



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:52 pm BST

PDB ID : 1R1O  
Title : Amino Acid Sulfonamides as Transition-State Analogue Inhibitors of Arginase  
Authors : Cama, E.; Shin, H.; Christianson, D.W.  
Deposited on : 2003-09-24  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

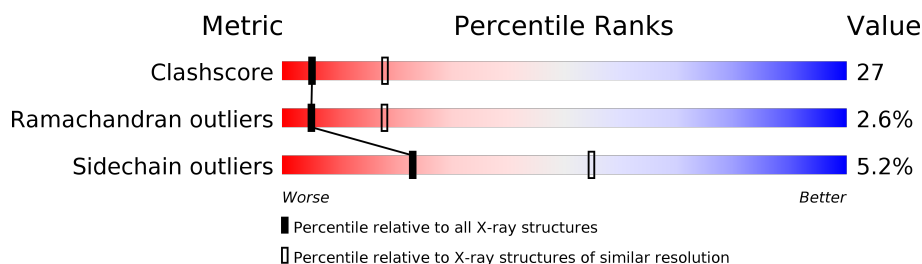
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	
1	C	323	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7271 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.

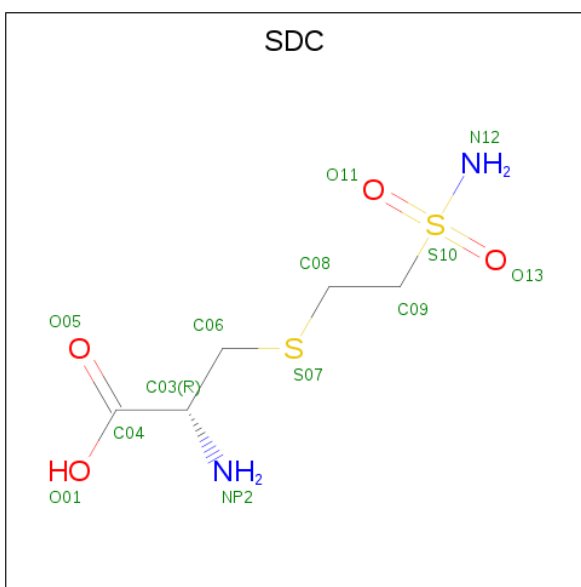
- Molecule 1 is a protein called Arginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			
1	B	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			
1	C	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is S-[2-(AMINOSULFONYL)ETHYL]-D-CYSTEINE (three-letter code: SDC) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>).

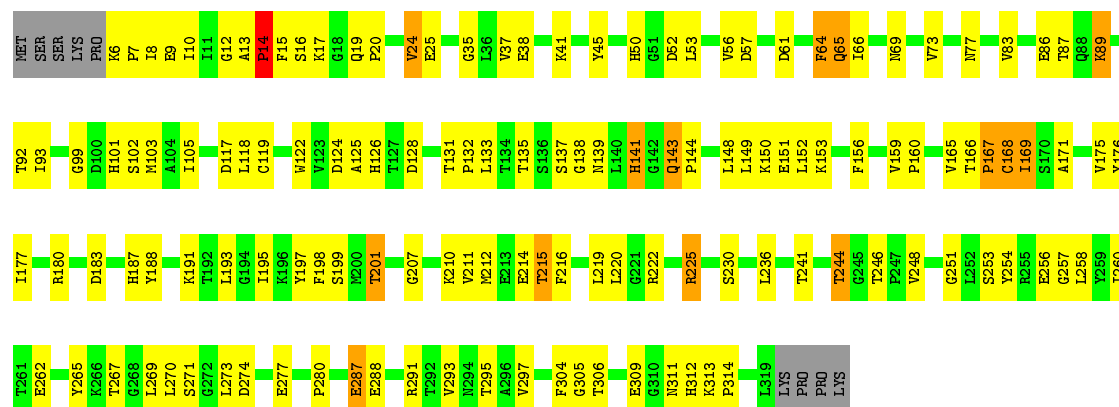


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	5	2	4	2		
3	B	1	Total	C	N	O	S	0	0
			13	5	2	4	2		
3	C	1	Total	C	N	O	S	0	0
			13	5	2	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	11	Total	O	0	0
			11	11		
4	C	13	Total	O	0	0
			13	13		





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.94Å 88.94Å 112.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.251 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	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: MN, SDC

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	0.42	0/2448	0.68	0/3325
1	B	0.44	0/2448	0.68	0/3325
1	C	0.44	0/2448	0.69	0/3325
All	All	0.43	0/7344	0.68	0/9975

There are no bond length outliers.

There are no bond angle outliers.

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	2395	0	2420	138	0
1	B	2395	0	2420	129	0
1	C	2395	0	2420	130	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	13	0	9	3	0
3	B	13	0	9	3	0
3	C	13	0	9	3	0
4	A	17	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	0	2	0
4	C	13	0	0	1	0
All	All	7271	0	7287	385	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 27.

All (385) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PRO:HD3	1:A:139:ASN:ND2	1.70	1.05
1:B:20:PRO:HD3	1:B:139:ASN:ND2	1.77	1.00
1:A:175:VAL:HG11	1:A:215:THR:HG22	1.46	0.97
1:C:20:PRO:HD3	1:C:139:ASN:ND2	1.82	0.94
1:C:175:VAL:HG11	1:C:215:THR:HG22	1.53	0.90
1:C:153:LYS:HD3	1:C:167:PRO:HG2	1.56	0.88
1:B:143:GLN:H	1:B:144:PRO:HD3	1.36	0.88
1:B:153:LYS:HD3	1:B:167:PRO:HG2	1.55	0.88
1:A:153:LYS:HD3	1:A:167:PRO:HG2	1.55	0.87
1:B:175:VAL:HG11	1:B:215:THR:HG22	1.53	0.87
1:C:143:GLN:H	1:C:144:PRO:HD3	1.38	0.87
1:A:143:GLN:H	1:A:144:PRO:HD3	1.42	0.85
1:A:175:VAL:HG11	1:A:215:THR:CG2	2.08	0.82
1:C:175:VAL:HG11	1:C:215:THR:CG2	2.12	0.79
1:B:169:ILE:H	1:B:169:ILE:HD13	1.48	0.79
1:C:12:GLY:HA3	1:C:52:ASP:OD1	1.84	0.78
1:C:212:MET:SD	1:C:260:ILE:HG13	2.23	0.78
1:B:175:VAL:HG11	1:B:215:THR:CG2	2.12	0.78
1:B:246:THR:HB	4:B:640:HOH:O	1.84	0.77
1:B:318:TYR:HB2	1:C:188:TYR:CD2	2.19	0.76
1:A:198:PHE:HE2	1:A:215:THR:HG23	1.50	0.75
1:A:35:GLY:HA2	1:A:38:GLU:OE1	1.86	0.75
1:B:230:SER:HA	1:B:274:ASP:HB2	1.67	0.74
1:A:169:ILE:H	1:A:169:ILE:HD13	1.52	0.74
1:C:13:ALA:N	1:C:14:PRO:CD	2.50	0.74
1:B:132:PRO:HD2	1:B:156:PHE:CD2	2.23	0.74
1:B:258:LEU:O	1:B:262:GLU:HG3	1.86	0.73
1:A:132:PRO:HD2	1:A:156:PHE:CD2	2.23	0.73
1:B:143:GLN:N	1:B:144:PRO:HD3	2.04	0.73
1:A:311:ASN:O	1:B:184:PRO:HA	1.89	0.73
1:B:35:GLY:HA2	1:B:38:GLU:OE1	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:GLN:N	1:C:144:PRO:HD3	2.04	0.72
1:C:180:ARG:NH1	1:C:248:VAL:O	2.23	0.72
1:C:230:SER:HA	1:C:274:ASP:HB2	1.72	0.71
1:C:35:GLY:HA2	1:C:38:GLU:OE1	1.88	0.71
1:B:253:SER:OG	1:B:256:GLU:HG3	1.90	0.71
1:A:20:PRO:HD3	1:A:139:ASN:HD21	1.54	0.71
1:B:180:ARG:NH1	1:B:248:VAL:O	2.24	0.71
1:A:12:GLY:HA3	1:A:52:ASP:OD1	1.89	0.71
1:B:143:GLN:N	1:B:144:PRO:CD	2.54	0.71
1:A:230:SER:HA	1:A:274:ASP:HB2	1.71	0.71
1:A:143:GLN:N	1:A:144:PRO:HD3	2.06	0.70
1:C:169:ILE:H	1:C:169:ILE:HD13	1.55	0.70
1:C:171:ALA:HB1	1:C:195:ILE:HG12	1.73	0.70
1:A:212:MET:SD	1:A:260:ILE:HG13	2.32	0.70
1:B:171:ALA:HB1	1:B:195:ILE:HG12	1.72	0.70
1:A:143:GLN:N	1:A:144:PRO:CD	2.56	0.69
1:C:180:ARG:CZ	1:C:251:GLY:HA3	2.23	0.69
1:C:143:GLN:N	1:C:144:PRO:CD	2.55	0.69
1:B:225:ARG:HG3	1:B:225:ARG:HH11	1.58	0.68
1:A:258:LEU:O	1:A:262:GLU:HG3	1.94	0.68
1:A:171:ALA:HB1	1:A:195:ILE:HG12	1.74	0.68
1:A:246:THR:HB	4:A:639:HOH:O	1.92	0.68
1:C:132:PRO:HD2	1:C:156:PHE:CD2	2.28	0.67
1:B:180:ARG:HD2	1:B:248:VAL:HG12	1.76	0.67
1:B:12:GLY:HA3	1:B:52:ASP:OD1	1.95	0.67
1:B:198:PHE:HE2	1:B:215:THR:HG23	1.58	0.67
1:A:198:PHE:CE2	1:A:215:THR:HG23	2.29	0.67
1:A:126:HIS:CG	3:A:1000:SDC:H091	2.30	0.67
1:B:212:MET:SD	1:B:260:ILE:HG13	2.34	0.67
1:B:126:HIS:CG	3:B:1001:SDC:H091	2.30	0.67
1:A:180:ARG:NH1	1:A:248:VAL:O	2.28	0.66
1:C:258:LEU:O	1:C:262:GLU:HG3	1.95	0.66
1:C:257:GLY:O	1:C:260:ILE:HG22	1.95	0.66
1:C:246:THR:HB	4:C:641:HOH:O	1.94	0.66
1:C:180:ARG:NH2	1:C:251:GLY:HA3	2.11	0.65
1:C:180:ARG:HD2	1:C:248:VAL:HG12	1.79	0.65
1:A:180:ARG:HD2	1:A:248:VAL:HG12	1.78	0.65
1:A:126:HIS:ND1	3:A:1000:SDC:H091	2.12	0.65
1:C:236:LEU:HD12	1:C:241:THR:CG2	2.27	0.64
1:A:257:GLY:O	1:A:260:ILE:HG22	1.97	0.64
1:C:13:ALA:N	1:C:14:PRO:HD3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:CZ	1:B:251:GLY:HA3	2.27	0.64
1:B:236:LEU:HD12	1:B:241:THR:CG2	2.28	0.64
1:C:198:PHE:HE2	1:C:215:THR:HG23	1.63	0.64
1:A:236:LEU:HD12	1:A:241:THR:CG2	2.28	0.64
1:B:207:GLY:O	1:B:211:VAL:HG23	1.97	0.64
1:A:253:SER:OG	1:A:256:GLU:HG3	1.98	0.63
1:B:126:HIS:ND1	3:B:1001:SDC:H091	2.13	0.63
1:B:225:ARG:NH1	1:B:225:ARG:HG3	2.12	0.63
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.64	0.63
1:B:64:PHE:O	1:B:65:GLN:HB2	1.99	0.62
1:A:16:SER:HB3	1:A:24:VAL:HG23	1.81	0.62
1:C:118:LEU:O	1:C:118:LEU:HD12	2.00	0.62
1:C:148:LEU:O	1:C:169:ILE:HD13	2.00	0.62
1:C:61:ASP:OD2	1:C:69:ASN:HA	1.99	0.62
1:C:15:PHE:O	1:C:99:GLY:HA3	1.99	0.62
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.35	0.62
1:A:184:PRO:HA	1:C:311:ASN:O	1.99	0.62
1:B:16:SER:CB	1:B:24:VAL:HG23	2.30	0.62
1:C:37:VAL:HG12	1:C:41:LYS:HE3	1.80	0.62
1:A:64:PHE:O	1:A:65:GLN:HB2	2.00	0.61
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.36	0.61
1:A:16:SER:CB	1:A:24:VAL:HG23	2.30	0.61
1:A:207:GLY:O	1:A:211:VAL:HG23	2.01	0.61
1:A:225:ARG:NH1	1:A:225:ARG:HG3	2.16	0.61
1:C:126:HIS:CG	3:C:1002:SDC:H091	2.36	0.61
1:A:148:LEU:O	1:A:169:ILE:HD13	2.01	0.61
1:A:37:VAL:HG12	1:A:41:LYS:HE3	1.83	0.60
1:B:15:PHE:O	1:B:99:GLY:HA3	2.01	0.60
1:B:180:ARG:NH2	1:B:251:GLY:HA3	2.16	0.60
1:A:15:PHE:O	1:A:99:GLY:HA3	2.01	0.60
1:A:180:ARG:CZ	1:A:251:GLY:HA3	2.32	0.60
1:C:253:SER:OG	1:C:256:GLU:HG3	2.00	0.60
1:A:61:ASP:OD2	1:A:69:ASN:HA	2.01	0.60
1:B:257:GLY:O	1:B:260:ILE:HG22	2.01	0.60
1:B:37:VAL:HG12	1:B:41:LYS:HE3	1.84	0.60
1:A:293:VAL:O	1:A:297:VAL:HG23	2.03	0.59
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.37	0.59
1:B:118:LEU:HD12	1:B:118:LEU:O	2.02	0.59
1:C:175:VAL:HG23	1:C:219:LEU:HD21	1.84	0.59
1:C:64:PHE:O	1:C:65:GLN:HB2	2.02	0.59
1:C:126:HIS:ND1	3:C:1002:SDC:H091	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ARG:HG3	1:C:248:VAL:HG11	1.85	0.59
1:B:198:PHE:CE2	1:B:215:THR:HG23	2.37	0.58
1:C:118:LEU:HD12	1:C:118:LEU:C	2.24	0.58
1:A:180:ARG:HG3	1:A:248:VAL:HG11	1.84	0.58
1:B:38:GLU:H	1:B:38:GLU:CD	2.07	0.58
1:C:16:SER:CB	1:C:24:VAL:HG23	2.33	0.58
1:A:210:LYS:HE3	1:A:214:GLU:OE2	2.03	0.58
1:C:150:LYS:HE3	1:C:168:CYS:O	2.04	0.58
1:A:118:LEU:C	1:A:118:LEU:HD12	2.25	0.58
1:A:118:LEU:O	1:A:118:LEU:HD12	2.05	0.57
1:B:293:VAL:O	1:B:297:VAL:HG23	2.04	0.57
1:A:291:ARG:O	1:A:295:THR:HG23	2.04	0.57
1:B:287:GLU:HG3	1:B:288:GLU:N	2.20	0.57
1:C:124:ASP:OD2	1:C:125:ALA:N	2.38	0.57
1:C:225:ARG:HG3	1:C:225:ARG:HH11	1.70	0.57
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.86	0.57
1:C:38:GLU:H	1:C:38:GLU:CD	2.07	0.57
1:C:16:SER:HB3	1:C:24:VAL:HG23	1.87	0.57
1:A:175:VAL:HG23	1:A:219:LEU:HD21	1.87	0.56
1:A:66:ILE:HG22	1:A:138:GLY:HA3	1.87	0.56
1:B:180:ARG:HG3	1:B:248:VAL:HG11	1.86	0.56
1:A:151:GLU:H	1:A:151:GLU:CD	2.08	0.56
1:A:287:GLU:HG3	1:A:288:GLU:N	2.20	0.56
1:B:187:HIS:O	1:B:191:LYS:HG2	2.05	0.56
1:A:7:PRO:HB2	1:A:92:THR:HG22	1.87	0.56
1:A:236:LEU:HD12	1:A:241:THR:HG23	1.88	0.56
1:B:118:LEU:HD12	1:B:118:LEU:C	2.26	0.56
1:A:38:GLU:H	1:A:38:GLU:CD	2.08	0.56
1:B:124:ASP:OD2	1:B:125:ALA:N	2.39	0.56
1:B:148:LEU:O	1:B:169:ILE:HD13	2.05	0.56
1:B:291:ARG:O	1:B:295:THR:HG23	2.06	0.56
1:B:16:SER:HB3	1:B:24:VAL:HG23	1.87	0.55
1:A:124:ASP:OD2	1:A:125:ALA:N	2.38	0.55
1:A:187:HIS:O	1:A:191:LYS:HG2	2.06	0.55
1:B:20:PRO:HD3	1:B:139:ASN:HD21	1.63	0.55
1:C:151:GLU:CD	1:C:151:GLU:N	2.60	0.55
1:C:207:GLY:O	1:C:211:VAL:HG23	2.06	0.55
1:C:198:PHE:CE2	1:C:215:THR:HG23	2.40	0.55
1:B:77:ASN:OD1	1:B:103:MET:HA	2.06	0.55
1:A:10:ILE:N	1:A:10:ILE:HD12	2.22	0.55
1:B:308:ARG:HB2	1:C:201:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TYR:HB2	1:A:197:TYR:CB	2.37	0.55
1:C:236:LEU:HD12	1:C:241:THR:HG23	1.88	0.55
1:B:176:TYR:HB2	1:B:197:TYR:CB	2.37	0.54
1:B:66:ILE:HG22	1:B:138:GLY:HA3	1.89	0.54
1:C:187:HIS:O	1:C:191:LYS:HG2	2.07	0.54
1:C:151:GLU:CD	1:C:151:GLU:H	2.09	0.54
1:C:291:ARG:O	1:C:295:THR:HG23	2.07	0.54
1:C:77:ASN:OD1	1:C:103:MET:HA	2.07	0.54
1:B:244:THR:HG23	1:B:277:GLU:O	2.07	0.54
1:B:236:LEU:HD12	1:B:241:THR:HG23	1.89	0.54
1:B:7:PRO:HB2	1:B:92:THR:HG22	1.89	0.54
1:C:128:ASP:HB3	1:C:144:PRO:HD2	1.88	0.54
1:B:169:ILE:HD13	1:B:169:ILE:N	2.22	0.54
1:C:176:TYR:HB2	1:C:197:TYR:CB	2.38	0.54
1:C:7:PRO:HB2	1:C:92:THR:HG22	1.89	0.54
1:C:143:GLN:H	1:C:144:PRO:CD	2.11	0.53
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.91	0.53
1:B:61:ASP:OD2	1:B:69:ASN:HA	2.09	0.53
1:C:225:ARG:NH1	1:C:225:ARG:HG3	2.22	0.53
1:C:212:MET:HA	1:C:215:THR:OG1	2.08	0.53
1:B:10:ILE:N	1:B:10:ILE:HD12	2.24	0.53
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.90	0.53
1:A:56:VAL:HG22	4:A:622:HOH:O	2.09	0.53
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.90	0.53
1:C:236:LEU:HD12	1:C:241:THR:HG21	1.91	0.53
1:C:287:GLU:HG3	1:C:288:GLU:N	2.24	0.53
1:C:15:PHE:HE2	1:C:73:VAL:HG22	1.73	0.53
1:A:151:GLU:N	1:A:151:GLU:CD	2.61	0.53
1:B:135:THR:HG21	1:B:143:GLN:NE2	2.24	0.53
1:A:15:PHE:HE2	1:A:73:VAL:HG22	1.72	0.53
1:C:66:ILE:HG22	1:C:138:GLY:HA3	1.90	0.53
1:C:10:ILE:HD12	1:C:10:ILE:N	2.24	0.52
1:A:128:ASP:HB3	1:A:144:PRO:HD2	1.92	0.52
1:C:210:LYS:HE3	1:C:214:GLU:OE2	2.08	0.52
1:B:117:ASP:O	1:B:225:ARG:NH1	2.42	0.52
1:A:77:ASN:OD1	1:A:103:MET:HA	2.09	0.52
1:B:6:LYS:HD2	1:B:7:PRO:CD	2.39	0.52
1:A:135:THR:HG21	1:A:143:GLN:NE2	2.25	0.52
1:C:13:ALA:O	1:C:15:PHE:N	2.43	0.52
1:A:176:TYR:HB2	1:A:197:TYR:HB2	1.91	0.52
1:B:15:PHE:HE2	1:B:73:VAL:HG22	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLN:HB2	1:C:20:PRO:HD2	1.92	0.51
1:C:93:ILE:HG23	1:C:271:SER:O	2.11	0.51
1:A:48:ARG:HA	4:A:607:HOH:O	2.10	0.51
1:B:6:LYS:HD2	1:B:7:PRO:HD2	1.93	0.51
1:A:212:MET:HA	1:A:215:THR:OG1	2.09	0.51
1:C:119:CYS:HB3	1:C:225:ARG:CZ	2.41	0.51
1:C:293:VAL:O	1:C:297:VAL:HG23	2.10	0.51
1:C:176:TYR:HB2	1:C:197:TYR:HB2	1.93	0.51
1:A:66:ILE:HG22	1:A:138:GLY:CA	2.41	0.51
1:A:75:LYS:HG3	4:A:622:HOH:O	2.11	0.51
1:A:93:ILE:HG23	1:A:271:SER:O	2.11	0.51
1:B:150:LYS:HE3	1:B:168:CYS:O	2.10	0.51
1:C:6:LYS:HD2	1:C:7:PRO:CD	2.41	0.51
1:A:180:ARG:NH2	1:A:251:GLY:HA3	2.26	0.50
1:B:210:LYS:HE3	1:B:214:GLU:OE2	2.11	0.50
1:A:19:GLN:HB3	1:A:141:HIS:CE1	2.47	0.50
1:C:86:GLU:O	1:C:89:LYS:HB3	2.11	0.50
1:B:45:TYR:CD2	1:B:304:PHE:HB3	2.47	0.50
1:C:6:LYS:HD2	1:C:7:PRO:HD2	1.93	0.50
1:C:137:SER:HB2	1:C:139:ASN:OD1	2.11	0.50
1:C:149:LEU:O	1:C:167:PRO:HB3	2.11	0.50
1:A:15:PHE:CE2	1:A:73:VAL:HG22	2.47	0.50
1:A:169:ILE:HD13	1:A:169:ILE:N	2.25	0.49
1:A:45:TYR:CD2	1:A:304:PHE:HB3	2.47	0.49
1:B:135:THR:HB	4:B:637:HOH:O	2.12	0.49
1:B:66:ILE:HG22	1:B:138:GLY:CA	2.41	0.49
1:C:102:SER:HA	1:C:144:PRO:HG3	1.95	0.49
1:A:149:LEU:O	1:A:167:PRO:HB3	2.11	0.49
1:A:262:GLU:OE1	1:B:201:THR:HB	2.13	0.49
1:B:236:LEU:HD12	1:B:241:THR:HG21	1.93	0.49
1:A:236:LEU:HD12	1:A:241:THR:HG21	1.95	0.49
1:B:212:MET:HA	1:B:215:THR:OG1	2.12	0.49
1:B:287:GLU:CG	1:B:291:ARG:HH21	2.24	0.49
1:A:199:SER:OG	1:A:201:THR:HG23	2.13	0.49
1:B:102:SER:HA	1:B:144:PRO:HG3	1.94	0.49
1:C:9:GLU:OE2	1:C:87:THR:HG21	2.13	0.49
1:B:19:GLN:HB3	1:B:141:HIS:CE1	2.47	0.49
1:A:102:SER:HA	1:A:144:PRO:HG3	1.95	0.48
1:B:151:GLU:CD	1:B:151:GLU:H	2.17	0.48
1:C:135:THR:HG21	1:C:143:GLN:NE2	2.28	0.48
1:C:66:ILE:HG22	1:C:138:GLY:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LEU:O	1:B:167:PRO:HB3	2.13	0.48
1:C:15:PHE:CE2	1:C:73:VAL:HG22	2.48	0.48
1:B:151:GLU:CD	1:B:151:GLU:N	2.67	0.48
1:B:175:VAL:HG23	1:B:219:LEU:HD21	1.94	0.48
1:A:101:HIS:CE1	1:A:122:TRP:CZ2	3.02	0.48
1:A:137:SER:HB2	1:A:139:ASN:OD1	2.12	0.48
1:A:19:GLN:HB3	1:A:141:HIS:ND1	2.29	0.48
1:B:129:ILE:HG23	1:B:129:ILE:O	2.13	0.48
1:B:16:SER:HB2	1:B:24:VAL:HG23	1.95	0.48
1:B:199:SER:OG	1:B:201:THR:HG23	2.13	0.48
1:A:312:HIS:O	1:A:314:PRO:HD3	2.14	0.48
1:A:8:ILE:HD13	1:A:93:ILE:HB	1.95	0.47
1:C:20:PRO:HD3	1:C:139:ASN:HD21	1.71	0.47
1:C:56:VAL:O	1:C:56:VAL:HG23	2.13	0.47
1:B:176:TYR:HB2	1:B:197:TYR:HB2	1.95	0.47
1:A:150:LYS:HE3	1:A:168:CYS:O	2.13	0.47
1:A:86:GLU:O	1:A:89:LYS:HB3	2.14	0.47
1:A:183:ASP:OD2	3:A:1000:SDC:NP2	2.43	0.47
1:B:101:HIS:CE1	1:B:122:TRP:CZ2	3.03	0.47
1:B:56:VAL:HG23	1:B:56:VAL:O	2.15	0.47
1:A:287:GLU:CG	1:A:291:ARG:HH21	2.28	0.47
1:A:259:TYR:CE1	1:B:205:LYS:HB2	2.50	0.47
1:C:117:ASP:O	1:C:225:ARG:NH1	2.47	0.47
1:A:180:ARG:HD2	1:A:248:VAL:CG1	2.45	0.47
1:A:225:ARG:CG	1:A:225:ARG:HH11	2.28	0.46
1:C:267:THR:O	1:C:269:LEU:HG	2.15	0.46
1:A:117:ASP:O	1:A:225:ARG:NH1	2.48	0.46
1:B:86:GLU:O	1:B:89:LYS:HB3	2.14	0.46
1:C:244:THR:HG23	1:C:277:GLU:O	2.14	0.46
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.97	0.46
1:C:53:LEU:CD2	1:C:83:VAL:HG21	2.46	0.46
1:A:105:ILE:HA	1:A:148:LEU:HD21	1.97	0.46
1:A:9:GLU:OE2	1:A:87:THR:HG21	2.16	0.46
1:B:15:PHE:CE2	1:B:73:VAL:HG22	2.50	0.46
1:B:210:LYS:HE3	1:B:214:GLU:HG3	1.98	0.46
1:A:177:ILE:HD12	1:A:260:ILE:HD11	1.98	0.46
1:C:287:GLU:CG	1:C:291:ARG:HH21	2.30	0.45
1:B:9:GLU:OE2	1:B:87:THR:HG21	2.15	0.45
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.98	0.45
1:A:309:GLU:OE2	1:B:187:HIS:NE2	2.28	0.45
1:B:165:VAL:HG12	1:B:166:THR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:HD2	1:B:248:VAL:CG1	2.43	0.45
1:B:150:LYS:HG2	1:B:167:PRO:O	2.17	0.45
1:B:93:ILE:HG23	1:B:271:SER:O	2.16	0.45
1:C:169:ILE:HD13	1:C:169:ILE:N	2.29	0.45
1:B:19:GLN:HB3	1:B:141:HIS:ND1	2.31	0.45
1:A:149:LEU:HA	1:A:149:LEU:HD23	1.86	0.45
1:B:105:ILE:HA	1:B:148:LEU:HD21	1.98	0.45
1:B:8:ILE:HD13	1:B:93:ILE:HB	1.97	0.45
1:C:6:LYS:HA	1:C:7:PRO:HD3	1.87	0.45
1:C:8:ILE:HD13	1:C:93:ILE:HB	1.99	0.44
1:A:237:ASP:N	1:A:252:LEU:O	2.46	0.44
1:C:131:THR:C	1:C:133:LEU:N	2.70	0.44
1:A:53:LEU:HD21	1:A:83:VAL:HG21	1.98	0.44
1:C:265:TYR:CZ	1:C:305:GLY:HA2	2.51	0.44
1:C:312:HIS:O	1:C:314:PRO:HD3	2.17	0.44
1:B:152:LEU:CD1	1:B:193:LEU:HD21	2.48	0.44
1:B:225:ARG:O	1:B:269:LEU:HD13	2.17	0.44
1:C:150:LYS:HG2	1:C:167:PRO:O	2.17	0.44
1:A:244:THR:HG23	1:A:277:GLU:O	2.17	0.44
1:B:119:CYS:HB3	1:B:225:ARG:CZ	2.47	0.44
1:B:265:TYR:CZ	1:B:305:GLY:HA2	2.53	0.44
1:B:262:GLU:OE1	1:C:201:THR:HB	2.18	0.44
1:C:216:PHE:CZ	1:C:267:THR:HG21	2.52	0.44
1:A:225:ARG:O	1:A:269:LEU:HD13	2.17	0.44
1:B:13:ALA:O	1:B:15:PHE:N	2.50	0.44
1:C:152:LEU:CD1	1:C:193:LEU:HD21	2.48	0.44
1:A:131:THR:C	1:A:133:LEU:H	2.21	0.44
1:A:166:THR:O	1:A:168:CYS:N	2.51	0.44
1:B:40:LEU:O	1:B:43:THR:HG23	2.17	0.44
1:B:86:GLU:OE2	1:B:89:LYS:HD2	2.17	0.44
1:A:13:ALA:O	1:A:15:PHE:N	2.49	0.43
1:C:131:THR:C	1:C:133:LEU:H	2.22	0.43
1:A:131:THR:C	1:A:133:LEU:N	2.69	0.43
1:A:56:VAL:HG23	1:A:56:VAL:O	2.18	0.43
1:B:131:THR:C	1:B:133:LEU:N	2.72	0.43
1:B:53:LEU:CD2	1:B:83:VAL:HG21	2.48	0.43
1:C:177:ILE:HD11	1:C:215:THR:HG21	2.00	0.43
1:A:180:ARG:HB3	1:A:200:MET:HG2	1.99	0.43
1:A:152:LEU:CD1	1:A:193:LEU:HD21	2.49	0.43
1:B:183:ASP:OD2	3:B:1001:SDC:NP2	2.49	0.43
1:C:199:SER:OG	1:C:201:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PRO:HD3	1:A:248:VAL:O	2.19	0.43
1:C:105:ILE:HA	1:C:148:LEU:HD21	2.01	0.43
1:C:270:LEU:HD23	1:C:304:PHE:CE1	2.53	0.43
1:B:132:PRO:CD	1:B:156:PHE:CD2	2.98	0.43
1:A:150:LYS:HG2	1:A:167:PRO:O	2.19	0.42
1:C:53:LEU:HD21	1:C:83:VAL:HG21	2.01	0.42
1:A:165:VAL:HG12	1:A:166:THR:N	2.35	0.42
1:A:53:LEU:CD2	1:A:83:VAL:HG21	2.48	0.42
1:B:149:LEU:HD23	1:B:149:LEU:HA	1.82	0.42
1:B:45:TYR:CE2	1:B:304:PHE:HB3	2.54	0.42
1:C:13:ALA:N	1:C:14:PRO:HD2	2.34	0.42
1:A:249:VAL:HG23	1:C:254:TYR:CE2	2.54	0.42
1:A:143:GLN:H	1:A:144:PRO:CD	2.16	0.42
1:A:229:LEU:HD13	1:A:264:ILE:CD1	2.49	0.42
1:C:19:GLN:HB3	1:C:141:HIS:CE1	2.55	0.42
1:C:24:VAL:HB	1:C:99:GLY:HA2	2.02	0.42
1:C:166:THR:O	1:C:168:CYS:N	2.53	0.42
1:C:225:ARG:O	1:C:269:LEU:HD13	2.20	0.42
1:C:45:TYR:CD2	1:C:304:PHE:HB3	2.55	0.42
1:A:10:ILE:N	1:A:10:ILE:CD1	2.82	0.42
1:A:216:PHE:CZ	1:A:267:THR:HG21	2.55	0.42
1:B:260:ILE:HG23	1:B:261:THR:N	2.35	0.42
1:C:19:GLN:HB3	1:C:141:HIS:ND1	2.35	0.42
1:A:23:GLY:O	1:A:26:LYS:HB2	2.20	0.42
1:B:185:GLY:O	1:B:188:TYR:HB3	2.20	0.42
1:A:267:THR:O	1:A:269:LEU:HG	2.20	0.41
1:A:64:PHE:O	1:A:65:GLN:CB	2.66	0.41
1:A:6:LYS:HD2	1:A:7:PRO:CD	2.50	0.41
1:B:148:LEU:HB3	1:B:169:ILE:HD11	2.02	0.41
1:B:32:ARG:NH1	1:B:52:ASP:OD1	2.54	0.41
1:C:101:HIS:CE1	1:C:122:TRP:CZ2	3.08	0.41
1:C:165:VAL:HG12	1:C:166:THR:N	2.34	0.41
1:B:6:LYS:HA	1:B:7:PRO:HD3	1.87	0.41
1:A:108:ILE:HB	1:A:148:LEU:HD13	2.03	0.41
1:A:141:HIS:C	1:A:141:HIS:CD2	2.92	0.41
1:A:265:TYR:CZ	1:A:305:GLY:HA2	2.55	0.41
1:A:131:THR:O	1:A:133:LEU:N	2.54	0.41
1:C:50:HIS:O	1:C:50:HIS:ND1	2.53	0.41
1:A:6:LYS:HD2	1:A:7:PRO:HD2	2.01	0.41
1:B:177:ILE:HD12	1:B:260:ILE:HD11	2.02	0.41
1:B:53:LEU:HD21	1:B:83:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:HIS:NE2	1:C:246:THR:HG21	2.36	0.41
1:A:232:ASP:OD2	1:A:234:ASP:OD2	2.39	0.41
1:B:10:ILE:CD1	1:B:10:ILE:N	2.83	0.41
1:A:132:PRO:CD	1:A:156:PHE:CD2	2.99	0.41
1:B:242:PRO:HD2	1:B:292:THR:OG1	2.21	0.41
1:B:308:ARG:HB2	1:C:201:THR:CG2	2.48	0.41
1:C:149:LEU:HA	1:C:149:LEU:HD23	1.79	0.41
1:C:183:ASP:OD2	3:C:1002:SDC:NP2	2.49	0.41
1:C:219:LEU:O	1:C:220:LEU:HD23	2.21	0.41
1:A:185:GLY:O	1:A:188:TYR:HB3	2.21	0.41
1:A:45:TYR:CE2	1:A:304:PHE:HB3	2.55	0.41
1:A:36:LEU:O	1:A:36:LEU:HD12	2.21	0.41
1:C:159:VAL:HA	1:C:160:PRO:HD3	1.90	0.41
1:C:25:GLU:CD	1:C:25:GLU:H	2.24	0.41
1:A:16:SER:HB2	1:A:24:VAL:HG23	2.03	0.40
1:C:225:ARG:HH11	1:C:225:ARG:CG	2.33	0.40
1:A:75:LYS:HE3	4:A:622:HOH:O	2.21	0.40
1:B:267:THR:O	1:B:269:LEU:HG	2.21	0.40
1:B:319:LEU:HG	1:C:188:TYR:HE2	1.85	0.40
1:C:180:ARG:CZ	1:C:251:GLY:CA	2.97	0.40
1:C:86:GLU:OE2	1:C:89:LYS:HD2	2.20	0.40
1:A:137:SER:OG	4:A:636:HOH:O	2.22	0.40
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.88	0.40
1:B:166:THR:O	1:B:168:CYS:N	2.54	0.40
1:B:64:PHE:O	1:B:65:GLN:CB	2.66	0.40
1:A:187:HIS:NE2	1:C:309:GLU:OE2	2.40	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/323 (97%)	279 (89%)	26 (8%)	7 (2%)	6	22
1	B	312/323 (97%)	280 (90%)	23 (7%)	9 (3%)	4	15
1	C	312/323 (97%)	276 (88%)	28 (9%)	8 (3%)	5	18
All	All	936/969 (97%)	835 (89%)	77 (8%)	24 (3%)	5	18

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	306	THR
1	B	65	GLN
1	C	65	GLN
1	A	64	PHE
1	B	64	PHE
1	B	100	ASP
1	B	143	GLN
1	C	14	PRO
1	C	306	THR
1	A	143	GLN
1	A	167	PRO
1	B	222	ARG
1	B	306	THR
1	C	64	PHE
1	C	143	GLN
1	C	222	ARG
1	A	280	PRO
1	B	167	PRO
1	C	167	PRO
1	C	280	PRO
1	B	280	PRO
1	A	14	PRO
1	B	14	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	264/273 (97%)	250 (95%)	14 (5%)	22	54
1	B	264/273 (97%)	251 (95%)	13 (5%)	25	57
1	C	264/273 (97%)	250 (95%)	14 (5%)	22	54
All	All	792/819 (97%)	751 (95%)	41 (5%)	23	55

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	57	ASP
1	A	89	LYS
1	A	127	THR
1	A	141	HIS
1	A	168	CYS
1	A	169	ILE
1	A	201	THR
1	A	215	THR
1	A	225	ARG
1	A	244	THR
1	A	273	LEU
1	A	287	GLU
1	A	313	LYS
1	B	24	VAL
1	B	57	ASP
1	B	89	LYS
1	B	127	THR
1	B	141	HIS
1	B	169	ILE
1	B	201	THR
1	B	215	THR
1	B	225	ARG
1	B	244	THR
1	B	273	LEU
1	B	287	GLU
1	B	313	LYS
1	C	14	PRO
1	C	24	VAL
1	C	57	ASP
1	C	89	LYS
1	C	141	HIS
1	C	168	CYS
1	C	169	ILE

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Mol	Chain	Res	Type
1	C	201	THR
1	C	215	THR
1	C	225	ARG
1	C	244	THR
1	C	273	LEU
1	C	287	GLU
1	C	313	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	SDC	B	1001	2	7,12,12	0.82	0	6,16,16	2.42	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SDC	C	1002	2	7,12,12	0.89	0	6,16,16	2.63	2 (33%)
3	SDC	A	1000	2	7,12,12	0.97	0	6,16,16	2.49	2 (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
3	SDC	B	1001	2	-	5/7/12/12	-
3	SDC	C	1002	2	-	5/7/12/12	-
3	SDC	A	1000	2	-	5/7/12/12	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	SDC	O13-S10-C09	5.19	116.07	107.84
3	B	1001	SDC	O13-S10-C09	4.81	115.46	107.84
3	A	1000	SDC	O13-S10-C09	4.28	114.63	107.84
3	A	1000	SDC	O11-S10-C09	3.51	113.41	107.84
3	C	1002	SDC	O11-S10-C09	2.86	112.37	107.84
3	B	1001	SDC	O11-S10-C09	2.59	111.95	107.84

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	SDC	C08-C09-S10-O11
3	B	1001	SDC	C08-C09-S10-O13
3	A	1000	SDC	C08-C09-S10-O11
3	A	1000	SDC	C08-C09-S10-O13
3	C	1002	SDC	C08-C09-S10-O11
3	C	1002	SDC	C08-C09-S10-O13
3	B	1001	SDC	C04-C03-C06-S07
3	A	1000	SDC	C04-C03-C06-S07
3	C	1002	SDC	C04-C03-C06-S07
3	C	1002	SDC	C09-C08-S07-C06
3	B	1001	SDC	C09-C08-S07-C06
3	A	1000	SDC	C09-C08-S07-C06

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Mol	Chain	Res	Type	Atoms
3	B	1001	SDC	NP2-C03-C06-S07
3	A	1000	SDC	NP2-C03-C06-S07
3	C	1002	SDC	NP2-C03-C06-S07

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	SDC	3	0
3	C	1002	SDC	3	0
3	A	1000	SDC	3	0

## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.