



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:01 am GMT

PDB ID : 2Z3R
Title : Crystal structure of the IL-15/IL-15Ra complex
Authors : Chirifu, M.; Yamagata, Y.; Davis, S.J.; Ikemizu, S.
Deposited on : 2007-06-05
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

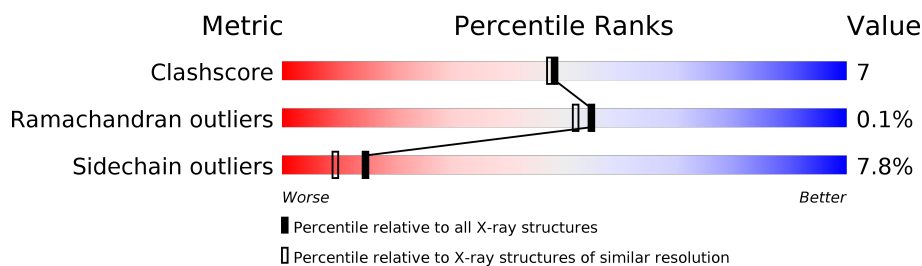
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)










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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	
1	C	119	
1	E	119	
1	G	119	
1	I	119	
1	K	119	
1	M	119	

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Mol	Chain	Length	Quality of chain
1	O	119	 77%20%..
2	B	107	 60%9%31%
2	D	107	 57%13%.29%
2	F	107	 61%. .32%
2	H	107	 59%12%.28%
2	J	107	 58%11%.27%
2	L	107	 59%9%.30%
2	N	107	 54%13%.29%
2	P	107	 55%11%.33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12517 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 Interleukin-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	0	0
			883	556	140	179	8			
1	C	116	Total	C	N	O	S	0	0	0
			904	568	143	185	8			
1	E	119	Total	C	N	O	S	0	0	0
			924	578	148	190	8			
1	G	119	Total	C	N	O	S	0	0	0
			924	578	148	190	8			
1	I	116	Total	C	N	O	S	0	0	0
			904	568	143	185	8			
1	K	116	Total	C	N	O	S	0	0	0
			904	568	143	185	8			
1	M	116	Total	C	N	O	S	0	0	0
			904	568	143	185	8			
1	O	118	Total	C	N	O	S	0	0	0
			917	575	147	187	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	EXPRESSION TAG	UNP P40933
A	-3	MET	-	EXPRESSION TAG	UNP P40933
A	-2	ALA	-	EXPRESSION TAG	UNP P40933
A	-1	ILE	-	EXPRESSION TAG	UNP P40933
A	0	SER	-	EXPRESSION TAG	UNP P40933
C	-4	ALA	-	EXPRESSION TAG	UNP P40933
C	-3	MET	-	EXPRESSION TAG	UNP P40933
C	-2	ALA	-	EXPRESSION TAG	UNP P40933
C	-1	ILE	-	EXPRESSION TAG	UNP P40933
C	0	SER	-	EXPRESSION TAG	UNP P40933
E	-4	ALA	-	EXPRESSION TAG	UNP P40933
E	-3	MET	-	EXPRESSION TAG	UNP P40933
E	-2	ALA	-	EXPRESSION TAG	UNP P40933

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ILE	-	EXPRESSION TAG	UNP P40933
E	0	SER	-	EXPRESSION TAG	UNP P40933
G	-4	ALA	-	EXPRESSION TAG	UNP P40933
G	-3	MET	-	EXPRESSION TAG	UNP P40933
G	-2	ALA	-	EXPRESSION TAG	UNP P40933
G	-1	ILE	-	EXPRESSION TAG	UNP P40933
G	0	SER	-	EXPRESSION TAG	UNP P40933
I	-4	ALA	-	EXPRESSION TAG	UNP P40933
I	-3	MET	-	EXPRESSION TAG	UNP P40933
I	-2	ALA	-	EXPRESSION TAG	UNP P40933
I	-1	ILE	-	EXPRESSION TAG	UNP P40933
I	0	SER	-	EXPRESSION TAG	UNP P40933
K	-4	ALA	-	EXPRESSION TAG	UNP P40933
K	-3	MET	-	EXPRESSION TAG	UNP P40933
K	-2	ALA	-	EXPRESSION TAG	UNP P40933
K	-1	ILE	-	EXPRESSION TAG	UNP P40933
K	0	SER	-	EXPRESSION TAG	UNP P40933
M	-4	ALA	-	EXPRESSION TAG	UNP P40933
M	-3	MET	-	EXPRESSION TAG	UNP P40933
M	-2	ALA	-	EXPRESSION TAG	UNP P40933
M	-1	ILE	-	EXPRESSION TAG	UNP P40933
M	0	SER	-	EXPRESSION TAG	UNP P40933
O	-4	ALA	-	EXPRESSION TAG	UNP P40933
O	-3	MET	-	EXPRESSION TAG	UNP P40933
O	-2	ALA	-	EXPRESSION TAG	UNP P40933
O	-1	ILE	-	EXPRESSION TAG	UNP P40933
O	0	SER	-	EXPRESSION TAG	UNP P40933

- Molecule 2 is a protein called Interleukin-15 receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	S	0	0	0
			584	367	106	106	5			
2	D	76	Total	C	N	O	S	0	0	0
			594	375	105	108	6			
2	F	73	Total	C	N	O	S	0	0	0
			573	361	102	105	5			
2	H	77	Total	C	N	O	S	0	0	0
			599	378	106	109	6			
2	J	78	Total	C	N	O	S	0	0	0
			610	384	110	110	6			
2	L	75	Total	C	N	O	S	0	0	0
			592	373	107	107	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	76	Total	C	N	O	S	0	0	0
			594	375	105	108	6			
2	P	72	Total	C	N	O	S	0	0	0
			564	356	100	103	5			

There are 40 discrepancies between the modelled and reference sequences:

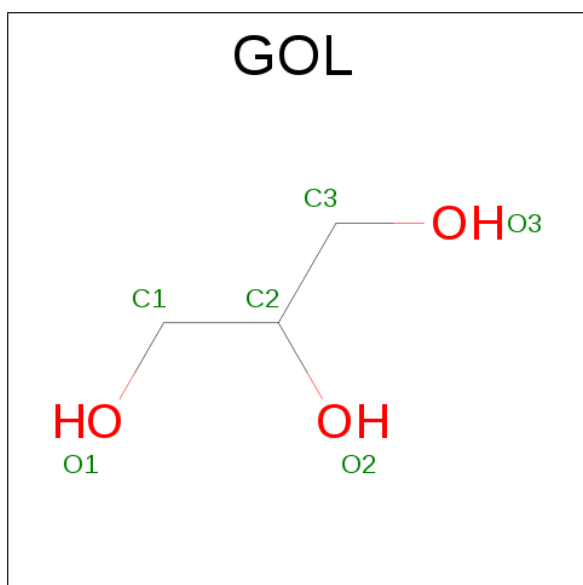
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	EXPRESSION TAG	UNP Q13261
B	-3	MET	-	EXPRESSION TAG	UNP Q13261
B	-2	ALA	-	EXPRESSION TAG	UNP Q13261
B	-1	ILE	-	EXPRESSION TAG	UNP Q13261
B	0	SER	-	EXPRESSION TAG	UNP Q13261
D	-4	ALA	-	EXPRESSION TAG	UNP Q13261
D	-3	MET	-	EXPRESSION TAG	UNP Q13261
D	-2	ALA	-	EXPRESSION TAG	UNP Q13261
D	-1	ILE	-	EXPRESSION TAG	UNP Q13261
D	0	SER	-	EXPRESSION TAG	UNP Q13261
F	-4	ALA	-	EXPRESSION TAG	UNP Q13261
F	-3	MET	-	EXPRESSION TAG	UNP Q13261
F	-2	ALA	-	EXPRESSION TAG	UNP Q13261
F	-1	ILE	-	EXPRESSION TAG	UNP Q13261
F	0	SER	-	EXPRESSION TAG	UNP Q13261
H	-4	ALA	-	EXPRESSION TAG	UNP Q13261
H	-3	MET	-	EXPRESSION TAG	UNP Q13261
H	-2	ALA	-	EXPRESSION TAG	UNP Q13261
H	-1	ILE	-	EXPRESSION TAG	UNP Q13261
H	0	SER	-	EXPRESSION TAG	UNP Q13261
J	-4	ALA	-	EXPRESSION TAG	UNP Q13261
J	-3	MET	-	EXPRESSION TAG	UNP Q13261
J	-2	ALA	-	EXPRESSION TAG	UNP Q13261
J	-1	ILE	-	EXPRESSION TAG	UNP Q13261
J	0	SER	-	EXPRESSION TAG	UNP Q13261
L	-4	ALA	-	EXPRESSION TAG	UNP Q13261
L	-3	MET	-	EXPRESSION TAG	UNP Q13261
L	-2	ALA	-	EXPRESSION TAG	UNP Q13261
L	-1	ILE	-	EXPRESSION TAG	UNP Q13261
L	0	SER	-	EXPRESSION TAG	UNP Q13261
N	-4	ALA	-	EXPRESSION TAG	UNP Q13261
N	-3	MET	-	EXPRESSION TAG	UNP Q13261
N	-2	ALA	-	EXPRESSION TAG	UNP Q13261
N	-1	ILE	-	EXPRESSION TAG	UNP Q13261

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Chain	Residue	Modelled	Actual	Comment	Reference
N	0	SER	-	EXPRESSION TAG	UNP Q13261
P	-4	ALA	-	EXPRESSION TAG	UNP Q13261
P	-3	MET	-	EXPRESSION TAG	UNP Q13261
P	-2	ALA	-	EXPRESSION TAG	UNP Q13261
P	-1	ILE	-	EXPRESSION TAG	UNP Q13261
P	0	SER	-	EXPRESSION TAG	UNP Q13261

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C O 6 3 3	0	0
3	O	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	32	Total O 32 32	0	0

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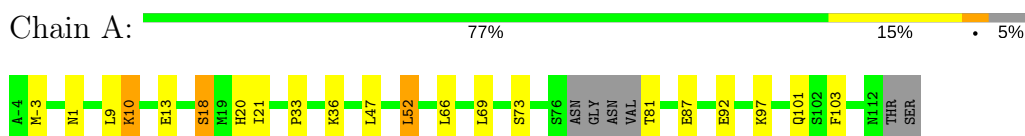
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	35	Total 35	O 35	0	0
4	D	26	Total 26	O 26	0	0
4	E	32	Total 32	O 32	0	0
4	F	43	Total 43	O 43	0	0
4	G	41	Total 41	O 41	0	0
4	H	43	Total 43	O 43	0	0
4	I	35	Total 35	O 35	0	0
4	J	37	Total 37	O 37	0	0
4	K	34	Total 34	O 34	0	0
4	L	45	Total 45	O 45	0	0
4	M	22	Total 22	O 22	0	0
4	N	21	Total 21	O 21	0	0
4	O	20	Total 20	O 20	0	0
4	P	36	Total 36	O 36	0	0

3 Residue-property plots [i](#)

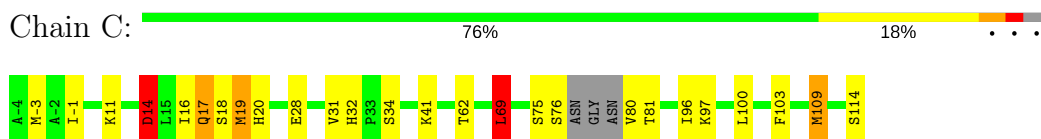
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

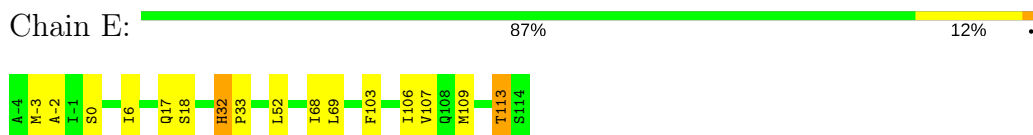
- Molecule 1: Interleukin-15



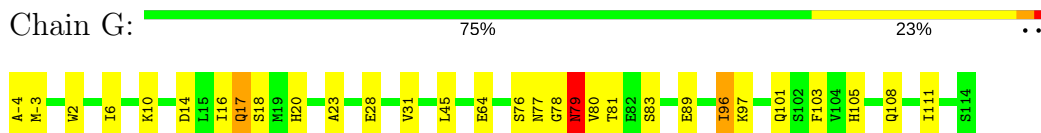
- Molecule 1: Interleukin-15



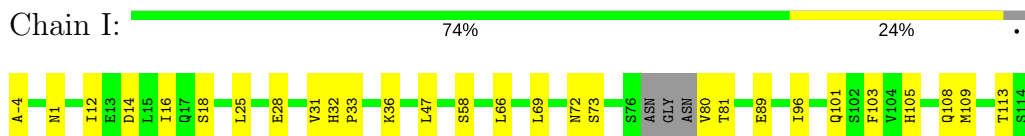
- Molecule 1: Interleukin-15



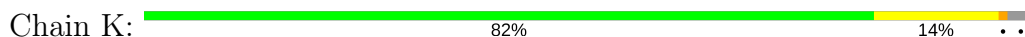
- Molecule 1: Interleukin-15

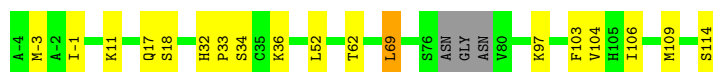


- Molecule 1: Interleukin-15



- Molecule 1: Interleukin-15





- Molecule 1: Interleukin-15

Chain M: 78% 18% ..



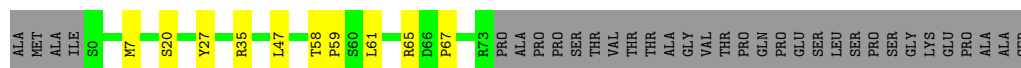
- Molecule 1: Interleukin-15

Chain O: 77% 20% ..



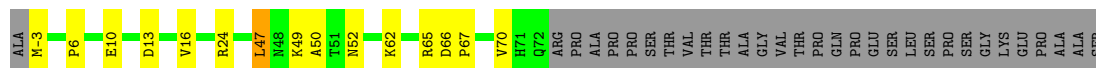
- Molecule 2: Interleukin-15 receptor alpha chain

Chain B: 60% 9% 31%



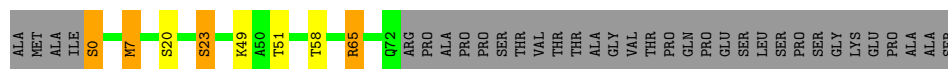
- Molecule 2: Interleukin-15 receptor alpha chain

Chain D: 57% 13% 29%



- Molecule 2: Interleukin-15 receptor alpha chain

Chain F: 61% 32%



- Molecule 2: Interleukin-15 receptor alpha chain

Chain H: 59% 12% 28%



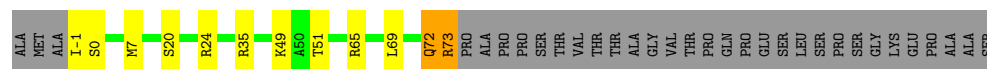
- Molecule 2: Interleukin-15 receptor alpha chain

Chain J: 58% 11% 27%



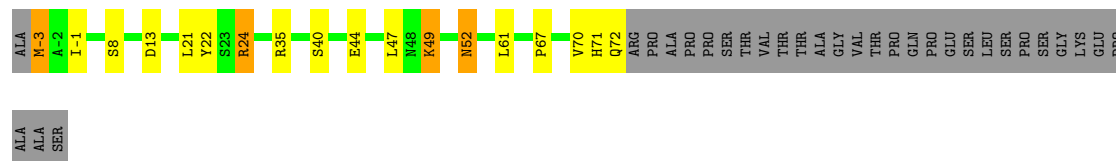
- Molecule 2: Interleukin-15 receptor alpha chain

Chain L:  59% 9% • 30%



- Molecule 2: Interleukin-15 receptor alpha chain

Chain N:  54% 13% . 29%



- Molecule 2: Interleukin-15 receptor alpha chain

Chain P:  55% 11% • 33%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.80Å 127.03Å 191.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.93 – 2.00	Depositor
% Data completeness (in resolution range)	100.0 (30.93-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12517	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.78	0/893	0.76	0/1205
1	C	0.84	0/914	0.84	2/1233 (0.2%)
1	E	0.82	0/935	0.78	0/1263
1	G	0.87	0/935	0.88	0/1263
1	I	0.99	1/914 (0.1%)	0.89	0/1233
1	K	0.94	0/914	0.84	1/1233 (0.1%)
1	M	0.81	0/914	0.79	0/1233
1	O	0.79	0/928	0.78	0/1255
2	B	0.84	0/599	0.86	0/814
2	D	0.80	0/609	0.85	0/828
2	F	0.94	0/588	0.85	1/800 (0.1%)
2	H	0.94	0/614	0.87	0/835
2	J	0.89	0/625	0.98	1/849 (0.1%)
2	L	0.90	0/607	0.85	1/825 (0.1%)
2	N	0.84	0/609	0.83	0/828
2	P	0.90	0/579	0.87	0/788
All	All	0.87	1/12177 (0.0%)	0.84	6/16485 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	-4	ALA	CA-CB	-6.77	1.38	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	7	MET	CB-CG-SD	6.84	132.92	112.40
1	K	69	LEU	CA-CB-CG	6.18	129.51	115.30
1	C	14	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	J	7	MET	CB-CG-SD	5.43	128.71	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	LEU	CB-CG-CD1	5.28	119.97	111.00
2	L	35	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	883	0	876	11	0
1	C	904	0	897	22	0
1	E	924	0	913	7	0
1	G	924	0	913	25	0
1	I	904	0	897	19	0
1	K	904	0	897	17	0
1	M	904	0	897	13	0
1	O	917	0	908	16	0
2	B	584	0	583	6	0
2	D	594	0	595	7	0
2	F	573	0	570	6	0
2	H	599	0	600	8	0
2	J	610	0	613	10	0
2	L	592	0	594	5	0
2	N	594	0	595	9	0
2	P	564	0	562	8	0
3	A	12	0	16	0	0
3	O	12	0	16	0	0
4	A	17	0	0	0	0
4	B	32	0	0	0	0
4	C	35	0	0	3	0
4	D	26	0	0	0	0
4	E	32	0	0	0	0
4	F	43	0	0	2	0
4	G	41	0	0	1	0
4	H	43	0	0	2	0
4	I	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	37	0	0	1	0
4	K	34	0	0	2	0
4	L	45	0	0	2	0
4	M	22	0	0	0	0
4	N	21	0	0	0	0
4	O	20	0	0	2	0
4	P	36	0	0	1	0
All	All	12517	0	11942	166	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 7.

All (166) 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:M:36:LYS:HE3	1:M:113:THR:HG21	1.21	1.18
1:C:-1:ILE:HD11	1:C:114:SER:OG	1.48	1.12
1:G:80:VAL:HG13	1:G:81:THR:HA	1.04	1.03
2:H:17:LYS:HD2	4:H:144:HOH:O	1.59	1.01
1:M:36:LYS:HE3	1:M:113:THR:CG2	1.92	0.98
1:G:80:VAL:CG1	1:G:81:THR:HA	1.95	0.96
2:D:67:PRO:HA	2:D:70:VAL:HG22	1.50	0.93
1:I:1:ASN:HD21	1:I:72:ASN:HD22	1.17	0.86
1:G:96:ILE:HD13	4:G:120:HOH:O	1.79	0.82
1:G:80:VAL:HG13	1:G:81:THR:CA	1.99	0.81
1:M:36:LYS:CE	1:M:113:THR:HG21	2.07	0.80
2:F:7:MET:HG2	4:F:137:HOH:O	1.81	0.80
1:C:75:SER:HB3	4:C:117:HOH:O	1.86	0.75
1:G:78:GLY:HA2	1:G:79:ASN:CB	2.17	0.74
2:H:13:ASP:HB2	4:H:142:HOH:O	1.88	0.73
1:G:78:GLY:HA2	1:G:79:ASN:HB2	1.70	0.73
1:C:-1:ILE:CD1	1:C:114:SER:OG	2.35	0.72
1:I:1:ASN:ND2	1:I:72:ASN:HD22	1.88	0.71
1:C:32:HIS:CD2	1:C:34:SER:H	2.10	0.70
1:G:105:HIS:HA	1:G:108:GLN:HE21	1.57	0.69
1:I:25:LEU:HD12	1:I:96:ILE:HD12	1.73	0.69
1:G:77:ASN:N	1:G:78:GLY:HA3	2.08	0.69
2:L:69:LEU:O	2:L:72:GLN:HG3	1.92	0.68
2:P:17:LYS:HE2	2:P:25:GLU:OE1	1.92	0.68
1:M:18:SER:HB2	1:O:18:SER:HB3	1.75	0.68
1:C:75:SER:CB	4:C:117:HOH:O	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:ALA:O	1:G:96:ILE:CD1	2.41	0.68
2:B:35:ARG:HG3	2:B:61:LEU:CD1	2.24	0.68
1:I:25:LEU:CD1	1:I:96:ILE:HD12	2.24	0.67
1:C:-1:ILE:HD11	1:C:114:SER:HG	1.59	0.67
1:I:1:ASN:HB2	1:I:73:SER:OG	1.94	0.66
1:E:32:HIS:ND1	1:E:33:PRO:HD2	2.13	0.64
1:O:22:ASP:HB3	2:P:26:ARG:HH11	1.62	0.64
1:K:36:LYS:HB3	1:K:109:MET:HE1	1.78	0.64
1:C:14:ASP:O	1:C:17:GLN:HB2	1.99	0.63
2:P:35:ARG:HG3	2:P:61:LEU:CD1	2.31	0.61
2:J:65:ARG:HG2	2:J:65:ARG:HH11	1.66	0.61
1:G:-4:ALA:HA	1:K:104:VAL:HG21	1.82	0.61
1:O:32:HIS:ND1	1:O:33:PRO:HD2	2.16	0.61
1:C:28:GLU:CG	1:C:31:VAL:HG22	2.31	0.61
1:O:66:LEU:HD23	1:O:66:LEU:C	2.22	0.60
1:A:52:LEU:HG	2:D:-3:MET:HE1	1.84	0.60
1:E:68:ILE:HG13	2:H:-1:ILE:HD11	1.84	0.60
1:E:106:ILE:HG13	1:E:109:MET:HE2	1.85	0.59
1:I:89:GLU:HB2	2:J:67:PRO:HG3	1.86	0.58
1:G:2:TRP:HB2	1:G:111:ILE:HG13	1.83	0.58
1:I:33:PRO:O	1:I:36:LYS:HG2	2.04	0.58
1:M:6:ILE:HG13	1:M:107:VAL:HG11	1.86	0.58
1:O:87:GLU:HG3	2:P:67:PRO:HB3	1.86	0.58
1:G:23:ALA:O	1:G:96:ILE:HD13	2.04	0.58
2:L:20:SER:HB3	4:L:136:HOH:O	2.05	0.57
1:C:31:VAL:O	1:C:109:MET:HE1	2.03	0.57
1:K:-1:ILE:HD11	1:K:114:SER:HB2	1.86	0.56
1:O:96:ILE:HG12	4:O:1016:HOH:O	2.05	0.56
1:E:109:MET:O	1:E:113:THR:HB	2.05	0.56
2:B:58:THR:HG21	2:D:50:ALA:HB2	1.88	0.56
1:G:76:SER:C	1:G:78:GLY:HA3	2.27	0.55
1:C:75:SER:O	1:C:76:SER:O	2.25	0.55
2:F:0:SER:N	1:G:64:GLU:OE2	2.40	0.54
1:A:97:LYS:O	1:A:101:GLN:HG3	2.07	0.54
2:F:20:SER:O	2:F:23:SER:HB2	2.08	0.53
1:G:78:GLY:CA	1:G:79:ASN:CB	2.87	0.53
1:K:32:HIS:CD2	1:K:34:SER:H	2.26	0.53
2:J:65:ARG:HH11	2:J:65:ARG:CG	2.20	0.53
1:O:111:ILE:O	1:O:112:ASN:CB	2.57	0.53
1:C:11:LYS:HE2	1:C:62:THR:OG1	2.08	0.53
1:I:18:SER:HB2	1:K:18:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:-1:ILE:HD11	1:K:114:SER:CB	2.38	0.53
2:N:-3:MET:HG2	2:N:52:ASN:HD21	1.73	0.53
1:I:12:ILE:O	1:I:16:ILE:HG23	2.08	0.53
2:D:66:ASP:O	2:D:70:VAL:HG13	2.09	0.53
1:C:28:GLU:HG3	1:C:31:VAL:HG22	1.92	0.52
1:M:14:ASP:O	1:M:17:GLN:HB2	2.09	0.52
1:O:45:LEU:O	1:O:48:GLN:HB2	2.08	0.52
1:G:6:ILE:O	1:G:10:LYS:HG2	2.10	0.52
1:C:32:HIS:HD2	1:C:34:SER:H	1.54	0.52
1:I:33:PRO:HA	1:I:109:MET:HE1	1.92	0.52
2:D:65:ARG:HB3	2:D:70:VAL:HG11	1.92	0.52
1:G:16:ILE:CD1	1:G:96:ILE:HG21	2.39	0.52
1:K:32:HIS:CD2	1:K:33:PRO:HD2	2.45	0.51
2:L:7:MET:HG2	4:L:140:HOH:O	2.09	0.51
1:G:89:GLU:HB2	2:H:67:PRO:HG3	1.92	0.51
1:K:97:LYS:CD	4:K:126:HOH:O	2.58	0.51
2:F:7:MET:HG2	4:F:108:HOH:O	2.10	0.51
2:J:21:LEU:O	2:J:22:TYR:HB2	2.11	0.51
1:O:10:LYS:HG2	4:O:1019:HOH:O	2.11	0.51
2:P:35:ARG:HG3	2:P:61:LEU:HD12	1.93	0.50
1:A:9:LEU:O	1:A:13:GLU:HG3	2.11	0.50
2:N:35:ARG:HG3	2:N:61:LEU:CD1	2.42	0.50
2:N:49:LYS:HG2	2:P:60:SER:HB3	1.93	0.50
1:O:97:LYS:HD2	1:O:101:GLN:NE2	2.28	0.49
1:G:16:ILE:HD13	1:G:96:ILE:HG21	1.93	0.49
1:K:32:HIS:HD2	1:K:33:PRO:HD2	1.77	0.49
1:G:28:GLU:HG3	1:G:31:VAL:HG22	1.94	0.48
1:C:41:LYS:NZ	4:C:145:HOH:O	2.35	0.48
2:F:65:ARG:HA	2:F:65:ARG:HD3	1.65	0.48
1:I:47:LEU:HD21	1:I:66:LEU:HD13	1.95	0.48
1:G:-4:ALA:HA	1:K:104:VAL:CG2	2.43	0.48
1:A:1:ASN:HB2	1:A:73:SER:OG	2.14	0.48
2:H:35:ARG:HG3	2:H:61:LEU:CD1	2.43	0.48
1:C:16:ILE:CD1	1:C:96:ILE:HG21	2.43	0.48
1:M:-1:ILE:O	1:M:3:VAL:HG23	2.14	0.48
2:L:72:GLN:O	2:L:73:ARG:HB3	2.13	0.47
1:I:32:HIS:ND1	1:I:33:PRO:HD2	2.28	0.47
1:O:73:SER:HA	1:O:76:SER:HB3	1.97	0.47
1:I:18:SER:CB	1:K:18:SER:HB2	2.44	0.47
1:A:10:LYS:O	1:A:10:LYS:HD3	2.15	0.47
2:B:35:ARG:HG3	2:B:61:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:ILE:HG13	1:M:109:MET:HE2	1.97	0.46
1:E:18:SER:HB2	1:G:18:SER:HB2	1.98	0.46
1:K:106:ILE:HG13	1:K:109:MET:HE2	1.97	0.46
1:C:100:LEU:HB3	1:O:-3:MET:HE1	1.98	0.46
1:K:36:LYS:CB	1:K:109:MET:HE1	2.44	0.46
1:M:89:GLU:HB2	2:N:67:PRO:HG3	1.98	0.46
1:A:33:PRO:O	1:A:36:LYS:HG2	2.16	0.46
1:I:25:LEU:CD1	1:I:96:ILE:CD1	2.92	0.46
1:E:-3:MET:CE	1:E:-2:ALA:H	2.29	0.46
2:B:27:TYR:CD2	2:B:59:PRO:HG3	2.51	0.46
2:J:51:THR:HB	2:J:53:VAL:HG23	1.98	0.46
2:J:65:ARG:HB3	2:J:70:VAL:HG21	1.97	0.46
1:I:105:HIS:O	1:I:108:GLN:HB2	2.16	0.45
2:L:65:ARG:HD3	2:L:65:ARG:HA	1.67	0.45
2:P:20:SER:O	2:P:23:SER:HB3	2.16	0.45
1:G:101:GLN:HE22	1:K:-3:MET:CE	2.29	0.45
2:N:70:VAL:CG1	2:N:70:VAL:O	2.64	0.45
2:J:66:ASP:HA	2:J:67:PRO:HD2	1.60	0.45
1:O:47:LEU:HD21	1:O:66:LEU:HD13	1.99	0.45
1:A:87:GLU:HG3	2:B:67:PRO:HB3	1.99	0.45
2:N:24:ARG:NH1	2:N:44:GLU:OE2	2.51	0.44
2:H:-1:ILE:HG12	2:H:0:SER:N	2.33	0.44
2:F:58:THR:HG21	2:H:50:ALA:HB2	2.00	0.44
1:O:97:LYS:HG3	1:O:98:GLU:N	2.30	0.44
1:O:37:VAL:HG21	1:O:80:VAL:HG11	2.00	0.44
1:A:47:LEU:HD21	1:A:66:LEU:HD13	1.98	0.44
1:M:87:GLU:HB2	1:M:90:GLU:HG3	1.99	0.44
1:I:16:ILE:CD1	1:I:96:ILE:HG21	2.48	0.43
2:N:40:SER:O	2:N:61:LEU:HB2	2.17	0.43
2:P:7:MET:HG2	4:P:122:HOH:O	2.17	0.43
1:M:11:LYS:HD3	1:M:62:THR:OG1	2.19	0.43
1:C:69:LEU:HD13	2:J:5:PRO:CD	2.49	0.42
2:H:3:CYS:HB3	2:H:4:PRO:HD2	2.00	0.42
2:J:48:ASN:C	2:J:48:ASN:HD22	2.22	0.42
1:I:28:GLU:CG	1:I:31:VAL:HG22	2.49	0.42
2:N:21:LEU:O	2:N:22:TYR:HB2	2.20	0.42
1:I:28:GLU:HG3	1:I:31:VAL:HG22	2.02	0.42
1:K:-1:ILE:CD1	1:K:114:SER:HB2	2.49	0.42
2:B:35:ARG:HG3	2:B:61:LEU:HD12	1.99	0.42
1:K:97:LYS:HD2	4:K:126:HOH:O	2.17	0.42
1:M:36:LYS:HB2	1:M:109:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HA	1:C:19:MET:HG3	2.00	0.42
1:A:52:LEU:HD21	2:D:47:LEU:HD12	2.02	0.41
1:A:66:LEU:C	1:A:66:LEU:HD23	2.41	0.41
1:E:6:ILE:HG13	1:E:107:VAL:HG11	2.02	0.41
1:K:11:LYS:HE2	1:K:62:THR:OG1	2.20	0.41
1:M:12:ILE:O	1:M:16:ILE:HG23	2.21	0.41
2:D:6:PRO:HG3	2:D:16:VAL:HG21	2.02	0.41
1:C:28:GLU:HG3	1:C:31:VAL:CG2	2.50	0.41
2:N:70:VAL:HG12	2:N:70:VAL:O	2.20	0.41
1:C:32:HIS:CD2	1:C:34:SER:OG	2.73	0.41
1:C:28:GLU:HG2	1:C:31:VAL:HG22	2.02	0.41
1:I:1:ASN:HD21	1:I:72:ASN:ND2	1.99	0.41
2:J:17:LYS:HD2	4:J:129:HOH:O	2.21	0.41
1:G:14:ASP:O	1:G:17:GLN:HB2	2.21	0.41
1:A:18:SER:HB2	1:C:18:SER:HB2	2.02	0.40
1:G:45:LEU:HA	1:G:45:LEU:HD23	1.91	0.40
1:O:3:VAL:CG2	1:O:111:ILE:HD11	2.52	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	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	C	112/119 (94%)	109 (97%)	3 (3%)	0	100	100
1	E	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
1	G	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	20	12
1	I	112/119 (94%)	108 (96%)	4 (4%)	0	100	100
1	K	112/119 (94%)	109 (97%)	3 (3%)	0	100	100
1	M	112/119 (94%)	109 (97%)	2 (2%)	1 (1%)	20	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
2	B	72/107 (67%)	66 (92%)	6 (8%)	0	100	100
2	D	74/107 (69%)	73 (99%)	1 (1%)	0	100	100
2	F	71/107 (66%)	69 (97%)	2 (3%)	0	100	100
2	H	75/107 (70%)	75 (100%)	0	0	100	100
2	J	76/107 (71%)	74 (97%)	2 (3%)	0	100	100
2	L	73/107 (68%)	70 (96%)	3 (4%)	0	100	100
2	N	74/107 (69%)	72 (97%)	2 (3%)	0	100	100
2	P	70/107 (65%)	69 (99%)	1 (1%)	0	100	100
All	All	1492/1808 (82%)	1448 (97%)	42 (3%)	2 (0%)	55	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	79	ASN
1	M	17	GLN

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	105/110 (96%)	95 (90%)	10 (10%)	10	5
1	C	108/110 (98%)	97 (90%)	11 (10%)	8	4
1	E	110/110 (100%)	103 (94%)	7 (6%)	20	15
1	G	110/110 (100%)	102 (93%)	8 (7%)	16	11
1	I	108/110 (98%)	100 (93%)	8 (7%)	16	10
1	K	108/110 (98%)	104 (96%)	4 (4%)	39	36
1	M	108/110 (98%)	103 (95%)	5 (5%)	31	27
1	O	109/110 (99%)	103 (94%)	6 (6%)	25	20
2	B	67/92 (73%)	63 (94%)	4 (6%)	22	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	68/92 (74%)	61 (90%)	7 (10%)	8	4
2	F	66/92 (72%)	61 (92%)	5 (8%)	15	10
2	H	68/92 (74%)	63 (93%)	5 (7%)	16	10
2	J	69/92 (75%)	61 (88%)	8 (12%)	6	3
2	L	68/92 (74%)	61 (90%)	7 (10%)	8	4
2	N	68/92 (74%)	58 (85%)	10 (15%)	3	1
2	P	65/92 (71%)	61 (94%)	4 (6%)	21	16
All	All	1405/1616 (87%)	1296 (92%)	109 (8%)	15	9

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	MET
1	A	10	LYS
1	A	18	SER
1	A	20	HIS
1	A	21	ILE
1	A	52	LEU
1	A	69	LEU
1	A	81	THR
1	A	92	GLU
1	A	103	PHE
2	B	7	MET
2	B	20	SER
2	B	47	LEU
2	B	65	ARG
1	C	-3	MET
1	C	14	ASP
1	C	17	GLN
1	C	19	MET
1	C	20	HIS
1	C	69	LEU
1	C	80	VAL
1	C	81	THR
1	C	97	LYS
1	C	103	PHE
1	C	109	MET
2	D	10	GLU
2	D	13	ASP
2	D	24	ARG

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Mol	Chain	Res	Type
2	D	47	LEU
2	D	49	LYS
2	D	52	ASN
2	D	62	LYS
1	E	0	SER
1	E	17	GLN
1	E	32	HIS
1	E	52	LEU
1	E	69	LEU
1	E	103	PHE
1	E	113	THR
2	F	0	SER
2	F	23	SER
2	F	49	LYS
2	F	51	THR
2	F	65	ARG
1	G	-3	MET
1	G	17	GLN
1	G	20	HIS
1	G	79	ASN
1	G	83	SER
1	G	96	ILE
1	G	97	LYS
1	G	103	PHE
2	H	-1	ILE
2	H	10	GLU
2	H	47	LEU
2	H	52	ASN
2	H	72	GLN
1	I	14	ASP
1	I	58	SER
1	I	69	LEU
1	I	80	VAL
1	I	81	THR
1	I	101	GLN
1	I	103	PHE
1	I	113	THR
2	J	-1	ILE
2	J	8	SER
2	J	47	LEU
2	J	48	ASN
2	J	53	VAL

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Mol	Chain	Res	Type
2	J	65	ARG
2	J	70	VAL
2	J	73	ARG
1	K	17	GLN
1	K	52	LEU
1	K	69	LEU
1	K	103	PHE
2	L	-1	ILE
2	L	0	SER
2	L	24	ARG
2	L	49	LYS
2	L	51	THR
2	L	72	GLN
2	L	73	ARG
1	M	58	SER
1	M	69	LEU
1	M	75	SER
1	M	80	VAL
1	M	103	PHE
2	N	-3	MET
2	N	-1	ILE
2	N	8	SER
2	N	13	ASP
2	N	24	ARG
2	N	47	LEU
2	N	49	LYS
2	N	52	ASN
2	N	71	HIS
2	N	72	GLN
1	O	10	LYS
1	O	17	GLN
1	O	52	LEU
1	O	69	LEU
1	O	97	LYS
1	O	103	PHE
2	P	0	SER
2	P	23	SER
2	P	47	LEU
2	P	51	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	101	GLN
1	A	105	HIS
2	B	30	ASN
2	B	71	HIS
1	C	32	HIS
1	C	48	GLN
2	D	30	ASN
2	D	71	HIS
1	E	20	HIS
1	E	108	GLN
2	F	30	ASN
1	G	20	HIS
1	G	101	GLN
1	G	108	GLN
2	H	30	ASN
2	H	55	HIS
1	I	48	GLN
1	I	72	ASN
2	J	30	ASN
2	J	48	ASN
2	J	55	HIS
1	K	32	HIS
2	L	72	GLN
1	M	32	HIS
1	M	48	GLN
1	M	108	GLN
2	N	30	ASN
2	N	52	ASN
1	O	79	ASN
1	O	101	GLN
1	O	108	GLN
2	P	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	1003	-	5,5,5	0.31	0	5,5,5	0.42	0
3	GOL	A	1004	-	5,5,5	0.38	0	5,5,5	0.46	0
3	GOL	O	1001	-	5,5,5	0.48	0	5,5,5	0.94	0
3	GOL	O	1002	-	5,5,5	0.35	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1004	-	-	0/4/4/4	0/0/0/0
3	GOL	O	1001	-	-	0/4/4/4	0/0/0/0
3	GOL	O	1002	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

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.