



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:33 AM GMT

PDB ID : 2IE3  
Title : Structure of the Protein Phosphatase 2A Core Enzyme Bound to Tumor-inducing Toxins  
Authors : Xing, Y.; Xu, Y.; Chen, Y.; Jeffrey, P.D.; Chao, Y.; Shi, Y.  
Deposited on : 2006-09-17  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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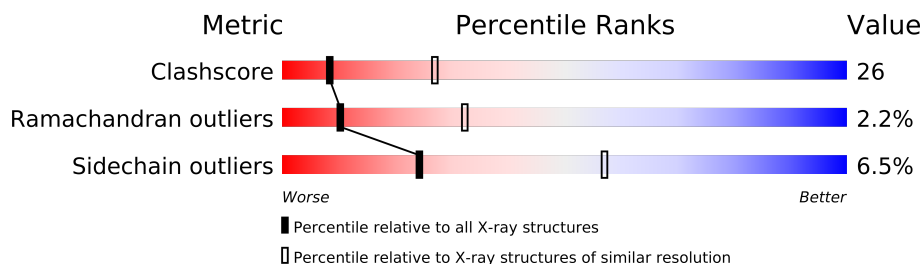
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	589	
2	C	309	
3	I	7	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6922 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4527	2877	763	860	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	288	Total	C	N	O	S	0	0	0
			2322	1471	396	440	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	LEU	VAL	CONFLICT	UNP P67775

- Molecule 3 is a protein called microcystin LR.

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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

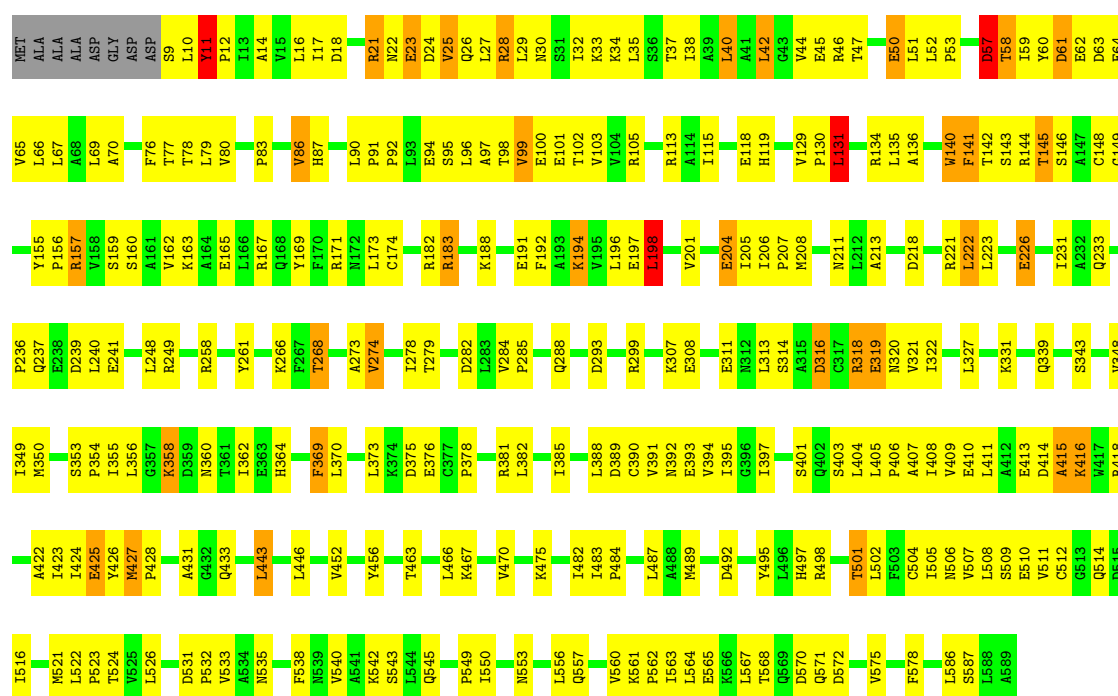
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

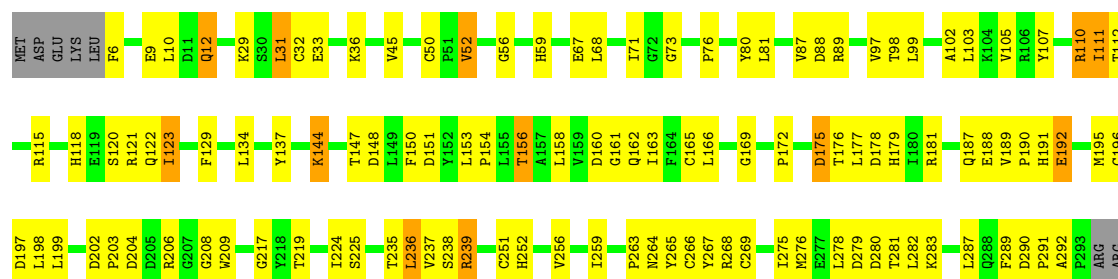
- Molecule 1: Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform

Chain A:



- Molecule 2: Serine/threonine-proteinphosphatase 2A catalytic subunit alpha isoform

Chain C:



GLY	GLU	PRO	HIS	VAL	THR	ARG	ARG	THR	PRO	ASP	TYR	PHE	LEU
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- Molecule 3: microcystin LR

Chain I:



L1	L2	D3	L7
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.07Å 195.09Å 201.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	92.9 (30.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

## 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	0.45	0/4601	0.71	4/6246 (0.1%)
2	C	0.51	0/2379	0.76	2/3227 (0.1%)
3	I	0.52	0/17	0.82	0/19
All	All	0.47	0/6997	0.73	6/9492 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	TYR	N-CA-C	6.67	129.00	111.00
1	A	11	TYR	C-N-CD	6.33	141.69	128.40
2	C	206	ARG	N-CA-C	-6.28	94.06	111.00
1	A	131	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	11	TYR	C-N-CA	-5.44	99.15	122.00
2	C	137	TYR	N-CA-C	-5.29	96.72	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4527	0	4633	259	0
2	C	2322	0	2223	107	0
3	I	71	0	67	3	0
4	C	2	0	0	0	0
All	All	6922	0	6923	361	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (361) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:VAL:HG12	1:A:100:GLU:H	1.05	1.11
1:A:526:LEU:HD22	1:A:563:ILE:HG13	1.51	0.91
2:C:115:ARG:HH12	2:C:151:ASP:HA	1.33	0.90
1:A:99:VAL:HG12	1:A:100:GLU:N	1.83	0.90
2:C:115:ARG:HH21	2:C:189:VAL:HG23	1.37	0.90
1:A:99:VAL:CG1	1:A:100:GLU:H	1.85	0.89
2:C:115:ARG:NH1	2:C:151:ASP:HA	1.88	0.88
2:C:118:HIS:CG	2:C:123:ILE:HD11	2.09	0.87
2:C:45:VAL:HA	2:C:156:THR:HG22	1.55	0.86
1:A:311:GLU:HG2	1:A:355:ILE:HD11	1.56	0.85
1:A:194:LYS:HD2	1:A:194:LYS:O	1.77	0.84
1:A:416:LYS:H	1:A:416:LYS:HD3	1.42	0.83
1:A:59:ILE:HG23	1:A:66:LEU:HD21	1.61	0.82
2:C:81:LEU:HD12	2:C:112:THR:HB	1.61	0.81
1:A:213:ALA:O	1:A:221:ARG:HD2	1.80	0.81
2:C:118:HIS:ND1	2:C:123:ILE:HD11	1.97	0.80
1:A:373:LEU:HD11	1:A:385:ILE:HD11	1.64	0.80
1:A:381:ARG:HD2	1:A:426:TYR:OH	1.82	0.80
2:C:281:THR:HG22	2:C:281:THR:O	1.83	0.79
1:A:27:LEU:HD13	1:A:32:ILE:HD11	1.64	0.79
2:C:175:ASP:H	2:C:179:HIS:HD2	1.30	0.78
2:C:176:THR:HG22	2:C:179:HIS:H	1.48	0.77
2:C:67:GLU:HB2	2:C:292:ALA:HB2	1.66	0.76
1:A:339:GLN:O	1:A:343:SER:HB2	1.86	0.75
1:A:105:ARG:HH21	1:A:145:THR:HG21	1.51	0.75
1:A:97:ALA:O	1:A:105:ARG:HD2	1.87	0.75
2:C:176:THR:CG2	2:C:178:ASP:H	2.00	0.74
1:A:29:LEU:HD11	1:A:64:GLU:HG2	1.69	0.74
1:A:226:GLU:OE2	1:A:266:LYS:HE3	1.88	0.74
1:A:42:LEU:HB2	1:A:46:ARG:HB2	1.69	0.73
1:A:57:ASP:O	1:A:59:ILE:HG13	1.89	0.72
2:C:275:ILE:HG22	2:C:287:LEU:HB2	1.71	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:564:LEU:O	1:A:568:THR:HG23	1.89	0.72
1:A:416:LYS:HD3	1:A:416:LYS:N	2.04	0.72
1:A:67:LEU:HD13	1:A:103:VAL:HG12	1.71	0.72
1:A:388:LEU:H	1:A:433:GLN:HE22	1.38	0.70
2:C:118:HIS:HA	2:C:123:ILE:CD1	2.22	0.70
1:A:28:ARG:HH11	1:A:30:ASN:HB2	1.58	0.69
1:A:204:GLU:O	1:A:208:MET:HG3	1.93	0.69
2:C:189:VAL:HA	2:C:195:MET:HE3	1.75	0.68
1:A:52:LEU:HB2	1:A:53:PRO:HD3	1.76	0.68
2:C:264:ASN:ND2	2:C:267:TYR:HA	2.09	0.68
2:C:290:ASP:HB3	2:C:291:PRO:HD2	1.74	0.68
1:A:285:PRO:HA	1:A:288:GLN:HE21	1.57	0.68
1:A:409:VAL:HG22	1:A:446:LEU:HD21	1.75	0.68
1:A:205:ILE:HD13	1:A:208:MET:HE3	1.75	0.68
1:A:446:LEU:HD12	1:A:446:LEU:H	1.58	0.68
2:C:122:GLN:HE22	2:C:191:HIS:HE1	1.40	0.67
2:C:176:THR:HG22	2:C:178:ASP:N	2.09	0.67
1:A:452:VAL:HG22	1:A:497:HIS:CE1	2.30	0.67
1:A:159:SER:OG	1:A:162:VAL:HG23	1.95	0.66
1:A:62:GLU:HA	1:A:62:GLU:OE2	1.96	0.65
2:C:190:PRO:HD3	2:C:195:MET:CE	2.26	0.65
1:A:284:VAL:O	1:A:288:GLN:HG3	1.97	0.65
2:C:283:LYS:HA	2:C:283:LYS:HE2	1.78	0.65
2:C:81:LEU:CD1	2:C:112:THR:HB	2.27	0.65
2:C:268:ARG:NH1	2:C:268:ARG:HB3	2.11	0.64
2:C:204:ASP:O	2:C:252:HIS:HE1	1.79	0.64
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.28	0.64
1:A:136:ALA:O	1:A:144:ARG:HG3	1.98	0.64
1:A:131:LEU:HD12	1:A:131:LEU:C	2.18	0.64
2:C:190:PRO:HD3	2:C:195:MET:HE2	1.79	0.63
1:A:378:PRO:HA	1:A:381:ARG:NH1	2.13	0.63
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.64	0.63
1:A:358:LYS:O	1:A:362:ILE:HG13	1.98	0.63
1:A:514:GLN:HG3	1:A:550:ILE:O	1.99	0.63
1:A:62:GLU:O	1:A:64:GLU:N	2.31	0.63
1:A:40:LEU:HD22	1:A:40:LEU:N	2.13	0.62
1:A:538:PHE:HB2	1:A:578:PHE:HD2	1.64	0.62
1:A:29:LEU:HD21	1:A:33:LYS:HE3	1.82	0.62
1:A:96:LEU:O	1:A:99:VAL:HG23	1.99	0.61
2:C:89:ARG:HD2	2:C:266:CYS:SG	2.39	0.61
1:A:23:GLU:HG3	1:A:26:GLN:OE1	1.99	0.61
2:C:176:THR:HG22	2:C:178:ASP:H	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:183:ARG:NH1	1:A:183:ARG:HG3	2.15	0.61
1:A:409:VAL:O	1:A:413:GLU:HG2	2.00	0.61
1:A:350:MET:HB3	1:A:391:VAL:HG23	1.83	0.60
1:A:29:LEU:HD23	1:A:29:LEU:C	2.22	0.60
2:C:281:THR:CG2	2:C:281:THR:O	2.49	0.60
1:A:37:THR:HA	1:A:40:LEU:HD23	1.83	0.60
1:A:349:ILE:HG23	1:A:350:MET:N	2.16	0.60
2:C:176:THR:HG23	2:C:178:ASP:H	1.67	0.60
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.84	0.60
1:A:475:LYS:HB2	1:A:516:ILE:HD12	1.84	0.59
2:C:115:ARG:NH1	2:C:150:PHE:O	2.33	0.59
1:A:390:CYS:O	1:A:394:VAL:HG23	2.01	0.59
2:C:225:SER:OG	2:C:252:HIS:HD2	1.84	0.59
2:C:177:LEU:O	2:C:181:ARG:HG3	2.01	0.59
1:A:129:VAL:HB	1:A:130:PRO:HD3	1.84	0.59
1:A:165:GLU:O	1:A:169:TYR:HD1	1.86	0.59
1:A:392:ASN:O	1:A:395:ILE:O	2.20	0.59
1:A:446:LEU:HD12	1:A:446:LEU:N	2.18	0.59
1:A:23:GLU:HG3	1:A:26:GLN:CD	2.23	0.59
1:A:240:LEU:HD13	1:A:274:VAL:HG23	1.84	0.59
1:A:62:GLU:HB3	1:A:65:VAL:HB	1.83	0.59
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.39	0.58
2:C:191:HIS:C	2:C:192:GLU:HG3	2.23	0.58
2:C:50:CYS:HA	2:C:52:VAL:HG22	1.85	0.58
2:C:188:GLU:HG3	2:C:189:VAL:N	2.17	0.58
1:A:509:SER:O	1:A:550:ILE:HD13	2.02	0.58
1:A:37:THR:OG1	1:A:38:ILE:HD12	2.03	0.58
1:A:307:LYS:O	1:A:311:GLU:HG3	2.03	0.58
1:A:507:VAL:O	1:A:510:GLU:HB2	2.04	0.58
1:A:241:GLU:OE2	1:A:249:ARG:NH2	2.37	0.57
1:A:489:MET:HB2	1:A:501:THR:OG1	2.05	0.57
1:A:318:ARG:O	1:A:321:VAL:HG22	2.05	0.57
2:C:176:THR:CG2	2:C:178:ASP:HB2	2.34	0.57
1:A:136:ALA:O	1:A:144:ARG:CG	2.52	0.57
2:C:208:GLY:C	2:C:224:ILE:HD11	2.25	0.57
1:A:586:LEU:O	1:A:587:SER:HB2	2.05	0.57
1:A:424:ILE:O	1:A:427:MET:HB2	2.05	0.57
1:A:388:LEU:H	1:A:433:GLN:NE2	2.04	0.56
2:C:158:LEU:HD21	2:C:161:GLY:HA2	1.87	0.56
2:C:59:HIS:HE1	2:C:118:HIS:CD2	2.23	0.56
1:A:206:ILE:HB	1:A:207:PRO:HD3	1.86	0.56
1:A:205:ILE:HD13	1:A:208:MET:CE	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:370:LEU:HD21	1:A:403:SER:O	2.06	0.56
2:C:68:LEU:HG	2:C:275:ILE:HD12	1.88	0.56
1:A:492:ASP:O	1:A:498:ARG:HD3	2.05	0.55
2:C:203:PRO:HD2	2:C:239:ARG:CZ	2.35	0.55
1:A:381:ARG:O	1:A:385:ILE:HG12	2.05	0.55
1:A:356:LEU:O	1:A:360:ASN:HB2	2.06	0.55
1:A:236:PRO:HG2	1:A:239:ASP:OD2	2.07	0.55
2:C:197:ASP:OD1	2:C:217:GLY:HA2	2.05	0.55
1:A:28:ARG:NH1	1:A:30:ASN:HD22	2.04	0.55
1:A:373:LEU:HD11	1:A:385:ILE:CD1	2.35	0.55
2:C:118:HIS:HA	2:C:123:ILE:HD11	1.88	0.55
1:A:59:ILE:HG22	1:A:59:ILE:O	2.06	0.54
1:A:350:MET:SD	1:A:369:PHE:HB2	2.47	0.54
1:A:542:LYS:NZ	1:A:578:PHE:CE1	2.76	0.54
1:A:502:LEU:HD11	1:A:540:VAL:HG23	1.90	0.54
1:A:353:SER:OG	1:A:391:VAL:HG22	2.08	0.54
2:C:268:ARG:HH11	2:C:268:ARG:HB3	1.73	0.54
1:A:553:ASN:O	1:A:557:GLN:HG2	2.08	0.54
1:A:194:LYS:CD	1:A:194:LYS:O	2.52	0.53
1:A:86:VAL:HG11	1:A:118:GLU:CB	2.39	0.53
1:A:28:ARG:NH1	1:A:30:ASN:HB2	2.22	0.53
1:A:60:TYR:O	1:A:62:GLU:N	2.41	0.53
1:A:155:TYR:CZ	1:A:196:LEU:HD22	2.44	0.53
1:A:205:ILE:HG22	1:A:231:ILE:HD13	1.90	0.53
2:C:169:GLY:O	2:C:198:LEU:HA	2.08	0.53
2:C:266:CYS:SG	3:I:2:LEU:HD12	2.48	0.53
1:A:113:ARG:NH1	1:A:149:GLY:O	2.42	0.53
1:A:572:ASP:OD2	2:C:110:ARG:NH2	2.42	0.53
2:C:118:HIS:HA	2:C:123:ILE:HD13	1.90	0.52
1:A:470:VAL:HG11	1:A:511:VAL:HG23	1.90	0.52
2:C:87:VAL:O	2:C:88:ASP:HB2	2.09	0.52
1:A:233:GLN:HG3	1:A:273:ALA:CB	2.40	0.52
1:A:86:VAL:HG11	1:A:118:GLU:HB2	1.91	0.52
1:A:233:GLN:HG3	1:A:273:ALA:HB1	1.92	0.52
1:A:258:ARG:O	1:A:261:TYR:HB3	2.09	0.52
1:A:59:ILE:HG23	1:A:66:LEU:CD2	2.34	0.52
2:C:162:GLN:HB3	2:C:235:THR:OG1	2.10	0.52
1:A:21:ARG:NH1	1:A:26:GLN:OE1	2.43	0.52
1:A:115:ILE:O	1:A:119:HIS:HD2	1.93	0.52
1:A:505:ILE:HG23	1:A:521:MET:HB3	1.91	0.52
1:A:32:ILE:O	1:A:32:ILE:HG22	2.09	0.52
1:A:467:LYS:HB2	1:A:507:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:466:LEU:HD22	1:A:482:ILE:HD13	1.91	0.52
1:A:404:LEU:HD11	1:A:408:ILE:HD11	1.91	0.51
2:C:268:ARG:NH1	3:I:2:LEU:HD21	2.25	0.51
1:A:83:PRO:O	1:A:86:VAL:HG22	2.10	0.51
1:A:102:THR:CG2	1:A:105:ARG:HH12	2.22	0.51
1:A:46:ARG:HD2	1:A:50:GLU:CD	2.31	0.51
1:A:44:VAL:HG13	1:A:45:GLU:N	2.26	0.51
1:A:44:VAL:HG23	1:A:80:VAL:C	2.30	0.51
1:A:282:ASP:O	1:A:285:PRO:HD2	2.11	0.51
1:A:90:LEU:HB2	1:A:91:PRO:HD3	1.92	0.51
2:C:165:CYS:HA	2:C:238:SER:O	2.10	0.51
2:C:80:TYR:HB2	2:C:111:ILE:HG22	1.93	0.51
1:A:506:ASN:HD21	1:A:543:SER:CB	2.24	0.51
1:A:40:LEU:CD2	1:A:40:LEU:N	2.73	0.51
2:C:176:THR:HG21	2:C:178:ASP:HB2	1.92	0.50
2:C:89:ARG:HG3	2:C:265:TYR:OH	2.11	0.50
2:C:121:ARG:HG2	2:C:147:THR:HB	1.93	0.50
1:A:145:THR:HG22	1:A:146:SER:N	2.26	0.50
2:C:251:CYS:O	2:C:252:HIS:HB2	2.12	0.50
1:A:58:THR:O	1:A:58:THR:HG22	2.11	0.50
1:A:155:TYR:CE1	1:A:163:LYS:HB3	2.46	0.50
1:A:57:ASP:O	1:A:58:THR:C	2.47	0.50
1:A:350:MET:HB3	1:A:391:VAL:CG2	2.41	0.50
2:C:279:ASP:OD2	2:C:283:LYS:HB2	2.11	0.50
1:A:157:ARG:HH11	1:A:157:ARG:HG2	1.77	0.50
1:A:197:GLU:CD	1:A:197:GLU:H	2.15	0.50
2:C:283:LYS:CA	2:C:283:LYS:HE2	2.42	0.50
1:A:102:THR:HA	1:A:105:ARG:NH1	2.27	0.50
1:A:313:LEU:HD13	1:A:321:VAL:CG2	2.42	0.49
1:A:354:PRO:HD3	1:A:390:CYS:SG	2.52	0.49
2:C:176:THR:HG22	2:C:179:HIS:N	2.23	0.49
2:C:263:PRO:O	2:C:264:ASN:C	2.49	0.49
1:A:136:ALA:O	1:A:144:ARG:HD2	2.12	0.49
1:A:452:VAL:CG2	1:A:497:HIS:CE1	2.95	0.49
2:C:237:VAL:HB	2:C:256:VAL:HG22	1.95	0.49
1:A:87:HIS:HA	1:A:90:LEU:HG	1.95	0.49
2:C:31:LEU:HD21	2:C:102:ALA:HA	1.94	0.49
1:A:80:VAL:HG12	1:A:80:VAL:O	2.12	0.49
2:C:115:ARG:NH2	2:C:189:VAL:HG23	2.18	0.49
1:A:141:PHE:CD1	1:A:141:PHE:C	2.84	0.49
1:A:38:ILE:HD12	1:A:38:ILE:N	2.27	0.49
1:A:542:LYS:NZ	1:A:578:PHE:CD1	2.81	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:THR:HG23	1:A:51:LEU:HD23	1.94	0.49
2:C:264:ASN:HA	2:C:269:CYS:O	2.13	0.48
1:A:42:LEU:HB2	1:A:46:ARG:CB	2.41	0.48
1:A:327:LEU:HG	1:A:331:LYS:HE3	1.95	0.48
2:C:187:GLN:HG3	2:C:188:GLU:O	2.13	0.48
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.76	0.48
2:C:144:LYS:HE3	2:C:148:ASP:OD2	2.13	0.48
1:A:25:VAL:HG12	1:A:25:VAL:O	2.13	0.48
1:A:94:GLU:OE1	1:A:134:ARG:NH2	2.43	0.48
1:A:9:SER:O	1:A:10:LEU:HD23	2.14	0.48
1:A:38:ILE:H	1:A:38:ILE:HD12	1.79	0.48
1:A:131:LEU:CD1	1:A:131:LEU:C	2.81	0.48
1:A:17:ILE:HG22	1:A:18:ASP:N	2.29	0.48
1:A:293:ASP:O	1:A:299:ARG:HD3	2.14	0.48
1:A:353:SER:N	1:A:354:PRO:HD2	2.29	0.48
1:A:522:LEU:N	1:A:523:PRO:CD	2.77	0.48
1:A:37:THR:CA	1:A:40:LEU:HD23	2.42	0.47
1:A:46:ARG:HD2	1:A:50:GLU:OE2	2.14	0.47
2:C:122:GLN:HG3	2:C:188:GLU:OE2	2.13	0.47
1:A:174:CYS:O	1:A:182:ARG:HD2	2.14	0.47
1:A:456:TYR:CD1	2:C:73:GLY:HA2	2.49	0.47
1:A:183:ARG:HH11	1:A:183:ARG:CG	2.27	0.47
1:A:509:SER:HB2	1:A:550:ILE:HD12	1.97	0.47
2:C:176:THR:O	2:C:179:HIS:HB2	2.15	0.47
1:A:92:PRO:O	1:A:95:SER:HB3	2.14	0.47
1:A:307:LYS:HE2	1:A:311:GLU:OE1	2.15	0.47
1:A:240:LEU:HD13	1:A:274:VAL:CG2	2.44	0.47
1:A:533:VAL:HG21	2:C:280:ASP:OD2	2.14	0.47
1:A:538:PHE:HB3	1:A:575:VAL:HA	1.96	0.47
1:A:140:TRP:N	1:A:140:TRP:CD1	2.82	0.47
1:A:188:LYS:HD2	1:A:191:GLU:OE2	2.14	0.47
1:A:567:LEU:O	1:A:570:ASP:HB2	2.15	0.46
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.98	0.46
2:C:120:SER:HB3	2:C:123:ILE:HG23	1.97	0.46
1:A:32:ILE:CG2	1:A:32:ILE:O	2.63	0.46
1:A:10:LEU:O	1:A:14:ALA:HB2	2.16	0.46
1:A:11:TYR:O	1:A:12:PRO:C	2.47	0.46
1:A:463:THR:HG23	1:A:504:CYS:SG	2.55	0.46
2:C:191:HIS:O	2:C:192:GLU:HG3	2.16	0.46
1:A:141:PHE:CD1	1:A:142:THR:N	2.84	0.46
1:A:69:LEU:O	1:A:69:LEU:HD12	2.15	0.46
1:A:311:GLU:CG	1:A:355:ILE:HD11	2.38	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:376:GLU:O	1:A:378:PRO:HD3	2.16	0.46
1:A:411:LEU:HB2	1:A:423:ILE:HG13	1.97	0.46
1:A:307:LYS:NZ	1:A:307:LYS:HB3	2.31	0.46
1:A:369:PHE:O	1:A:373:LEU:HB2	2.16	0.46
1:A:279:THR:O	1:A:284:VAL:HG23	2.16	0.46
1:A:422:ALA:O	1:A:425:GLU:HG2	2.15	0.46
1:A:322:ILE:HG21	1:A:356:LEU:HD21	1.98	0.45
1:A:102:THR:HG22	1:A:105:ARG:HH12	1.80	0.45
1:A:483:ILE:N	1:A:484:PRO:CD	2.79	0.45
1:A:35:LEU:C	1:A:37:THR:H	2.18	0.45
1:A:171:ARG:HH12	1:A:204:GLU:CG	2.29	0.45
1:A:318:ARG:O	1:A:320:ASN:N	2.49	0.45
1:A:369:PHE:HZ	1:A:404:LEU:HB2	1.81	0.45
1:A:411:LEU:C	1:A:413:GLU:H	2.20	0.45
2:C:268:ARG:HH11	2:C:268:ARG:CB	2.29	0.45
1:A:206:ILE:CB	1:A:207:PRO:HD3	2.47	0.45
1:A:248:LEU:HD12	1:A:248:LEU:O	2.16	0.45
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.98	0.45
2:C:281:THR:HG22	2:C:283:LYS:HE3	1.98	0.45
1:A:425:GLU:O	1:A:428:PRO:HD2	2.17	0.45
2:C:115:ARG:HB2	2:C:153:LEU:HB2	1.99	0.45
1:A:349:ILE:CG2	1:A:350:MET:N	2.79	0.45
1:A:44:VAL:HG13	1:A:45:GLU:H	1.81	0.45
1:A:561:LYS:O	1:A:565:GLU:HG3	2.17	0.45
1:A:99:VAL:CG1	1:A:100:GLU:N	2.55	0.45
1:A:378:PRO:CB	1:A:381:ARG:HH12	2.30	0.45
1:A:407:ALA:O	1:A:410:GLU:HB3	2.17	0.45
2:C:190:PRO:HD3	2:C:195:MET:HE3	1.97	0.44
1:A:401:SER:O	1:A:405:LEU:HB2	2.17	0.44
1:A:268:THR:HG21	1:A:308:GLU:CG	2.47	0.44
1:A:391:VAL:O	1:A:395:ILE:HG12	2.18	0.44
1:A:34:LYS:O	1:A:38:ILE:CD1	2.65	0.44
2:C:89:ARG:NH2	3:I:3:ACB:O	2.47	0.44
1:A:67:LEU:CD1	1:A:103:VAL:HG12	2.43	0.44
2:C:202:ASP:O	2:C:219:THR:HA	2.17	0.44
1:A:556:LEU:HD23	1:A:560:VAL:HG21	1.99	0.44
1:A:350:MET:CE	1:A:369:PHE:HB2	2.48	0.44
1:A:77:THR:HG23	1:A:86:VAL:HG13	2.00	0.44
2:C:166:LEU:N	2:C:166:LEU:HD23	2.33	0.44
1:A:130:PRO:O	1:A:134:ARG:HG3	2.18	0.44
1:A:389:ASP:O	1:A:393:GLU:OE1	2.36	0.44
1:A:148:CYS:SG	1:A:173:LEU:HD13	2.57	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:418:ARG:NH2	2:C:67:GLU:OE1	2.51	0.44
1:A:427:MET:CE	1:A:443:LEU:HG	2.48	0.44
1:A:414:ASP:OD1	1:A:415:ALA:N	2.51	0.44
2:C:97:VAL:HG13	2:C:98:THR:N	2.32	0.44
2:C:81:LEU:HD12	2:C:112:THR:CB	2.41	0.43
1:A:155:TYR:OH	1:A:167:ARG:NH1	2.51	0.43
2:C:29:LYS:O	2:C:33:GLU:HG3	2.17	0.43
1:A:545:GLN:HG2	1:A:545:GLN:O	2.18	0.43
1:A:198:LEU:O	1:A:201:VAL:N	2.50	0.43
1:A:446:LEU:CD1	1:A:446:LEU:H	2.28	0.43
1:A:218:ASP:OD1	1:A:258:ARG:NH1	2.51	0.43
1:A:80:VAL:CG1	1:A:80:VAL:O	2.66	0.43
1:A:135:LEU:HD23	1:A:143:SER:OG	2.19	0.43
1:A:318:ARG:HG2	1:A:319:GLU:N	2.33	0.43
1:A:375:ASP:O	1:A:381:ARG:NH2	2.51	0.43
1:A:571:GLN:HG2	1:A:572:ASP:N	2.34	0.43
1:A:96:LEU:HA	1:A:99:VAL:HG23	2.01	0.43
2:C:32:CYS:O	2:C:36:LYS:HG3	2.19	0.43
2:C:10:LEU:HD11	2:C:105:VAL:HG12	1.99	0.43
1:A:78:THR:C	1:A:80:VAL:H	2.21	0.43
2:C:276:MET:CE	2:C:278:LEU:HD21	2.49	0.43
1:A:487:LEU:HD22	1:A:524:THR:OG1	2.19	0.43
1:A:70:ALA:HB2	1:A:96:LEU:HD13	2.01	0.43
1:A:61:ASP:HA	1:A:66:LEU:HD11	2.00	0.43
1:A:42:LEU:HD22	1:A:42:LEU:H	1.84	0.43
1:A:411:LEU:C	1:A:413:GLU:N	2.72	0.43
1:A:508:LEU:O	1:A:512:CYS:HB2	2.18	0.43
1:A:561:LYS:N	1:A:562:PRO:CD	2.82	0.43
1:A:456:TYR:CG	2:C:73:GLY:HA2	2.54	0.43
1:A:313:LEU:HD13	1:A:321:VAL:HG21	1.99	0.42
2:C:282:LEU:HD23	2:C:282:LEU:HA	1.82	0.42
2:C:115:ARG:HG2	2:C:199:LEU:HD21	2.02	0.42
1:A:102:THR:HG22	1:A:105:ARG:NH1	2.34	0.42
2:C:99:LEU:O	2:C:102:ALA:HB3	2.18	0.42
1:A:392:ASN:HD21	1:A:397:ILE:HA	1.84	0.42
1:A:406:PRO:O	1:A:410:GLU:HB2	2.19	0.42
2:C:56:GLY:HA3	2:C:259:ILE:O	2.19	0.42
1:A:105:ARG:CZ	1:A:142:THR:HG22	2.49	0.42
1:A:77:THR:HG23	1:A:86:VAL:CG1	2.50	0.42
2:C:76:PRO:HG3	2:C:107:TYR:CE1	2.55	0.42
2:C:97:VAL:CG1	2:C:98:THR:N	2.82	0.42
1:A:222:LEU:HD23	1:A:223:LEU:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:45:VAL:HG22	2:C:156:THR:CG2	2.50	0.42
1:A:196:LEU:CD1	1:A:205:ILE:HD11	2.50	0.42
1:A:98:THR:O	1:A:98:THR:HG22	2.19	0.42
2:C:6:PHE:O	2:C:9:GLU:HB3	2.20	0.42
2:C:45:VAL:HG22	2:C:156:THR:HG21	2.01	0.42
1:A:397:ILE:O	1:A:401:SER:HB2	2.20	0.42
2:C:176:THR:HB	2:C:179:HIS:CD2	2.54	0.42
1:A:538:PHE:C	1:A:538:PHE:CD1	2.93	0.42
2:C:76:PRO:HB2	2:C:110:ARG:HG3	2.02	0.42
2:C:10:LEU:HA	2:C:10:LEU:HD23	1.83	0.42
2:C:190:PRO:O	2:C:196:CYS:HB2	2.20	0.41
1:A:136:ALA:O	1:A:144:ARG:CD	2.67	0.41
1:A:192:PHE:CE1	1:A:196:LEU:HD21	2.55	0.41
2:C:71:ILE:CD1	2:C:289:PHE:HB3	2.50	0.41
1:A:201:VAL:HA	1:A:205:ILE:CG1	2.50	0.41
1:A:17:ILE:CG2	1:A:18:ASP:N	2.84	0.41
1:A:284:VAL:N	1:A:285:PRO:CD	2.84	0.41
2:C:163:ILE:HG23	2:C:236:LEU:HD23	2.03	0.41
1:A:78:THR:O	1:A:80:VAL:N	2.53	0.41
1:A:38:ILE:O	1:A:42:LEU:HD22	2.20	0.41
2:C:225:SER:OG	2:C:252:HIS:CD2	2.70	0.41
1:A:44:VAL:HG23	1:A:80:VAL:O	2.21	0.41
1:A:327:LEU:HD21	1:A:364:HIS:HB3	2.03	0.41
1:A:314:SER:C	1:A:316:ASP:N	2.73	0.41
2:C:172:PRO:HA	2:C:209:TRP:CZ2	2.56	0.41
1:A:196:LEU:HD11	1:A:205:ILE:HD11	2.03	0.41
1:A:100:GLU:O	1:A:101:GLU:C	2.59	0.40
1:A:531:ASP:CG	1:A:532:PRO:HD2	2.41	0.40
1:A:321:VAL:HG23	1:A:322:ILE:N	2.37	0.40
2:C:103:LEU:O	2:C:111:ILE:HD11	2.20	0.40
2:C:9:GLU:O	2:C:12:GLN:HB3	2.21	0.40
1:A:318:ARG:HD3	1:A:355:ILE:CG2	2.51	0.40
1:A:427:MET:HE2	1:A:443:LEU:HG	2.03	0.40
1:A:318:ARG:HD3	1:A:355:ILE:HG23	2.03	0.40
1:A:240:LEU:HD12	1:A:278:ILE:HD12	2.04	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	579/589 (98%)	499 (86%)	62 (11%)	18 (3%)	7	21
2	C	286/309 (93%)	255 (89%)	30 (10%)	1 (0%)	50	84
3	I	1/7 (14%)	1 (100%)	0	0	100	100
All	All	866/905 (96%)	755 (87%)	92 (11%)	19 (2%)	10	32

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	63	ASP
1	A	319	GLU
1	A	21	ARG
1	A	23	GLU
1	A	57	ASP
1	A	79	LEU
1	A	140	TRP
1	A	316	ASP
1	A	431	ALA
2	C	129	PHE
1	A	198	LEU
1	A	415	ALA
1	A	25	VAL
1	A	58	THR
1	A	318	ARG
1	A	22	ASN
1	A	99	VAL
1	A	348	VAL

### 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	508/512 (99%)	473 (93%)	35 (7%)	22	53
2	C	254/274 (93%)	239 (94%)	15 (6%)	28	62
3	I	2/2 (100%)	2 (100%)	0	100	100
All	All	764/788 (97%)	714 (94%)	50 (6%)	24	57

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	16	LEU
1	A	24	ASP
1	A	28	ARG
1	A	40	LEU
1	A	42	LEU
1	A	50	GLU
1	A	57	ASP
1	A	76	PHE
1	A	86	VAL
1	A	131	LEU
1	A	141	PHE
1	A	145	THR
1	A	157	ARG
1	A	160	SER
1	A	183	ARG
1	A	194	LYS
1	A	198	LEU
1	A	204	GLU
1	A	211	ASN
1	A	222	LEU
1	A	226	GLU
1	A	237	GLN
1	A	268	THR
1	A	274	VAL
1	A	358	LYS
1	A	369	PHE
1	A	382	LEU
1	A	416	LYS
1	A	425	GLU
1	A	427	MET
1	A	443	LEU

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Mol	Chain	Res	Type
1	A	495	TYR
1	A	501	THR
1	A	549	PRO
2	C	12	GLN
2	C	31	LEU
2	C	52	VAL
2	C	110	ARG
2	C	111	ILE
2	C	123	ILE
2	C	134	LEU
2	C	144	LYS
2	C	154	PRO
2	C	156	THR
2	C	160	ASP
2	C	175	ASP
2	C	192	GLU
2	C	236	LEU
2	C	239	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	30	ASN
1	A	119	HIS
1	A	200	ASN
1	A	237	GLN
1	A	271	GLN
1	A	288	GLN
1	A	364	HIS
1	A	392	ASN
1	A	402	GLN
1	A	433	GLN
1	A	465	ASN
1	A	506	ASN
2	C	16	GLN
2	C	122	GLN
2	C	179	HIS
2	C	191	HIS
2	C	252	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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$
3	DAL	I	1	3	4,4,5	8.94	2 (50%)	3,4,6	3.82	1 (33%)
3	ACB	I	3	3	8,8,9	6.82	3 (37%)	9,10,12	16.49	1 (11%)
3	1ZN	I	5	3	23,23,24	4.12	4 (17%)	28,29,31	9.53	3 (10%)
3	FGA	I	6	3	8,8,9	7.59	4 (50%)	7,9,11	1.76	2 (28%)
3	DAM	I	7	3,2	4,5,6	3.43	1 (25%)	2,5,7	2.73	2 (100%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	6	FGA	OE1-CD	20.48	1.25	1.11
3	I	3	ACB	OD1-CG	18.59	1.24	1.11
3	I	5	1ZN	O3-C20	18.43	1.24	1.11
3	I	1	DAL	O-C	17.01	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	7	DAM	CA-N	5.99	1.45	1.34
3	I	1	DAL	CA-C	5.40	1.58	1.48
3	I	6	FGA	O-C	4.25	1.36	1.22
3	I	5	1ZN	C3-C2	3.80	1.57	1.52
3	I	3	ACB	CA-N	3.56	1.60	1.47
3	I	3	ACB	CB-CA	2.82	1.58	1.55
3	I	6	FGA	CG-CD	2.73	1.55	1.47
3	I	6	FGA	CB-CG	2.67	1.59	1.52
3	I	5	1ZN	C9-C4	2.40	1.44	1.38
3	I	5	1ZN	C18-C17	-2.24	1.52	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5	1ZN	O3-C20-C18	-50.06	120.82	176.50
3	I	3	ACB	OD1-CG-CB	-49.41	121.54	176.50
3	I	1	DAL	C-CA-N	-6.37	112.55	113.27
3	I	5	1ZN	C19-C18-C20	3.74	110.13	108.46
3	I	6	FGA	OXT-C-CA	3.69	125.16	116.88
3	I	7	DAM	CM-N-CA	-2.90	116.21	124.79
3	I	6	FGA	O-C-CA	-2.78	110.33	118.36
3	I	5	1ZN	C17-C16-C15	-2.65	119.50	123.80
3	I	7	DAM	CB-CA-N	-2.54	120.41	126.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.