HG13	1:C:126:VAL:HG12	1.74	0.69
1:B:3:LYS:HG2	1:B:78:VAL:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLN:H	1:A:348:GLN:NE2	1.90	0.68
1:A:121:ASP:OD1	1:A:332:VAL:HG21	1.92	0.68
1:A:339:ILE:HG13	1:A:407:CYS:HB3	1.76	0.68
1:B:339:ILE:HG13	1:B:407:CYS:HB3	1.76	0.67
1:A:120:ARG:HH11	1:A:144:LEU:HG	1.59	0.67
1:A:70:VAL:HG13	1:A:126:VAL:HG12	1.76	0.67
1:C:3:LYS:HG2	1:C:78:VAL:HB	1.76	0.67
1:C:37:TYR:HD1	1:C:418:CYS:HG	1.44	0.66
1:B:70:VAL:HG13	1:B:126:VAL:HG12	1.78	0.66
1:A:120:ARG:NE	1:A:332:VAL:O	2.25	0.65
1:D:70:VAL:HG13	1:D:126:VAL:HG12	1.77	0.65
1:A:3:LYS:HG2	1:A:78:VAL:HB	1.78	0.64
1:A:358:LYS:NZ	1:A:361:GLU:OE1	2.23	0.64
1:B:20:ARG:HH11	1:B:354:THR:HG21	1.62	0.64
1:C:339:ILE:HG13	1:C:407:CYS:HB3	1.79	0.64
1:B:87:GLY:HA3	1:B:140:HIS:HB2	1.80	0.63
1:A:117:ASP:OD1	1:A:120:ARG:NH2	2.32	0.63
1:C:20:ARG:HH11	1:C:354:THR:HG21	1.64	0.63
1:B:120:ARG:NH1	1:B:334:LEU:HG	2.14	0.63
1:B:20:ARG:NH1	1:B:354:THR:HG21	2.14	0.62
1:B:246:GLU:HG2	1:B:249:LYS:HE3	1.81	0.62
1:C:246:GLU:HG2	1:C:249:LYS:HE3	1.82	0.62
1:D:358:LYS:HD2	1:D:359:PRO:HD2	1.80	0.61
1:C:20:ARG:NH1	1:C:354:THR:HG21	2.16	0.61
1:D:246:GLU:HG2	1:D:249:LYS:HE3	1.81	0.61
1:D:215:GLU:HB2	1:D:397:GLN:O	2.01	0.61
1:B:344:CYS:HB2	1:B:348:GLN:HG3	1.84	0.60
1:D:344:CYS:HB2	1:D:348:GLN:HG3	1.83	0.60
1:D:37:TYR:HD1	1:D:418:CYS:HG	1.48	0.60
1:B:281:ASN:HA	1:B:284:GLU:HG3	1.83	0.59
1:C:220:ILE:HG12	1:C:355:PRO:HA	1.84	0.59
1:A:281:ASN:HA	1:A:284:GLU:HG3	1.84	0.59
1:C:281:ASN:HA	1:C:284:GLU:HG3	1.83	0.59
1:A:246:GLU:HG2	1:A:249:LYS:HE3	1.84	0.59
1:B:309:VAL:HG12	1:B:313:MET:HG2	1.85	0.58
1:D:281:ASN:HA	1:D:284:GLU:HG3	1.85	0.58
1:D:150:GLU:O	1:D:384:ARG:NH2	2.36	0.58
1:A:373:ILE:O	1:A:377:THR:HG23	2.04	0.58
1:A:309:VAL:HG12	1:A:313:MET:HG2	1.85	0.58
1:D:131:ARG:NH2	2:D:501:SO4:O1	2.35	0.58
1:B:387:VAL:HG21	1:B:405:LEU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:GLU:CB	1:D:329:ARG:HD2	2.34	0.57
1:D:276:LYS:HE2	1:D:287:LEU:HD12	1.87	0.57
1:B:373:ILE:O	1:B:377:THR:HG23	2.04	0.57
1:C:373:ILE:O	1:C:377:THR:HG23	2.04	0.57
1:C:120:ARG:HD2	1:C:332:VAL:O	2.03	0.57
1:D:309:VAL:HG12	1:D:313:MET:HG2	1.87	0.57
1:C:309:VAL:HG12	1:C:313:MET:HG2	1.86	0.57
1:D:387:VAL:HG21	1:D:405:LEU:HB2	1.87	0.57
1:C:20:ARG:HD3	1:C:359:PRO:CB	2.29	0.57
1:C:280:GLY:O	1:C:282:GLY:N	2.38	0.56
1:A:344:CYS:HB2	1:A:348:GLN:HG3	1.86	0.56
1:C:276:LYS:HE2	1:C:287:LEU:HD12	1.87	0.56
1:C:101:GLY:C	1:C:102:PHE:HD1	2.09	0.56
1:C:132:MET:O	1:C:339:ILE:HG22	2.05	0.56
1:A:37:TYR:HD1	1:A:418:CYS:SG	2.28	0.56
1:B:121:ASP:OD1	1:B:332:VAL:HG21	2.06	0.56
1:D:345:GLN:O	1:D:347:ASP:N	2.37	0.56
1:A:386:MET:HG2	1:A:416:PHE:CE1	2.40	0.56
1:D:121:ASP:OD1	1:D:332:VAL:HG21	2.06	0.55
1:B:276:LYS:HE2	1:B:287:LEU:HD12	1.88	0.55
1:C:23:VAL:HG13	1:C:48:ILE:HD13	1.89	0.55
1:B:101:GLY:C	1:B:102:PHE:HD1	2.10	0.55
1:A:101:GLY:C	1:A:102:PHE:HD1	2.10	0.55
1:C:344:CYS:HB2	1:C:348:GLN:HG3	1.87	0.55
1:D:101:GLY:C	1:D:102:PHE:HD1	2.10	0.55
1:A:89:ARG:HD2	1:A:104:GLU:HG2	1.89	0.55
1:B:276:LYS:HE3	1:B:283:GLU:HB3	1.89	0.55
1:C:343:GLY:HA2	1:C:366:MET:HG3	1.89	0.55
1:A:139:CYS:SG	1:A:226:SER:HB2	2.47	0.55
1:B:386:MET:HG2	1:B:416:PHE:CE1	2.42	0.55
1:A:132:MET:O	1:A:339:ILE:HG22	2.06	0.55
1:A:280:GLY:O	1:A:282:GLY:N	2.40	0.55
1:B:280:GLY:O	1:B:282:GLY:N	2.39	0.55
1:B:37:TYR:HD1	1:B:418:CYS:SG	2.30	0.55
1:C:386:MET:HG2	1:C:416:PHE:CE1	2.41	0.55
1:A:276:LYS:HE2	1:A:287:LEU:HD12	1.89	0.54
1:C:123:VAL:HG22	1:C:132:MET:SD	2.47	0.54
1:D:151:GLN:HB3	1:D:405:LEU:HB3	1.89	0.54
1:A:345:GLN:O	1:A:347:ASP:N	2.36	0.54
1:C:387:VAL:HG21	1:C:405:LEU:HB2	1.88	0.54
1:B:132:MET:O	1:B:339:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:MET:HG2	1:D:416:PHE:CE1	2.43	0.54
1:D:37:TYR:HD1	1:D:418:CYS:SG	2.30	0.54
1:D:280:GLY:O	1:D:282:GLY:N	2.40	0.54
1:B:89:ARG:HD2	1:B:104:GLU:HG2	1.89	0.53
1:C:37:TYR:HD1	1:C:418:CYS:SG	2.31	0.53
1:A:343:GLY:HA2	1:A:366:MET:HG3	1.89	0.53
1:B:58:THR:OG1	1:B:61:ASN:OD1	2.27	0.53
1:C:276:LYS:HE3	1:C:283:GLU:HB3	1.89	0.53
1:D:120:ARG:NE	1:D:332:VAL:O	2.38	0.53
1:D:150:GLU:HG3	1:D:412:ALA:HB2	1.91	0.53
1:D:99:ASP:OD1	1:D:325:ALA:N	2.42	0.52
1:B:139:CYS:SG	1:B:226:SER:HB2	2.48	0.52
1:C:151:GLN:HB3	1:C:405:LEU:HB3	1.91	0.52
1:C:89:ARG:HD2	1:C:104:GLU:HG2	1.91	0.52
1:A:120:ARG:NH1	1:A:144:LEU:HA	2.25	0.52
1:A:344:CYS:HB2	1:A:348:GLN:HE21	1.75	0.52
1:B:343:GLY:HA2	1:B:366:MET:HG3	1.92	0.52
1:C:137:ASP:O	1:C:225:LYS:HE2	2.10	0.52
1:D:139:CYS:SG	1:D:226:SER:HB2	2.49	0.52
1:A:120:ARG:CZ	1:A:144:LEU:HA	2.39	0.52
1:C:210:LYS:O	1:C:222:ALA:N	2.42	0.52
1:B:244:ASN:HD21	1:B:249:LYS:HZ2	1.58	0.51
1:A:87:GLY:HA3	1:A:140:HIS:HB2	1.92	0.51
1:A:276:LYS:HE3	1:A:283:GLU:HB3	1.91	0.51
1:B:360:THR:HG21	1:C:238:GLN:HG2	1.91	0.51
1:D:344:CYS:HB2	1:D:348:GLN:CG	2.39	0.51
1:B:92:ALA:HB2	1:B:325:ALA:HB3	1.92	0.51
1:C:281:ASN:HA	1:C:284:GLU:CG	2.41	0.51
1:C:345:GLN:O	1:C:347:ASP:N	2.37	0.51
1:A:23:VAL:HG13	1:A:48:ILE:HD13	1.91	0.51
1:A:387:VAL:HG21	1:A:405:LEU:HB2	1.92	0.51
1:D:339:ILE:HG13	1:D:407:CYS:HB3	1.92	0.51
1:D:276:LYS:HE3	1:D:283:GLU:HB3	1.92	0.50
1:D:372:THR:O	1:D:376:GLU:HG3	2.10	0.50
1:A:151:GLN:HB3	1:A:405:LEU:HB3	1.93	0.50
1:B:255:PHE:CG	1:B:270:MET:HG3	2.46	0.50
1:B:345:GLN:O	1:B:347:ASP:N	2.36	0.50
1:D:255:PHE:CG	1:D:270:MET:HG3	2.46	0.50
1:C:255:PHE:CG	1:C:270:MET:HG3	2.47	0.50
1:D:321:GLU:HB3	1:D:329:ARG:HD2	1.92	0.50
1:D:219:THR:O	1:D:355:PRO:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:OG1	1:A:61:ASN:OD1	2.27	0.50
1:B:344:CYS:HB2	1:B:348:GLN:HE21	1.76	0.50
1:C:123:VAL:O	1:C:126:VAL:HG13	2.12	0.50
1:A:99:ASP:OD1	1:A:325:ALA:N	2.41	0.50
1:B:281:ASN:HA	1:B:284:GLU:CG	2.42	0.50
1:B:344:CYS:HB2	1:B:348:GLN:CG	2.41	0.50
1:C:281:ASN:HA	1:C:284:GLU:HB2	1.94	0.50
1:A:255:PHE:CG	1:A:270:MET:HG3	2.47	0.49
1:A:344:CYS:HB2	1:A:348:GLN:CG	2.42	0.49
1:C:382:SER:OG	1:C:385:GLU:HG3	2.12	0.49
1:A:382:SER:OG	1:A:385:GLU:HG3	2.12	0.49
1:A:123:VAL:HG22	1:A:132:MET:SD	2.52	0.49
1:A:244:ASN:HD21	1:A:249:LYS:NZ	2.11	0.49
1:B:244:ASN:HD21	1:B:249:LYS:NZ	2.10	0.49
1:D:89:ARG:HD2	1:D:104:GLU:HG2	1.93	0.49
1:D:102:PHE:O	1:D:326:GLY:HA2	2.13	0.49
1:D:343:GLY:HA2	1:D:366:MET:HG3	1.94	0.49
1:A:130:CYS:O	1:A:132:MET:N	2.46	0.49
1:A:222:ALA:HA	1:A:352:ASP:O	2.12	0.49
1:B:23:VAL:HG13	1:B:48:ILE:HD13	1.94	0.49
1:B:382:SER:OG	1:B:385:GLU:HG3	2.13	0.49
1:C:344:CYS:HB2	1:C:348:GLN:CG	2.42	0.49
1:B:123:VAL:HG22	1:B:132:MET:SD	2.52	0.49
1:C:344:CYS:HB2	1:C:348:GLN:HE21	1.78	0.49
1:A:339:ILE:HD12	1:A:411:TYR:HB3	1.95	0.48
1:D:123:VAL:HG22	1:D:132:MET:SD	2.53	0.48
1:D:244:ASN:HD21	1:D:249:LYS:NZ	2.11	0.48
1:B:281:ASN:HA	1:B:284:GLU:HB2	1.95	0.48
1:C:90:LEU:HD11	1:C:250:ILE:HG21	1.95	0.48
1:D:63:ARG:NH1	1:D:122:LEU:HD11	2.28	0.48
1:D:321:GLU:HG3	1:D:324:TYR:CE2	2.48	0.48
1:B:151:GLN:HB3	1:B:405:LEU:HB3	1.95	0.48
1:A:281:ASN:HA	1:A:284:GLU:CG	2.43	0.48
1:B:339:ILE:HD12	1:B:411:TYR:HB3	1.95	0.48
1:C:89:ARG:HB3	1:C:102:PHE:HD2	1.79	0.48
1:C:139:CYS:SG	1:C:226:SER:HB2	2.52	0.48
1:D:281:ASN:HA	1:D:284:GLU:CG	2.43	0.48
1:D:132:MET:O	1:D:339:ILE:HG22	2.13	0.48
1:D:281:ASN:HA	1:D:284:GLU:HB2	1.94	0.48
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.73	0.48
1:B:212:ILE:HB	1:B:221:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:HB3	1:B:102:PHE:HD2	1.79	0.48
1:A:150:GLU:O	1:A:384:ARG:NH2	2.47	0.48
1:C:115:THR:HG22	1:C:117:ASP:H	1.79	0.47
1:C:121:ASP:OD1	1:C:332:VAL:HG21	2.13	0.47
1:C:130:CYS:O	1:C:132:MET:N	2.48	0.47
1:C:87:GLY:HA3	1:C:140:HIS:HB2	1.96	0.47
1:C:385:GLU:O	1:C:389:ARG:HG3	2.13	0.47
1:D:385:GLU:O	1:D:389:ARG:HG3	2.14	0.47
1:A:385:GLU:O	1:A:389:ARG:HG3	2.14	0.47
1:B:240:THR:O	1:B:242:ASN:N	2.48	0.47
1:B:385:GLU:O	1:B:389:ARG:HG3	2.14	0.47
1:D:344:CYS:HB2	1:D:348:GLN:HE21	1.79	0.47
1:B:321:GLU:HG3	1:B:324:TYR:CE2	2.49	0.47
1:C:58:THR:OG1	1:C:61:ASN:OD1	2.31	0.47
1:D:339:ILE:HA	1:D:407:CYS:HB3	1.96	0.47
1:D:355:PRO:HD3	1:D:362:ALA:HA	1.96	0.47
1:A:120:ARG:HD3	1:A:144:LEU:HA	1.96	0.47
1:A:281:ASN:HA	1:A:284:GLU:HB2	1.96	0.47
1:B:130:CYS:O	1:B:132:MET:N	2.47	0.47
1:C:131:ARG:HH21	1:C:418:CYS:HA	1.80	0.47
1:C:339:ILE:HD12	1:C:411:TYR:HB3	1.97	0.47
1:D:236:LEU:HD23	1:D:236:LEU:HA	1.73	0.47
1:D:249:LYS:HZ1	1:D:292:GLY:HA3	1.80	0.47
1:D:90:LEU:HD11	1:D:250:ILE:HG21	1.96	0.47
1:C:236:LEU:HD23	1:C:236:LEU:HA	1.71	0.47
1:D:339:ILE:HD12	1:D:411:TYR:HB3	1.97	0.46
1:C:121:ASP:CG	1:C:332:VAL:HG21	2.36	0.46
1:D:291:LEU:O	1:D:295:ALA:HB3	2.15	0.46
1:A:144:LEU:HD23	1:A:334:LEU:HD21	1.98	0.46
1:B:52:GLU:HG2	1:C:50:THR:O	2.16	0.46
1:A:212:ILE:HG13	1:A:221:HIS:CD2	2.51	0.46
1:A:240:THR:O	1:A:242:ASN:N	2.49	0.46
1:C:236:LEU:HB3	1:C:245:ILE:HD13	1.97	0.46
1:D:240:THR:O	1:D:242:ASN:N	2.49	0.46
1:D:291:LEU:HD23	1:D:291:LEU:HA	1.71	0.46
1:B:89:ARG:HH21	1:B:102:PHE:HB2	1.81	0.46
1:D:384:ARG:O	1:D:388:THR:OG1	2.28	0.46
1:A:93:GLU:OE2	1:A:250:ILE:HB	2.16	0.45
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.86	0.45
1:C:240:THR:O	1:C:242:ASN:N	2.49	0.45
1:A:5:ALA:HB3	1:A:44:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:THR:OG1	1:D:61:ASN:OD1	2.32	0.45
1:D:130:CYS:O	1:D:132:MET:N	2.49	0.45
1:C:123:VAL:HG12	1:C:335:PRO:HG2	1.97	0.45
1:C:244:ASN:HD21	1:C:249:LYS:NZ	2.14	0.45
1:C:249:LYS:HZ1	1:C:292:GLY:HA3	1.81	0.45
1:A:291:LEU:O	1:A:295:ALA:HB3	2.17	0.45
1:C:281:ASN:ND2	1:C:284:GLU:OE2	2.50	0.45
1:D:123:VAL:O	1:D:126:VAL:HG13	2.17	0.45
1:B:116:ASP:O	1:B:120:ARG:HG3	2.15	0.45
1:B:150:GLU:O	1:B:384:ARG:NH2	2.49	0.45
1:D:89:ARG:HH21	1:D:102:PHE:HB2	1.81	0.45
1:A:89:ARG:HH21	1:A:102:PHE:HB2	1.82	0.45
1:C:16:LYS:HB2	1:C:16:LYS:HE2	1.55	0.45
1:C:150:GLU:O	1:C:384:ARG:NH2	2.49	0.45
1:C:228:PRO:HG2	1:C:231:THR:OG1	2.17	0.45
1:B:137:ASP:O	1:B:225:LYS:HE2	2.17	0.45
1:C:118:ASP:OD1	1:C:264:PRO:HB2	2.16	0.45
1:C:332:VAL:HA	1:C:333:PRO:HD2	1.78	0.45
1:A:249:LYS:HZ1	1:A:292:GLY:HA3	1.82	0.45
1:D:50:THR:OG1	1:D:53:SER:HB3	2.17	0.45
1:C:294:LEU:HD12	1:C:294:LEU:HA	1.70	0.44
1:A:228:PRO:HG2	1:A:231:THR:OG1	2.17	0.44
1:C:5:ALA:HB3	1:C:44:ILE:HG12	1.99	0.44
1:D:281:ASN:ND2	1:D:284:GLU:OE2	2.50	0.44
1:D:294:LEU:HD12	1:D:294:LEU:HA	1.71	0.44
1:B:294:LEU:HD12	1:B:294:LEU:HA	1.72	0.44
1:A:89:ARG:HB3	1:A:102:PHE:HD2	1.81	0.44
1:A:281:ASN:ND2	1:A:284:GLU:OE2	2.51	0.44
1:D:131:ARG:HH21	1:D:418:CYS:HA	1.83	0.44
1:A:244:ASN:HD21	1:A:249:LYS:HZ2	1.66	0.44
1:C:99:ASP:HB2	1:C:324:TYR:CG	2.52	0.44
1:D:244:ASN:HD21	1:D:249:LYS:HZ2	1.66	0.44
1:C:20:ARG:NH1	2:C:501:SO4:O4	2.50	0.44
1:B:5:ALA:HB3	1:B:44:ILE:HG12	1.99	0.44
1:C:140:HIS:CE1	1:C:226:SER:OG	2.71	0.44
1:C:374:LEU:HD23	1:C:374:LEU:HA	1.75	0.44
1:A:12:TYR:OH	1:A:107:VAL:O	2.25	0.43
1:A:321:GLU:HG3	1:A:324:TYR:CE2	2.54	0.43
1:C:372:THR:O	1:C:376:GLU:HG3	2.17	0.43
1:D:212:ILE:HB	1:D:221:HIS:HD2	1.84	0.43
1:A:372:THR:O	1:A:376:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD11	1:B:250:ILE:HG21	1.99	0.43
1:C:210:LYS:HB2	1:C:221:HIS:HB3	2.00	0.43
1:A:92:ALA:HB2	1:A:325:ALA:HB3	2.00	0.43
1:A:396:LYS:HG3	1:A:397:GLN:HE21	1.83	0.43
1:B:6:VAL:HG23	1:B:69:LEU:HD22	2.00	0.43
1:B:236:LEU:HB3	1:B:245:ILE:HD13	2.00	0.43
1:C:291:LEU:O	1:C:295:ALA:HB3	2.19	0.43
1:D:124:ASP:HA	1:D:335:PRO:HG2	2.00	0.43
1:B:131:ARG:HH21	1:B:418:CYS:HA	1.84	0.43
1:B:281:ASN:ND2	1:B:284:GLU:OE2	2.51	0.43
1:B:349:THR:O	1:B:401:GLN:HB3	2.19	0.43
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.73	0.43
1:D:137:ASP:O	1:D:225:LYS:HE2	2.19	0.43
1:B:30:TYR:OH	1:B:41:GLU:HB3	2.18	0.43
1:B:372:THR:O	1:B:376:GLU:HG3	2.18	0.43
1:A:19:LEU:HD23	1:A:223:LYS:HD3	2.01	0.43
1:A:30:TYR:OH	1:A:41:GLU:HB3	2.19	0.43
1:B:150:GLU:HG3	1:B:412:ALA:HB2	2.01	0.43
1:C:116:ASP:O	1:C:120:ARG:HG3	2.19	0.43
1:D:333:PRO:O	1:D:335:PRO:HD3	2.19	0.43
1:D:354:THR:HA	1:D:355:PRO:HD3	1.87	0.43
1:A:236:LEU:HB3	1:A:245:ILE:HD13	2.00	0.42
1:C:349:THR:O	1:C:401:GLN:HB3	2.18	0.42
1:D:122:LEU:HD23	1:D:122:LEU:HA	1.88	0.42
1:D:332:VAL:HA	1:D:333:PRO:HD2	1.66	0.42
1:D:377:THR:H	1:D:377:THR:HG23	1.60	0.42
1:C:260:ASP:O	1:C:267:LYS:HE2	2.19	0.42
1:D:382:SER:OG	1:D:385:GLU:HG3	2.19	0.42
1:A:349:THR:O	1:A:401:GLN:HB3	2.19	0.42
1:D:349:THR:O	1:D:401:GLN:HB3	2.19	0.42
1:C:93:GLU:OE2	1:C:250:ILE:HB	2.19	0.42
1:C:244:ASN:HD21	1:C:249:LYS:HZ2	1.67	0.42
1:D:5:ALA:HB3	1:D:44:ILE:HG12	2.01	0.42
1:A:260:ASP:O	1:A:267:LYS:HE2	2.20	0.42
1:B:228:PRO:HG2	1:B:231:THR:OG1	2.19	0.42
1:B:238:GLN:CD	1:C:357:GLY:HA3	2.40	0.42
1:C:70:VAL:HG13	1:C:126:VAL:CG1	2.46	0.42
1:C:99:ASP:OD1	1:C:325:ALA:N	2.53	0.42
1:D:6:VAL:HG23	1:D:69:LEU:HD22	2.01	0.42
1:D:228:PRO:HG2	1:D:231:THR:OG1	2.20	0.42
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD11	1:A:250:ILE:HG21	2.01	0.42
1:C:145:ILE:HG21	1:C:406:TYR:CB	2.46	0.42
1:C:220:ILE:HG23	1:C:354:THR:H	1.85	0.42
1:A:123:VAL:O	1:A:126:VAL:HG13	2.20	0.41
1:A:137:ASP:O	1:A:225:LYS:HE2	2.20	0.41
1:D:260:ASP:O	1:D:267:LYS:HE2	2.20	0.41
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.77	0.41
1:D:93:GLU:OE2	1:D:250:ILE:HB	2.20	0.41
1:B:93:GLU:OE2	1:B:250:ILE:HB	2.19	0.41
1:C:30:TYR:OH	1:C:41:GLU:HB3	2.21	0.41
1:B:99:ASP:OD1	1:B:325:ALA:N	2.45	0.41
1:D:30:TYR:OH	1:D:41:GLU:HB3	2.20	0.41
1:D:396:LYS:HG3	1:D:397:GLN:HE21	1.85	0.41
1:D:130:CYS:O	1:D:337:SER:OG	2.39	0.41
1:A:332:VAL:HA	1:A:333:PRO:HD2	1.80	0.41
1:B:239:GLN:HA	1:C:358:LYS:CE	2.51	0.41
1:C:6:VAL:HG23	1:C:69:LEU:HD22	2.03	0.41
1:C:233:ILE:O	1:C:237:LYS:HG3	2.21	0.41
1:A:221:HIS:O	1:A:354:THR:HG22	2.20	0.41
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.73	0.41
1:B:92:ALA:HA	1:B:325:ALA:HB2	2.02	0.41
1:B:124:ASP:HA	1:B:335:PRO:HG2	2.02	0.41
1:B:260:ASP:O	1:B:267:LYS:HE2	2.21	0.41
1:B:18:GLU:O	1:B:223:LYS:HE2	2.20	0.41
1:B:123:VAL:O	1:B:126:VAL:HG13	2.21	0.41
1:C:89:ARG:HH21	1:C:102:PHE:HB2	1.86	0.41
1:C:150:GLU:HG3	1:C:412:ALA:HB2	2.01	0.41
1:A:145:ILE:HG12	1:A:406:TYR:CD2	2.56	0.40
1:A:325:ALA:C	1:A:327:GLY:H	2.25	0.40
1:D:236:LEU:HB3	1:D:245:ILE:HD13	2.03	0.40
1:B:4:LYS:O	1:B:79:LEU:HA	2.21	0.40
1:B:373:ILE:HD11	1:B:390:ALA:HA	2.03	0.40
1:A:150:GLU:HG3	1:A:412:ALA:HB2	2.04	0.40
1:D:10:ILE:HG12	1:D:57:PRO:CG	2.50	0.40
1:D:70:VAL:HG13	1:D:126:VAL:CG1	2.49	0.40
1:A:294:LEU:HA	1:A:294:LEU:HD12	1.68	0.40
1:A:373:ILE:HD11	1:A:390:ALA:HA	2.03	0.40
1:C:104:GLU:HB3	1:C:140:HIS:O	2.21	0.40
1:C:321:GLU:HG3	1:C:324:TYR:CE2	2.57	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	358/426 (84%)	324 (90%)	28 (8%)	6 (2%)	9	40
1	B	351/426 (82%)	318 (91%)	27 (8%)	6 (2%)	9	40
1	C	355/426 (83%)	320 (90%)	28 (8%)	7 (2%)	7	37
1	D	352/426 (83%)	319 (91%)	25 (7%)	8 (2%)	6	34
All	All	1416/1704 (83%)	1281 (90%)	108 (8%)	27 (2%)	8	37

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	ARG
1	A	212	ILE
1	A	327	GLY
1	A	346	THR
1	A	356	ALA
1	B	131	ARG
1	B	327	GLY
1	B	346	THR
1	B	356	ALA
1	C	131	ARG
1	C	346	THR
1	C	356	ALA
1	D	50	THR
1	D	131	ARG
1	D	346	THR
1	D	360	THR
1	A	241	GLY
1	B	212	ILE
1	B	241	GLY
1	C	210	LYS
1	C	241	GLY
1	D	241	GLY

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Mol	Chain	Res	Type
1	D	356	ALA
1	C	146	ASP
1	C	208	GLU
1	D	146	ASP
1	D	339	ILE

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	300/357 (84%)	291 (97%)	9 (3%)	41	70
1	B	297/357 (83%)	288 (97%)	9 (3%)	41	70
1	C	301/357 (84%)	291 (97%)	10 (3%)	38	68
1	D	299/357 (84%)	291 (97%)	8 (3%)	44	72
All	All	1197/1428 (84%)	1161 (97%)	36 (3%)	41	70

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	141	SER
1	A	145	ILE
1	A	151	GLN
1	A	209	THR
1	A	236	LEU
1	A	283	GLU
1	A	300	GLU
1	A	306	GLU
1	B	16	LYS
1	B	64	ARG
1	B	151	GLN
1	B	209	THR
1	B	211	GLU
1	B	236	LEU
1	B	283	GLU

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Mol	Chain	Res	Type
1	B	300	GLU
1	B	306	GLU
1	C	16	LYS
1	C	64	ARG
1	C	151	GLN
1	C	206	GLU
1	C	208	GLU
1	C	209	THR
1	C	236	LEU
1	C	283	GLU
1	C	300	GLU
1	C	306	GLU
1	D	64	ARG
1	D	151	GLN
1	D	209	THR
1	D	210	LYS
1	D	236	LEU
1	D	283	GLU
1	D	300	GLU
1	D	306	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	HIS
1	A	244	ASN
1	A	281	ASN
1	A	314	GLN
1	A	345	GLN
1	A	348	GLN
1	A	397	GLN
1	B	244	ASN
1	B	281	ASN
1	B	314	GLN
1	B	345	GLN
1	B	348	GLN
1	B	397	GLN
1	C	140	HIS
1	C	221	HIS
1	C	244	ASN
1	C	281	ASN
1	C	314	GLN

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Mol	Chain	Res	Type
1	C	345	GLN
1	C	348	GLN
1	C	397	GLN
1	D	56	GLN
1	D	244	ASN
1	D	281	ASN
1	D	314	GLN
1	D	345	GLN
1	D	348	GLN
1	D	397	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	SO4	C	503	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.06	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	SO4	1	0
2	D	501	SO4	1	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.

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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	362/426 (84%)	0.36	19 (5%)	27	26	43, 86, 129, 185	0
1	B	357/426 (83%)	0.43	23 (6%)	19	19	50, 92, 144, 216	0
1	C	361/426 (84%)	0.36	11 (3%)	50	47	41, 84, 136, 182	0
1	D	358/426 (84%)	0.52	24 (6%)	17	18	49, 102, 150, 196	0
All	All	1438/1704 (84%)	0.42	77 (5%)	25	25	41, 90, 141, 216	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	378	ASP	7.2
1	A	282	GLY	7.0
1	A	281	ASN	6.1
1	C	379	GLY	5.0
1	B	146	ASP	4.7
1	B	281	ASN	4.7
1	A	280	GLY	4.7
1	B	213	GLU	4.5
1	D	283	GLU	4.5
1	D	98	ASP	4.4
1	B	283	GLU	4.1
1	B	378	ASP	4.0
1	D	213	GLU	3.8
1	A	283	GLU	3.7
1	D	286	GLY	3.6
1	D	97	ASP	3.5
1	D	329	ARG	3.5
1	D	151	GLN	3.4
1	B	419	VAL	3.4
1	C	377	THR	3.3
1	B	219	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	3	LYS	3.2
1	B	211	GLU	3.2
1	B	380	GLU	3.1
1	C	214	LEU	3.1
1	B	280	GLY	3.1
1	C	282	GLY	3.0
1	B	282	GLY	3.0
1	B	212	ILE	2.9
1	A	397	GLN	2.9
1	D	318	GLY	2.9
1	A	98	ASP	2.9
1	B	98	ASP	2.8
1	A	398	GLY	2.8
1	D	398	GLY	2.8
1	C	211	GLU	2.8
1	A	151	GLN	2.7
1	A	213	GLU	2.7
1	A	284	GLU	2.7
1	D	282	GLY	2.6
1	C	244	ASN	2.6
1	A	378	ASP	2.6
1	C	290	MET	2.6
1	D	146	ASP	2.6
1	D	321	GLU	2.5
1	A	318	GLY	2.5
1	A	97	ASP	2.5
1	D	147	GLU	2.5
1	A	144	LEU	2.5
1	C	380	GLU	2.5
1	D	3	LYS	2.5
1	B	218	GLU	2.5
1	A	72	SER	2.4
1	A	380	GLU	2.4
1	B	355	PRO	2.4
1	B	318	GLY	2.4
1	D	333	PRO	2.3
1	A	143	GLY	2.3
1	C	389	ARG	2.3
1	A	209	THR	2.3
1	D	276	LYS	2.3
1	C	206	GLU	2.3
1	B	306	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	284	GLU	2.2
1	D	102	PHE	2.2
1	D	215	GLU	2.2
1	D	347	ASP	2.2
1	D	40	SER	2.2
1	B	357	GLY	2.2
1	A	2	THR	2.1
1	D	39	PHE	2.1
1	D	317	VAL	2.1
1	B	379	GLY	2.1
1	B	97	ASP	2.0
1	B	329	ARG	2.0
1	D	418	CYS	2.0
1	D	281	ASN	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 ⓘ

There are no monosaccharides 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. 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
2	SO4	A	501	5/5	0.75	0.34	126,126,126,126	0
2	SO4	C	503	5/5	0.77	0.41	153,153,153,153	0
2	SO4	A	502	5/5	0.80	0.24	143,143,143,143	0
2	SO4	B	501	5/5	0.83	0.38	117,117,117,117	0
2	SO4	A	503	5/5	0.87	0.28	137,137,137,137	0
2	SO4	C	502	5/5	0.88	0.19	118,118,118,118	0
2	SO4	C	501	5/5	0.89	0.22	116,116,116,116	0
2	SO4	D	501	5/5	0.89	0.39	141,141,141,141	0

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6.5 Other polymers (i)

There are no such residues in this entry.