



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2017 – 11:20 AM EDT

PDB ID : 3FGA  
Title : Structural Basis of PP2A and Sgo interaction  
Authors : Xu, Z.; Xu, W.  
Deposited on : unknown  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

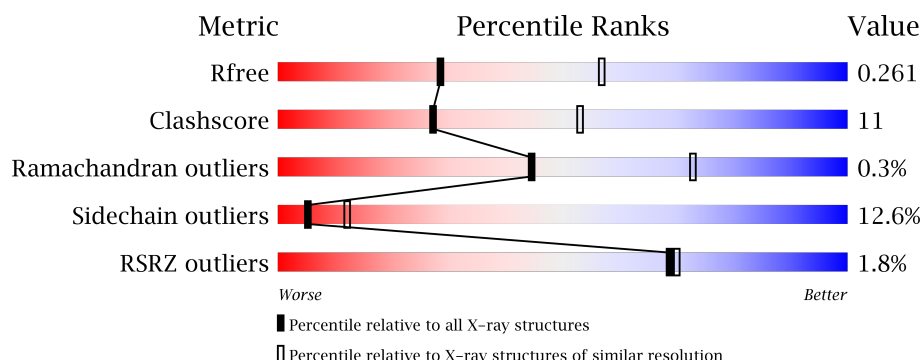
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	<div> <div>73%</div> <div>22%</div> <div>••</div> </div>
2	B	403	<div> <div>3%</div> <div>68%</div> <div>26%</div> <div>6%</div> </div>
3	C	309	<div> <div>%</div> <div>64%</div> <div>29%</div> <div>5%</div> <div>•</div> </div>
4	D	47	<div> <div>6%</div> <div>74%</div> <div>26%</div> </div>
5	E	7	<div> <div>14%</div> <div>57%</div> <div>29%</div> <div>14%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10810 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4532	2881	764	860	27			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3287	2149	540	582	16			

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total	C	N	O	S	0	0	0
			2446	1549	421	461	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	ASN	ASP	ENGINEERED	UNP P67775

- Molecule 4 is a protein called Shugoshin-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	47	Total	C	N	O	S	0	0	0
			380	239	64	74	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	50	PRO	-	INSERTION	UNP Q5FBB7

- Molecule 5 is a protein called MICROCYSTIN-LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	7	Total	C	N	O	0	0	0
			71	49	10	12			

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	Mn	0	0
			2	2		

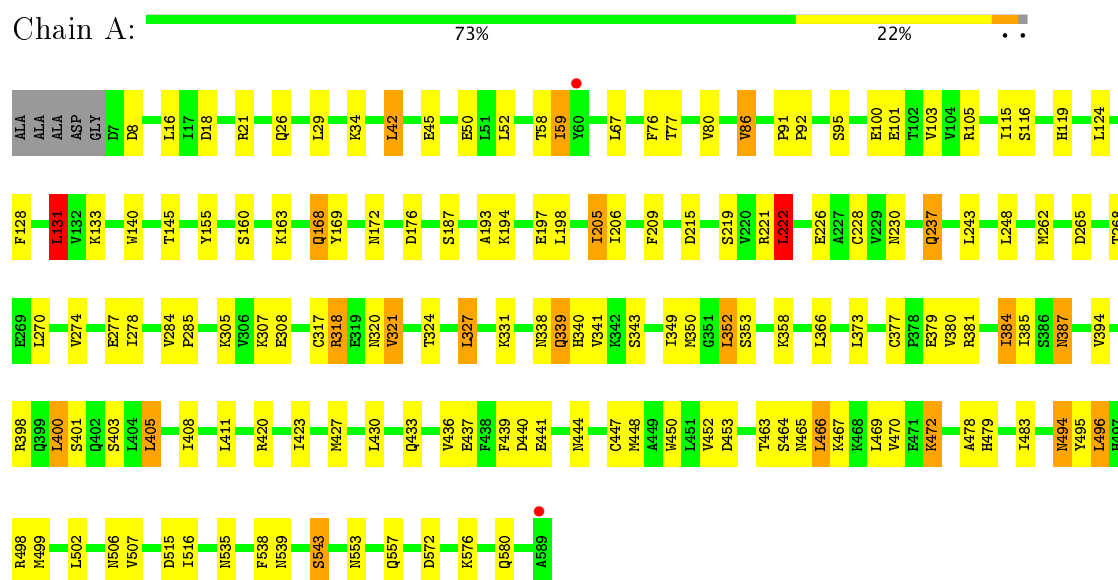
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	36	Total	O	0	0
			36	36		
7	B	11	Total	O	0	0
			11	11		
7	C	44	Total	O	0	0
			44	44		
7	D	1	Total	O	0	0
			1	1		

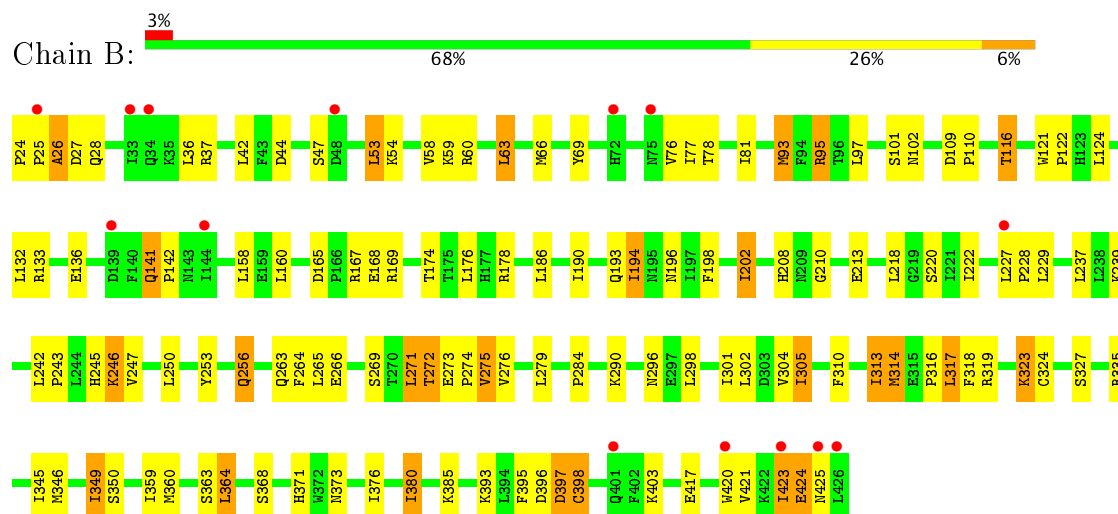
### 3 Residue-property plots

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.

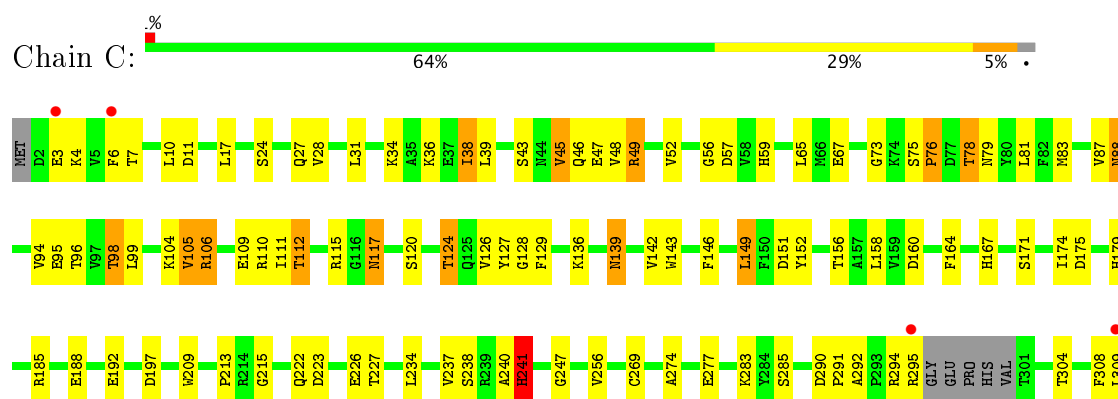
- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



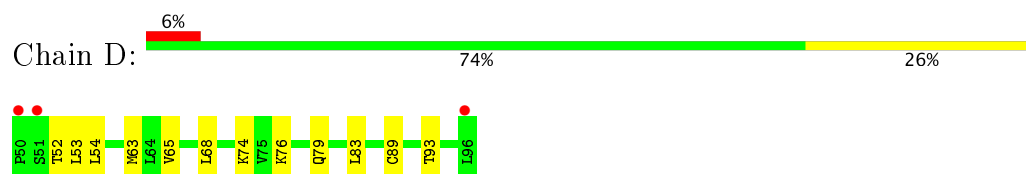
- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform



- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



• Molecule 4: Shugoshin-like 1



• Molecule 5: MICROCYSTIN-LR



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.94Å 145.86Å 294.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 2.70 49.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.8 (49.03-2.70) 92.8 (49.03-2.70)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.228 , 0.277 0.220 , 0.261	Depositor DCC
$R_{free}$ test set	2898 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: ACB, DAL, DAM, MN, 1ZN, FGA

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	0.50	0/4606	0.67	8/6255 (0.1%)
2	B	0.50	0/3378	0.67	5/4582 (0.1%)
3	C	0.54	0/2505	0.75	4/3396 (0.1%)
4	D	0.51	0/382	0.63	0/510
5	E	0.43	0/17	0.77	0/19
All	All	0.51	0/10888	0.69	17/14762 (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
5	E	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	ASP	N-CA-C	-5.91	95.05	111.00
2	B	26	ALA	N-CA-CB	-5.86	101.89	110.10
1	A	131	LEU	CB-CG-CD1	5.83	120.91	111.00
1	A	42	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	400	LEU	CA-CB-CG	5.60	128.17	115.30
3	C	241	HIS	N-CA-CB	-5.58	100.55	110.60
1	A	498	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	8	ASP	N-CA-CB	5.46	120.42	110.60
3	C	241	HIS	N-CA-C	5.46	125.73	111.00
1	A	222	LEU	CA-CB-CG	5.42	127.75	115.30
2	B	26	ALA	N-CA-C	5.30	125.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	131	LEU	CA-CB-CG	5.08	126.97	115.30
3	C	87	VAL	C-N-CA	-5.07	109.04	121.70
2	B	424	GLU	N-CA-C	-5.04	97.38	111.00
3	C	88	ASN	N-CA-C	5.00	124.51	111.00
1	A	318	ARG	CB-CA-C	-5.00	100.40	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	4	ARG	Sidechain

## 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	4532	0	4628	85	0
2	B	3287	0	3232	92	0
3	C	2446	0	2335	68	0
4	D	380	0	398	3	0
5	E	71	0	69	7	0
6	C	2	0	0	0	0
7	A	36	0	0	0	0
7	B	11	0	0	0	0
7	C	44	0	0	1	0
7	D	1	0	0	0	0
All	All	10810	0	10662	244	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 11.

All (244) 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)
3:C:269:CYS:SG	5:E:7:DAM:CB	2.25	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:VAL:O	3:C:98:THR:HG22	1.59	1.02
3:C:124:THR:CG2	3:C:143:TRP:HE1	1.73	1.01
2:B:208:HIS:HD2	2:B:210:GLY:H	1.09	0.99
3:C:269:CYS:SG	5:E:7:DAM:HB1	2.12	0.87
3:C:94:VAL:O	3:C:98:THR:CG2	2.24	0.85
3:C:124:THR:HG21	3:C:143:TRP:HE1	1.40	0.85
1:A:353:SER:HB3	1:A:394:VAL:HG11	1.57	0.84
3:C:24:SER:H	3:C:27:GLN:HE21	1.24	0.83
1:A:274:VAL:CG1	1:A:278:ILE:HB	2.11	0.81
2:B:208:HIS:CD2	2:B:210:GLY:H	1.96	0.81
3:C:167:HIS:NE2	3:C:241:HIS:HB2	1.96	0.80
3:C:175:ASP:H	3:C:179:HIS:HD2	1.29	0.78
2:B:218:LEU:O	2:B:222:ILE:HG12	1.84	0.77
1:A:427:MET:HE1	1:A:439:PHE:HE2	1.47	0.77
3:C:167:HIS:CE1	3:C:241:HIS:HB2	2.18	0.76
2:B:269:SER:O	2:B:272:THR:HG23	1.86	0.75
4:D:89:CYS:O	4:D:93:THR:HG22	1.88	0.74
2:B:36:LEU:HD23	2:B:66:MET:HE1	1.70	0.73
2:B:385:LYS:HG3	4:D:93:THR:HG21	1.71	0.73
2:B:59:LYS:O	2:B:63:LEU:HD23	1.90	0.71
1:A:274:VAL:HG13	1:A:278:ILE:HB	1.72	0.69
1:A:494:ASN:ND2	1:A:496:LEU:H	1.90	0.69
2:B:101:SER:HB2	2:B:116:THR:HG21	1.74	0.69
2:B:227:LEU:CB	2:B:228:PRO:CD	2.71	0.68
3:C:38:ILE:HD11	3:C:104:LYS:HE3	1.75	0.68
1:A:401:SER:HA	1:A:405:LEU:HB2	1.75	0.67
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.25	0.67
2:B:371:HIS:CE1	2:B:376:ILE:HD11	2.30	0.66
2:B:364:LEU:H	2:B:364:LEU:HD22	1.61	0.66
1:A:467:LYS:HB2	1:A:507:VAL:HG13	1.76	0.66
3:C:139:ASN:HD22	3:C:139:ASN:C	1.99	0.65
3:C:79:ASN:HD21	3:C:110:ARG:HD3	1.61	0.65
3:C:79:ASN:ND2	3:C:110:ARG:HD3	2.12	0.65
2:B:276:VAL:HG11	2:B:313:ILE:HG13	1.78	0.65
3:C:24:SER:H	3:C:27:GLN:NE2	1.95	0.64
1:A:320:ASN:O	1:A:324:THR:HG22	1.97	0.64
1:A:427:MET:HG3	1:A:450:TRP:CH2	2.32	0.64
3:C:152:TYR:O	3:C:185:ARG:NH2	2.29	0.64
1:A:427:MET:HE1	1:A:439:PHE:CE2	2.31	0.64
1:A:339:GLN:H	1:A:339:GLN:HE21	1.46	0.64
3:C:49:ARG:CD	3:C:49:ARG:H	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASN:HD22	1:A:495:TYR:N	1.96	0.63
3:C:73:GLY:HA3	3:C:78:THR:HG21	1.80	0.62
2:B:396:ASP:C	2:B:398:CYS:H	2.03	0.62
3:C:49:ARG:HD2	3:C:49:ARG:H	1.64	0.62
3:C:124:THR:HG21	3:C:143:TRP:NE1	2.12	0.62
3:C:126:VAL:HG22	3:C:127:TYR:CE2	2.36	0.61
1:A:427:MET:CE	1:A:439:PHE:HE2	2.14	0.61
3:C:10:LEU:HD11	3:C:105:VAL:HG22	1.82	0.60
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.82	0.60
3:C:308:PHE:O	3:C:309:LEU:HB2	2.02	0.60
1:A:268:THR:HG21	1:A:308:GLU:HB3	1.84	0.60
3:C:215:GLY:HA3	5:E:5:1ZN:H14	1.83	0.60
3:C:213:PRO:HB2	5:E:4:ARG:HH11	1.67	0.59
2:B:26:ALA:C	2:B:28:GLN:H	2.05	0.59
3:C:98:THR:HB	3:C:146:PHE:HZ	1.67	0.59
3:C:164:PHE:HB2	3:C:234:LEU:HD13	1.84	0.59
1:A:381:ARG:O	1:A:385:ILE:HG12	2.03	0.59
1:A:91:PRO:HB2	1:A:92:PRO:HD3	1.85	0.59
2:B:165:ASP:OD2	2:B:167:ARG:HD3	2.03	0.59
2:B:213:GLU:N	2:B:213:GLU:OE2	2.28	0.59
2:B:265:LEU:HD22	2:B:272:THR:HG22	1.85	0.58
1:A:317:CYS:O	1:A:321:VAL:HG12	2.03	0.58
2:B:424:GLU:CD	2:B:424:GLU:N	2.56	0.58
2:B:227:LEU:CB	2:B:228:PRO:HD3	2.33	0.58
3:C:11:ASP:OD1	3:C:106:ARG:HD2	2.04	0.58
3:C:43:SER:H	3:C:46:GLN:HE21	1.52	0.58
2:B:304:VAL:HG12	2:B:304:VAL:O	2.03	0.57
2:B:26:ALA:C	2:B:28:GLN:N	2.55	0.57
2:B:222:ILE:HD12	2:B:264:PHE:CE1	2.39	0.57
2:B:318:PHE:HB2	2:B:359:ILE:HD11	1.85	0.57
1:A:339:GLN:H	1:A:339:GLN:NE2	2.02	0.57
1:A:265:ASP:O	1:A:305:LYS:NZ	2.38	0.57
3:C:167:HIS:CD2	3:C:241:HIS:HB2	2.40	0.56
1:A:193:ALA:HB2	1:A:205:ILE:HD12	1.86	0.56
1:A:576:LYS:HG2	1:A:580:GLN:HE21	1.70	0.56
1:A:572:ASP:OD2	3:C:110:ARG:NH1	2.38	0.56
1:A:494:ASN:C	1:A:494:ASN:HD22	2.09	0.56
3:C:45:VAL:HB	3:C:156:THR:OG1	2.06	0.56
3:C:167:HIS:O	3:C:241:HIS:HB3	2.06	0.56
1:A:506:ASN:ND2	1:A:543:SER:OG	2.39	0.56
2:B:373:ASN:HD22	2:B:376:ILE:H	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:O	1:A:352:LEU:HB2	2.06	0.56
2:B:78:THR:O	2:B:81:ILE:HG13	2.07	0.55
2:B:397:ASP:O	2:B:397:ASP:OD2	2.25	0.54
2:B:423:ILE:O	2:B:425:ASN:HB3	2.06	0.54
3:C:269:CYS:SG	5:E:7:DAM:CA	2.89	0.54
2:B:318:PHE:CB	2:B:359:ILE:HD11	2.36	0.54
3:C:73:GLY:HA3	3:C:78:THR:CG2	2.38	0.54
1:A:427:MET:HG3	1:A:450:TRP:HH2	1.71	0.54
2:B:44:ASP:OD2	2:B:47:SER:HB3	2.06	0.54
1:A:168:GLN:HE22	1:A:172:ASN:HD21	1.53	0.54
2:B:284:PRO:HG2	2:B:290:LYS:HB3	1.90	0.53
3:C:124:THR:CG2	3:C:143:TRP:NE1	2.58	0.53
2:B:194:ILE:HD11	2:B:218:LEU:HD21	1.90	0.53
2:B:345:ILE:O	2:B:349:ILE:HG12	2.07	0.53
2:B:424:GLU:CD	2:B:424:GLU:H	2.10	0.53
2:B:69:TYR:CE1	2:B:76:VAL:HG11	2.43	0.53
1:A:516:ILE:HD12	1:A:516:ILE:H	1.73	0.53
3:C:117:ASN:HD22	3:C:167:HIS:CD2	2.26	0.53
2:B:121:TRP:N	2:B:122:PRO:HD2	2.23	0.52
1:A:119:HIS:HB2	1:A:124:LEU:HD13	1.91	0.52
3:C:117:ASN:H	3:C:117:ASN:HD22	1.57	0.52
1:A:499:MET:HE3	1:A:535:ASN:HB3	1.91	0.52
1:A:539:ASN:O	1:A:543:SER:HB2	2.09	0.52
2:B:93:MET:CE	2:B:124:LEU:HD22	2.40	0.52
3:C:48:VAL:HG22	3:C:112:THR:HG21	1.92	0.52
1:A:408:ILE:HG23	1:A:423:ILE:HD12	1.91	0.52
2:B:190:ILE:O	2:B:194:ILE:HG23	2.09	0.52
2:B:24:PRO:HB2	2:B:25:PRO:CD	2.40	0.52
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.91	0.51
2:B:36:LEU:HD23	2:B:66:MET:CE	2.40	0.51
3:C:126:VAL:HG22	3:C:127:TYR:CD2	2.45	0.51
1:A:470:VAL:HG22	1:A:478:ALA:HB2	1.92	0.51
1:A:338:ASN:ND2	1:A:340:HIS:H	2.09	0.51
1:A:128:PHE:O	1:A:131:LEU:HB3	2.11	0.50
1:A:133:LYS:HD3	1:A:169:TYR:CZ	2.46	0.50
3:C:83:MET:HE1	3:C:238:SER:OG	2.10	0.50
2:B:396:ASP:C	2:B:398:CYS:N	2.62	0.50
2:B:169:ARG:HD2	2:B:213:GLU:OE1	2.12	0.50
2:B:319:ARG:O	2:B:323:LYS:HG2	2.12	0.50
2:B:271:LEU:O	2:B:275:VAL:HG13	2.12	0.50
3:C:36:LYS:HG3	3:C:149:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:MET:CE	1:A:539:ASN:ND2	2.74	0.50
1:A:463:THR:O	1:A:466:LEU:HB2	2.12	0.49
2:B:360:MET:O	2:B:364:LEU:HD22	2.13	0.49
1:A:194:LYS:HE2	1:A:230:ASN:ND2	2.28	0.49
1:A:576:LYS:HG2	1:A:580:GLN:NE2	2.28	0.49
2:B:136:GLU:OE1	2:B:178:ARG:NH2	2.39	0.49
2:B:376:ILE:O	2:B:380:ILE:HG22	2.13	0.48
1:A:219:SER:HA	1:A:222:LEU:HD13	1.95	0.48
2:B:417:GLU:O	2:B:421:VAL:HG23	2.14	0.48
1:A:516:ILE:HD12	1:A:516:ILE:N	2.27	0.48
3:C:79:ASN:HD21	3:C:110:ARG:HH21	1.62	0.48
1:A:101:GLU:OE2	2:B:246:LYS:NZ	2.46	0.48
1:A:385:ILE:HD11	1:A:411:LEU:HD13	1.95	0.47
2:B:193:GLN:NE2	2:B:196:ASN:HD22	2.12	0.47
1:A:353:SER:CB	1:A:394:VAL:HG11	2.36	0.47
1:A:427:MET:HG3	1:A:450:TRP:CZ3	2.49	0.47
1:A:327:LEU:CD1	1:A:331:LYS:HE3	2.44	0.47
2:B:24:PRO:CB	2:B:25:PRO:CD	2.93	0.47
2:B:310:PHE:O	2:B:314:MET:HG2	2.14	0.47
1:A:366:LEU:HD21	1:A:403:SER:HB3	1.97	0.47
1:A:59:ILE:HG23	1:A:59:ILE:O	2.14	0.47
3:C:120:SER:HB2	3:C:188:GLU:OE2	2.15	0.47
1:A:440:ASP:HA	1:A:444:ASN:HB2	1.97	0.47
2:B:393:LYS:C	2:B:395:PHE:H	2.18	0.47
2:B:26:ALA:O	2:B:28:GLN:N	2.47	0.47
3:C:88:ASN:HD22	3:C:129:PHE:H	1.62	0.47
2:B:53:LEU:H	2:B:53:LEU:HD22	1.80	0.47
1:A:268:THR:HG21	1:A:308:GLU:CB	2.45	0.46
2:B:273:GLU:HB3	2:B:274:PRO:HD3	1.97	0.46
1:A:366:LEU:HD21	1:A:403:SER:CB	2.46	0.46
1:A:77:THR:HG23	1:A:86:VAL:HG13	1.97	0.46
2:B:371:HIS:HE1	2:B:376:ILE:HD11	1.76	0.46
1:A:350:MET:CE	1:A:384:ILE:O	2.64	0.46
1:A:499:MET:HE2	1:A:539:ASN:ND2	2.30	0.46
2:B:305:ILE:HG12	2:B:310:PHE:HB2	1.97	0.46
1:A:494:ASN:HD21	1:A:496:LEU:HB2	1.80	0.46
1:A:553:ASN:O	1:A:557:GLN:HB2	2.16	0.45
2:B:313:ILE:O	2:B:316:PRO:HD2	2.15	0.45
2:B:368:SER:HA	2:B:380:ILE:HD11	1.98	0.45
2:B:242:LEU:O	2:B:245:HIS:HB2	2.15	0.45
2:B:121:TRP:CD1	2:B:167:ARG:NH1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ASN:HD22	2:B:335:ARG:HE	1.65	0.45
3:C:6:PHE:CE1	3:C:34:LYS:HD2	2.51	0.45
1:A:350:MET:HE3	1:A:387:ASN:HB3	1.98	0.45
1:A:34:LYS:HD2	2:B:420:TRP:HZ2	1.81	0.45
2:B:313:ILE:O	2:B:317:LEU:HB2	2.15	0.45
3:C:56:GLY:HA2	3:C:240:ALA:HB1	1.99	0.45
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.51	0.45
3:C:139:ASN:C	3:C:139:ASN:ND2	2.70	0.45
3:C:17:LEU:HD13	3:C:99:LEU:HA	1.99	0.45
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.98	0.45
1:A:155:TYR:CE2	1:A:163:LYS:HE3	2.52	0.45
2:B:253:TYR:O	2:B:256:GLN:HG2	2.16	0.45
3:C:222:GLN:HG2	3:C:226:GLU:OE2	2.18	0.44
1:A:420:ARG:NH1	1:A:453:ASP:OD1	2.50	0.44
1:A:472:LYS:HE3	1:A:472:LYS:HB3	1.65	0.44
1:A:194:LYS:HE2	1:A:230:ASN:HD22	1.82	0.44
1:A:447:CYS:HA	1:A:450:TRP:CE3	2.52	0.44
2:B:24:PRO:HB2	2:B:25:PRO:HD2	1.98	0.44
2:B:296:ASN:ND2	2:B:335:ARG:HH21	2.16	0.44
1:A:133:LYS:HD3	1:A:169:TYR:CE1	2.52	0.44
2:B:198:PHE:O	2:B:202:ILE:HG23	2.17	0.44
3:C:209:TRP:CB	4:D:65:VAL:HG21	2.48	0.44
1:A:284:VAL:HB	1:A:285:PRO:HD3	2.00	0.43
2:B:346:MET:HA	2:B:349:ILE:HG13	1.99	0.43
3:C:213:PRO:CB	5:E:4:ARG:HH11	2.31	0.43
1:A:248:LEU:HD11	1:A:270:LEU:HD22	2.00	0.43
2:B:202:ILE:CD1	2:B:246:LYS:HD3	2.49	0.43
3:C:95:GLU:OE2	3:C:136:LYS:HE2	2.19	0.43
1:A:206:ILE:HG21	1:A:243:LEU:HB3	2.00	0.43
1:A:494:ASN:ND2	1:A:496:LEU:HB2	2.34	0.43
2:B:109:ASP:HA	2:B:110:PRO:HD2	1.89	0.43
2:B:250:LEU:HD23	2:B:290:LYS:HG2	1.99	0.43
3:C:128:GLY:HA3	7:C:335:HOH:O	2.18	0.43
2:B:242:LEU:HB2	2:B:243:PRO:HD3	2.00	0.42
3:C:237:VAL:O	3:C:256:VAL:HA	2.18	0.42
1:A:433:GLN:HB2	1:A:433:GLN:HE21	1.63	0.42
3:C:171:SER:HB2	3:C:197:ASP:HB2	2.02	0.42
2:B:314:MET:O	2:B:318:PHE:HD1	2.03	0.42
2:B:93:MET:HE3	2:B:93:MET:HA	2.01	0.42
2:B:95:ARG:NH2	2:B:168:GLU:OE1	2.48	0.42
1:A:197:GLU:CD	1:A:197:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:LYS:HA	3:C:111:ILE:CG2	2.50	0.42
1:A:209:PHE:CE1	1:A:228:CYS:HB2	2.55	0.42
3:C:6:PHE:CZ	3:C:34:LYS:HD2	2.55	0.42
2:B:298:LEU:HA	2:B:301:ILE:HD12	2.01	0.42
2:B:313:ILE:HG12	2:B:313:ILE:O	2.20	0.41
2:B:54:LYS:O	2:B:58:VAL:HG23	2.19	0.41
1:A:237:GLN:HE21	1:A:237:GLN:HB3	1.74	0.41
2:B:349:ILE:HG12	2:B:349:ILE:H	1.73	0.41
2:B:121:TRP:N	2:B:122:PRO:CD	2.82	0.41
1:A:115:ILE:O	1:A:119:HIS:HD2	2.03	0.41
1:A:479:HIS:HA	1:A:483:ILE:HG13	2.01	0.41
2:B:36:LEU:CD2	2:B:66:MET:CE	2.98	0.41
2:B:279:LEU:HD12	2:B:298:LEU:HD13	2.01	0.41
2:B:141:GLN:HE21	2:B:141:GLN:HB2	1.64	0.41
3:C:65:LEU:HD22	3:C:96:THR:HG23	2.03	0.41
1:A:116:SER:HA	1:A:119:HIS:CD2	2.55	0.41
2:B:271:LEU:O	2:B:275:VAL:CG1	2.68	0.41
3:C:48:VAL:CG2	3:C:112:THR:HG21	2.51	0.41
3:C:88:ASN:ND2	3:C:129:PHE:H	2.19	0.41
1:A:100:GLU:O	1:A:105:ARG:NH1	2.53	0.41
1:A:215:ASP:O	1:A:221:ARG:HD3	2.21	0.41
1:A:226:GLU:HG2	1:A:262:MET:CE	2.51	0.41
1:A:506:ASN:HD21	1:A:543:SER:HA	1.85	0.41
3:C:115:ARG:NH1	3:C:151:ASP:HA	2.35	0.41
2:B:132:LEU:HA	2:B:132:LEU:HD23	1.89	0.41
3:C:75:SER:N	3:C:76:PRO:CD	2.84	0.41
1:A:499:MET:CE	1:A:539:ASN:HD22	2.34	0.41
1:A:168:GLN:HE22	1:A:172:ASN:ND2	2.18	0.40
2:B:178:ARG:HD3	2:B:178:ARG:HA	1.81	0.40
2:B:271:LEU:O	2:B:274:PRO:HD2	2.22	0.40
2:B:368:SER:CA	2:B:380:ILE:HD11	2.50	0.40
2:B:165:ASP:OD1	2:B:167:ARG:NH2	2.54	0.40
3:C:57:ASP:HB3	3:C:59:HIS:CD2	2.57	0.40
5:E:5:1ZN:H21	5:E:5:1ZN:H17	1.91	0.40
2:B:36:LEU:CD2	2:B:66:MET:HE1	2.47	0.40
3:C:247:GLY:O	3:C:274:ALA:HB3	2.22	0.40
1:A:377:CYS:SG	1:A:380:VAL:HG23	2.61	0.40
2:B:324:CYS:O	2:B:327:SER:HB3	2.21	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	581/588 (99%)	557 (96%)	24 (4%)	0	100	100
2	B	401/403 (100%)	379 (94%)	19 (5%)	3 (1%)	25	53
3	C	299/309 (97%)	282 (94%)	16 (5%)	1 (0%)	44	73
4	D	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
5	E	1/7 (14%)	1 (100%)	0	0	100	100
All	All	1327/1354 (98%)	1262 (95%)	61 (5%)	4 (0%)	44	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	27	ASP
3	C	76	PRO
2	B	77	ILE
2	B	142	PRO

### 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	506/511 (99%)	445 (88%)	61 (12%)	6	13
2	B	353/375 (94%)	309 (88%)	44 (12%)	5	12
3	C	265/274 (97%)	231 (87%)	34 (13%)	5	12
4	D	44/45 (98%)	35 (80%)	9 (20%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	2/2 (100%)	2 (100%)	0	100	100
All	All	1170/1207 (97%)	1022 (87%)	148 (13%)	5	12

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	18	ASP
1	A	21	ARG
1	A	26	GLN
1	A	29	LEU
1	A	42	LEU
1	A	45	GLU
1	A	50	GLU
1	A	52	LEU
1	A	58	THR
1	A	59	ILE
1	A	67	LEU
1	A	76	PHE
1	A	80	VAL
1	A	86	VAL
1	A	95	SER
1	A	103	VAL
1	A	131	LEU
1	A	140	TRP
1	A	145	THR
1	A	160	SER
1	A	168	GLN
1	A	176	ASP
1	A	187	SER
1	A	198	LEU
1	A	205	ILE
1	A	222	LEU
1	A	237	GLN
1	A	277	GLU
1	A	307	LYS
1	A	318	ARG
1	A	321	VAL
1	A	327	LEU
1	A	339	GLN
1	A	341	VAL
1	A	343	SER

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Mol	Chain	Res	Type
1	A	352	LEU
1	A	358	LYS
1	A	373	LEU
1	A	379	GLU
1	A	384	ILE
1	A	387	ASN
1	A	398	ARG
1	A	400	LEU
1	A	405	LEU
1	A	430	LEU
1	A	436	VAL
1	A	437	GLU
1	A	441	GLU
1	A	448	MET
1	A	452	VAL
1	A	464	SER
1	A	465	ASN
1	A	466	LEU
1	A	469	LEU
1	A	472	LYS
1	A	494	ASN
1	A	496	LEU
1	A	502	LEU
1	A	515	ASP
1	A	543	SER
2	B	37	ARG
2	B	42	LEU
2	B	53	LEU
2	B	60	ARG
2	B	93	MET
2	B	95	ARG
2	B	97	LEU
2	B	102	ASN
2	B	116	THR
2	B	133	ARG
2	B	141	GLN
2	B	158	LEU
2	B	160	LEU
2	B	174	THR
2	B	176	LEU
2	B	186	LEU
2	B	194	ILE

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Mol	Chain	Res	Type
2	B	202	ILE
2	B	220	SER
2	B	229	LEU
2	B	237	LEU
2	B	239	LYS
2	B	246	LYS
2	B	247	VAL
2	B	256	GLN
2	B	263	GLN
2	B	266	GLU
2	B	271	LEU
2	B	272	THR
2	B	275	VAL
2	B	302	LEU
2	B	305	ILE
2	B	313	ILE
2	B	314	MET
2	B	317	LEU
2	B	323	LYS
2	B	349	ILE
2	B	350	SER
2	B	363	SER
2	B	364	LEU
2	B	380	ILE
2	B	398	CYS
2	B	403	LYS
2	B	423	ILE
3	C	3	GLU
3	C	4	LYS
3	C	7	THR
3	C	31	LEU
3	C	38	ILE
3	C	39	LEU
3	C	45	VAL
3	C	47	GLU
3	C	49	ARG
3	C	52	VAL
3	C	78	THR
3	C	81	LEU
3	C	98	THR
3	C	105	VAL
3	C	106	ARG

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Mol	Chain	Res	Type
3	C	109	GLU
3	C	112	THR
3	C	117	ASN
3	C	124	THR
3	C	139	ASN
3	C	149	LEU
3	C	158	LEU
3	C	160	ASP
3	C	174	ILE
3	C	192	GLU
3	C	223	ASP
3	C	227	THR
3	C	241	HIS
3	C	277	GLU
3	C	283	LYS
3	C	285	SER
3	C	294	ARG
3	C	295	ARG
3	C	304	THR
4	D	52	THR
4	D	53	LEU
4	D	54	LEU
4	D	63	MET
4	D	68	LEU
4	D	74	LYS
4	D	76	LYS
4	D	79	GLN
4	D	83	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	30	ASN
1	A	119	HIS
1	A	172	ASN
1	A	211	ASN
1	A	217	GLN
1	A	230	ASN
1	A	237	GLN
1	A	250	GLN
1	A	338	ASN

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Mol	Chain	Res	Type
1	A	339	GLN
1	A	360	ASN
1	A	387	ASN
1	A	392	ASN
1	A	433	GLN
1	A	454	HIS
1	A	465	ASN
1	A	494	ASN
1	A	506	ASN
1	A	520	HIS
1	A	539	ASN
1	A	580	GLN
2	B	141	GLN
2	B	193	GLN
2	B	208	HIS
2	B	223	ASN
2	B	254	HIS
2	B	296	ASN
2	B	373	ASN
3	C	27	GLN
3	C	46	GLN
3	C	79	ASN
3	C	88	ASN
3	C	139	ASN
3	C	179	HIS
3	C	272	GLN
4	D	56	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
5	DAL	E	1	5	4,4,5	3.04	1 (25%)	1,4,6	0.28	0
5	ACB	E	3	5	4,8,9	3.79	2 (50%)	3,10,12	0.81	0
5	1ZN	E	5	5	22,23,24	1.12	2 (9%)	24,29,31	0.89	0
5	FGA	E	6	5	3,8,9	1.66	1 (33%)	2,9,11	0.80	0
5	DAM	E	7	5	5,5,6	2.47	2 (40%)	3,5,7	3.31	1 (33%)

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	DAL	E	1	5	-	0/0/2/4	0/0/0/0
5	ACB	E	3	5	-	0/5/10/12	0/0/0/0
5	1ZN	E	5	5	-	0/22/25/27	0/1/1/1
5	FGA	E	6	5	-	0/3/8/9	0/0/0/0
5	DAM	E	7	5	-	0/0/4/6	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6	FGA	CG-CD	2.17	1.55	1.49
5	E	5	1ZN	C3-C2	2.21	1.55	1.52
5	E	5	1ZN	C5-C4	2.28	1.43	1.38
5	E	7	DAM	C-CA	3.15	1.50	1.45
5	E	7	DAM	CA-N	4.13	1.45	1.34
5	E	3	ACB	CB-CA	4.23	1.59	1.55
5	E	1	DAL	CA-C	6.00	1.58	1.50
5	E	3	ACB	CA-N	6.19	1.60	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	7	DAM	O-C-CA	-5.40	118.40	125.07

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
5	E	5	1ZN	2	0
5	E	7	DAM	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	583/588 (99%)	-0.14	2 (0%) 93 94	29, 42, 62, 77	0
2	B	403/403 (100%)	0.12	14 (3%) 44 44	31, 55, 90, 103	0
3	C	303/309 (98%)	-0.12	4 (1%) 77 78	24, 38, 55, 84	0
4	D	47/47 (100%)	0.40	3 (6%) 20 18	37, 49, 74, 83	0
5	E	2/7 (28%)	2.03	1 (50%) 0 0	91, 91, 91, 103	0
All	All	1338/1354 (98%)	-0.04	24 (1%) 69 70	24, 44, 81, 103	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	48	ASP	5.3
2	B	426	LEU	4.4
4	D	51	SER	4.4
1	A	589	ALA	3.7
4	D	50	PRO	3.5
2	B	25	PRO	3.4
1	A	60	TYR	3.4
3	C	309	LEU	3.3
2	B	227	LEU	3.2
2	B	144	ILE	3.2
2	B	34	GLN	3.1
2	B	423	ILE	3.1
2	B	33	ILE	3.0
2	B	425	ASN	3.0
2	B	420	TRP	2.9
2	B	139	ASP	2.7
5	E	4	ARG	2.7
3	C	6	PHE	2.3
2	B	72	HIS	2.2
2	B	75	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	3	GLU	2.1
2	B	401	GLN	2.1
4	D	96	LEU	2.0
3	C	295	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	DAL	E	1	5/6	0.89	0.28	-	77,77,80,80	0
5	DAM	E	7	6/7	0.83	0.34	-	76,80,81,82	0
5	1ZN	E	5	23/24	0.86	0.33	-	64,70,89,93	0
5	ACB	E	3	9/10	0.88	0.24	-	93,97,99,101	0
5	FGA	E	6	9/10	0.79	0.26	-	81,90,97,100	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MN	C	312	1/1	0.98	0.19	0.55	26,26,26,26	0
6	MN	C	311	1/1	0.94	0.18	0.25	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.