



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:22 am BST

PDB ID : 3KQA  
Title : MurA dead-end complex with terreic acid  
Authors : Schonbrunn, E.  
Deposited on : 2009-11-17  
Resolution : 2.25 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) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

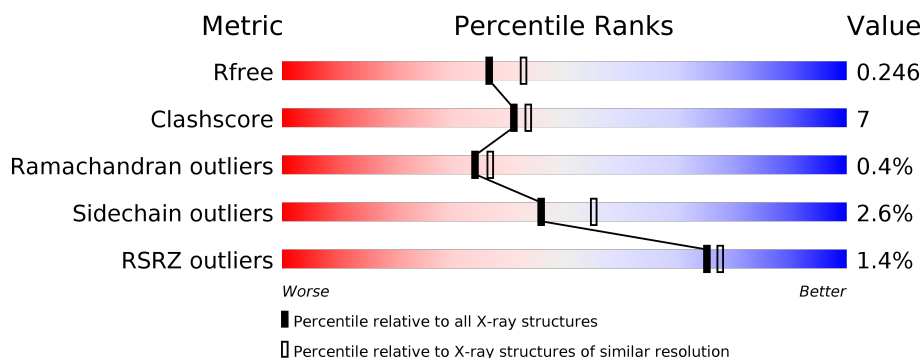
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\leq 5\%$ . 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	419	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> </div> </div> <div>87% 13%</div> </div>
1	B	419	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 85%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> </div> </div> <div>85% 14%</div> </div>
1	C	419	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 16%; height: 10px; background-color: yellow;"></div> </div> </div> <div>84% 16%</div> </div>
1	D	419	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 79%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: yellow;"></div> </div> </div> <div>79% 20%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13150 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.

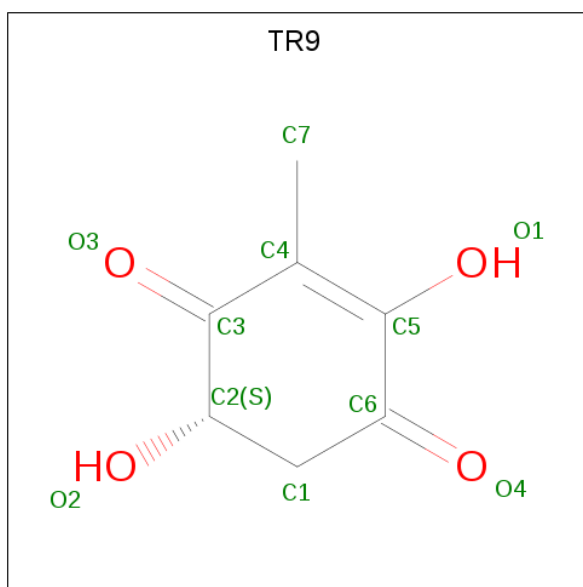
- Molecule 1 is a protein called UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3143	1976	554	599	14			
1	B	419	Total	C	N	O	S	0	0	0
			3143	1976	554	599	14			
1	C	419	Total	C	N	O	S	0	0	0
			3143	1976	554	599	14			
1	D	419	Total	C	N	O	S	0	0	0
			3143	1976	554	599	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	SEE REMARK 999	UNP P33038
B	67	IAS	ASN	SEE REMARK 999	UNP P33038
C	67	IAS	ASN	SEE REMARK 999	UNP P33038
D	67	IAS	ASN	SEE REMARK 999	UNP P33038

- Molecule 2 is (5S)-2,5-dihydroxy-3-methylcyclohex-2-ene-1,4-dione (three-letter code: TR9) (formula: C<sub>7</sub>H<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 7 4	0	0
2	B	1	Total C O 11 7 4	0	0
2	C	1	Total C O 11 7 4	0	0
2	D	1	Total C O 11 7 4	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Ca 4 4	0	0
3	A	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	146	Total O 146 146	0	0

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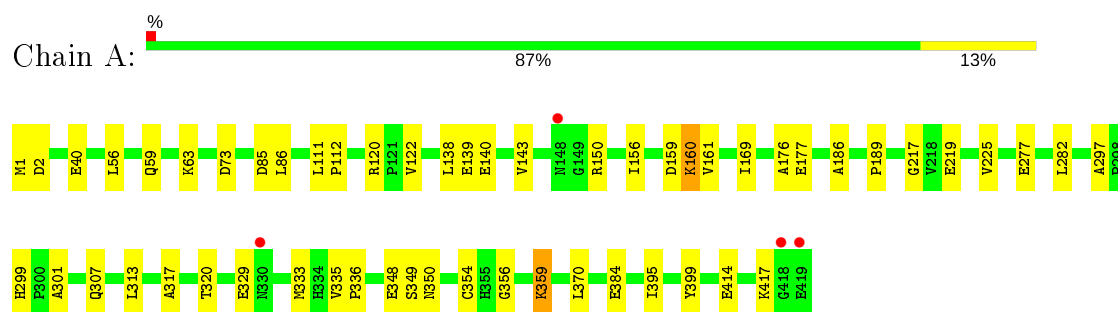
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	177	Total 177	O 177	0	0
4	C	125	Total 125	O 125	0	0
4	D	76	Total 76	O 76	0	0

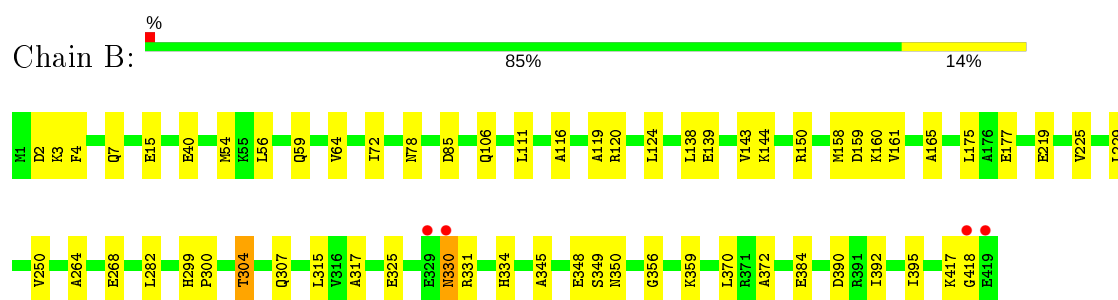
### 3 Residue-property plots [i](#)

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.

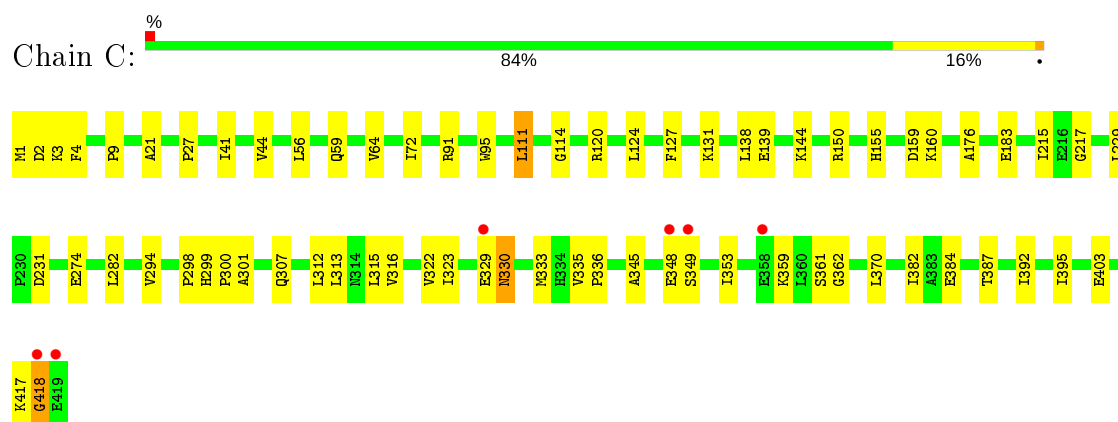
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



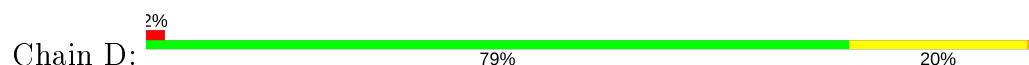
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

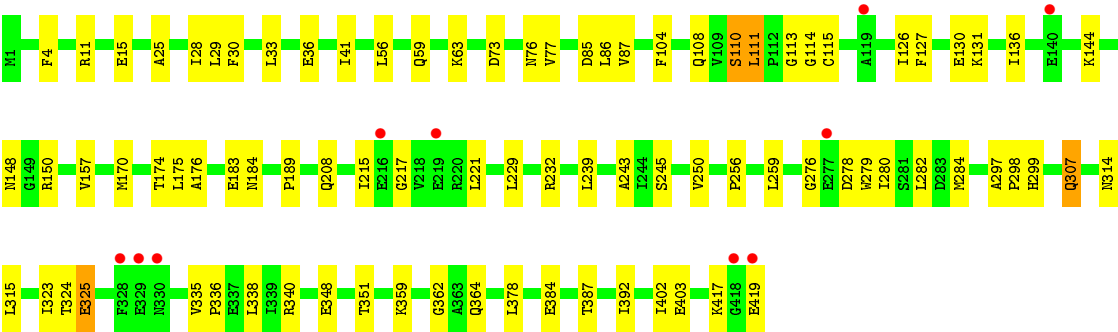


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.27Å 115.27Å 277.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.25 14.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.25) 99.8 (14.98-2.25)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.44 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.195 , 0.254 0.190 , 0.246	Depositor DCC
$R_{free}$ test set	1063 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2803e-03.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TR9, CA, IAS

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	0.55	0/3179	0.71	1/4305 (0.0%)
1	B	0.57	0/3179	0.74	0/4305
1	C	0.53	0/3179	0.71	0/4305
1	D	0.45	0/3179	0.67	0/4305
All	All	0.53	0/12716	0.71	1/17220 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	VAL	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3143	0	3215	43	0
1	B	3143	0	3215	38	0
1	C	3143	0	3215	48	0
1	D	3143	0	3215	53	0
2	A	11	0	5	3	0
2	B	11	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	11	0	6	0	0
2	D	11	0	5	1	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	146	0	0	2	0
4	B	177	0	0	2	0
4	C	125	0	0	3	0
4	D	76	0	0	0	0
All	All	13150	0	12881	180	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 (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ASN:HD22	1:B:330:ASN:H	1.13	0.89
1:C:111:LEU:HD13	1:C:114:GLY:HA3	1.56	0.86
1:C:359:LYS:HD3	1:C:384:GLU:HB2	1.57	0.85
1:A:277:GLU:HG2	1:C:274:GLU:OE1	1.80	0.81
1:B:150:ARG:HD2	1:B:177:GLU:HG3	1.64	0.79
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.68	0.76
1:D:15:GLU:HG2	1:D:250:VAL:HB	1.68	0.75
1:B:138:LEU:HD22	2:B:500:TR9:H2	1.69	0.74
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.71	0.72
1:B:150:ARG:HD2	1:B:177:GLU:CG	2.19	0.72
1:A:138:LEU:HD22	2:A:500:TR9:H2	1.70	0.72
1:B:330:ASN:N	1:B:330:ASN:HD22	1.84	0.70
1:A:40:GLU:HB3	1:A:225:VAL:HG22	1.73	0.70
1:B:15:GLU:HG2	1:B:250:VAL:HB	1.73	0.69
1:C:127:PHE:O	1:C:131:LYS:HG2	1.93	0.69
1:B:304:THR:HG22	1:B:325:GLU:OE2	1.93	0.68
1:B:219:GLU:HG3	4:B:494:HOH:O	1.94	0.68
1:A:150:ARG:NH2	1:A:219:GLU:HA	2.09	0.67
1:A:120:ARG:HD2	4:A:446:HOH:O	1.93	0.66
1:D:63:LYS:HE3	1:D:76:ASN:HD22	1.59	0.65
1:C:329:GLU:O	1:C:330:ASN:HB3	1.96	0.65
1:B:330:ASN:H	1:B:330:ASN:ND2	1.89	0.65
1:B:116:ALA:HB3	1:B:120:ARG:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:HD21	1:C:345:ALA:HB2	1.79	0.64
1:A:176:ALA:O	1:A:217:GLY:HA3	1.98	0.64
1:B:124:LEU:HB3	1:B:165:ALA:HB2	1.79	0.63
1:B:317:ALA:O	1:B:356:GLY:HA3	1.99	0.63
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.81	0.62
1:B:304:THR:HB	1:B:331:ARG:NH1	2.15	0.62
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.15	0.61
1:B:161:VAL:HG23	4:B:536:HOH:O	2.00	0.61
1:C:150:ARG:HH11	1:C:150:ARG:HG2	1.66	0.60
1:D:176:ALA:O	1:D:217:GLY:HA3	2.00	0.60
1:D:110:SER:O	1:D:111:LEU:HG	2.02	0.59
1:C:56:LEU:HD23	1:C:56:LEU:C	2.23	0.59
1:D:315:LEU:HD12	1:D:338:LEU:HD13	1.84	0.58
1:A:2:ASP:OD1	1:A:417:LYS:HD3	2.04	0.58
1:D:87:VAL:HG21	1:D:110:SER:O	2.04	0.58
1:D:157:VAL:HG22	1:D:183:GLU:HG3	1.84	0.58
1:D:63:LYS:HE3	1:D:76:ASN:ND2	2.18	0.57
1:D:4:PHE:CD1	1:D:392:ILE:HG21	2.39	0.57
1:D:189:PRO:HD3	1:D:299:HIS:CD2	2.39	0.57
1:B:359:LYS:HD3	1:B:384:GLU:HB2	1.87	0.56
1:D:276:GLY:HA3	1:D:279:TRP:CE2	2.41	0.56
1:B:330:ASN:N	1:B:330:ASN:ND2	2.49	0.55
1:D:157:VAL:HA	1:D:183:GLU:HB2	1.88	0.55
1:A:348:GLU:O	1:A:349:SER:HB3	2.07	0.55
1:B:54:MET:HG2	1:B:64:VAL:HG11	1.89	0.55
1:C:111:LEU:CD1	1:C:114:GLY:HA3	2.33	0.55
1:C:333:MET:HE3	1:C:333:MET:HA	1.88	0.55
1:D:150:ARG:HD2	1:D:175:LEU:O	2.07	0.55
1:D:127:PHE:O	1:D:131:LYS:HG2	2.07	0.54
1:B:2:ASP:OD1	1:B:417:LYS:HD3	2.07	0.54
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.89	0.54
1:D:113:GLY:O	1:D:115:CYS:N	2.40	0.54
1:A:313:LEU:C	1:A:313:LEU:HD23	2.28	0.54
1:D:282:LEU:C	1:D:282:LEU:HD23	2.28	0.53
1:D:108:GLN:OE1	1:D:144:LYS:HE2	2.08	0.53
1:C:139:GLU:HG3	1:C:144:LYS:HE3	1.89	0.53
1:A:189:PRO:HD3	1:A:299:HIS:CD2	2.44	0.52
1:C:329:GLU:O	1:C:330:ASN:CB	2.57	0.52
1:B:139:GLU:HG3	1:B:144:LYS:HE3	1.92	0.52
1:D:243:ALA:HA	1:D:284:MET:CG	2.40	0.51
1:B:64:VAL:HG13	1:B:72:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:HIS:HE1	1:C:183:GLU:OE2	1.94	0.51
1:D:362:GLY:HA2	1:D:387:THR:OG1	2.12	0.51
1:D:402:ILE:HG23	1:D:403:GLU:N	2.26	0.50
1:A:317:ALA:O	1:A:356:GLY:HA3	2.12	0.50
1:A:56:LEU:O	1:A:56:LEU:HD23	2.12	0.50
1:C:150:ARG:NH1	4:C:459:HOH:O	2.44	0.50
1:D:108:GLN:HG3	1:D:144:LYS:HG2	1.92	0.49
1:D:28:ILE:HG22	1:D:41:ILE:HD13	1.93	0.49
1:D:115:CYS:HA	2:D:500:TR9:H2	1.94	0.49
1:A:160:LYS:NZ	1:A:160:LYS:HB2	2.28	0.49
1:A:333:MET:HG3	4:A:515:HOH:O	2.12	0.49
1:B:282:LEU:HD23	1:B:282:LEU:C	2.33	0.49
1:A:370:LEU:CD1	1:A:395:ILE:HA	2.43	0.48
1:D:359:LYS:HD3	1:D:384:GLU:HB2	1.95	0.48
1:A:150:ARG:HD2	1:A:177:GLU:HB2	1.94	0.48
1:D:77:VAL:HB	1:D:104:PHE:CZ	2.49	0.48
1:D:232:ARG:HB2	1:D:259:LEU:HD21	1.96	0.48
1:B:40:GLU:HB3	1:B:225:VAL:HG22	1.95	0.48
1:B:264:ALA:O	1:B:268:GLU:HG3	2.13	0.48
1:D:340:ARG:NH2	1:D:364:GLN:O	2.47	0.48
1:D:59:GLN:HG2	1:D:86:LEU:HD12	1.95	0.48
1:C:138:LEU:N	1:C:138:LEU:HD22	2.29	0.47
1:A:139:GLU:O	1:A:140:GLU:HG2	2.14	0.47
1:C:21:ALA:HB2	1:C:231:ASP:HA	1.95	0.47
1:D:30:PHE:O	1:D:33:LEU:HB2	2.14	0.47
1:A:150:ARG:HH22	1:A:219:GLU:HA	1.78	0.47
1:B:299:HIS:CG	1:B:300:PRO:HA	2.49	0.47
1:B:150:ARG:HD2	1:B:177:GLU:HG2	1.96	0.47
1:C:120:ARG:NH2	1:D:348:GLU:OE1	2.48	0.47
1:C:91:ARG:HG2	1:C:91:ARG:HH11	1.79	0.46
1:B:348:GLU:O	1:B:349:SER:HB3	2.15	0.46
1:A:63:LYS:HB2	1:A:73:ASP:HB3	1.98	0.46
1:A:282:LEU:HD23	1:A:282:LEU:C	2.36	0.46
1:C:348:GLU:O	1:C:349:SER:HB3	2.16	0.46
1:D:11:ARG:HA	1:D:245:SER:HB2	1.98	0.46
1:A:156:ILE:HD13	1:A:169:ILE:HG21	1.98	0.46
1:B:150:ARG:HD3	1:B:175:LEU:O	2.16	0.45
1:B:304:THR:CG2	1:B:325:GLU:OE2	2.64	0.45
1:A:297:ALA:HB3	1:A:301:ALA:CB	2.47	0.45
1:C:124:LEU:CD1	1:C:124:LEU:N	2.79	0.45
1:B:4:PHE:CD1	1:B:392:ILE:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:HA	1:C:120:ARG:HD3	1.84	0.45
1:C:2:ASP:OD1	1:C:417:LYS:HD3	2.17	0.45
1:A:160:LYS:NZ	1:A:160:LYS:CB	2.79	0.45
1:D:215:ILE:HD12	1:D:215:ILE:N	2.31	0.45
1:C:294:VAL:HB	1:C:323:ILE:HD13	1.99	0.45
1:C:150:ARG:NH1	1:C:150:ARG:HG2	2.32	0.45
1:B:315:LEU:HD21	1:B:345:ALA:HB2	1.99	0.45
1:C:215:ILE:HD12	1:C:215:ILE:N	2.31	0.45
1:D:29:LEU:HD23	1:D:41:ILE:HD12	1.99	0.44
1:A:56:LEU:C	1:A:56:LEU:HD23	2.38	0.44
1:D:126:ILE:HG23	1:D:136:ILE:HG13	2.00	0.44
1:B:370:LEU:HD12	1:B:395:ILE:HA	1.99	0.44
1:A:359:LYS:CE	1:A:384:GLU:HB2	2.47	0.44
1:C:27:PRO:HD3	1:C:95:TRP:CZ3	2.52	0.44
1:C:333:MET:O	1:C:336:PRO:HD2	2.17	0.44
1:D:256:PRO:HG3	1:D:280:ILE:CG1	2.48	0.44
1:A:59:GLN:HG2	1:A:86:LEU:HD12	2.00	0.44
1:C:403:GLU:CB	4:C:446:HOH:O	2.65	0.43
1:C:176:ALA:O	1:C:217:GLY:HA3	2.18	0.43
1:D:56:LEU:HD23	1:D:56:LEU:O	2.19	0.43
1:C:124:LEU:HD12	1:C:124:LEU:N	2.34	0.43
1:A:161:VAL:CG1	1:A:186:ALA:HA	2.49	0.43
1:C:160:LYS:HB2	1:C:160:LYS:NZ	2.34	0.43
1:C:313:LEU:HD23	1:C:313:LEU:C	2.38	0.43
1:C:64:VAL:HG13	1:C:72:ILE:HD13	2.01	0.43
1:B:325:GLU:O	1:B:350:ASN:ND2	2.44	0.43
1:C:299:HIS:CG	1:C:300:PRO:HA	2.54	0.43
1:D:278:ASP:OD2	1:D:278:ASP:N	2.52	0.43
1:C:282:LEU:HD23	1:C:282:LEU:C	2.40	0.42
1:C:294:VAL:HB	1:C:323:ILE:CD1	2.49	0.42
1:C:370:LEU:HD12	1:C:395:ILE:HA	2.01	0.42
1:C:403:GLU:HB3	4:C:446:HOH:O	2.17	0.42
1:B:56:LEU:HD23	1:B:56:LEU:C	2.39	0.42
1:C:417:LYS:O	1:C:418:GLY:O	2.36	0.42
1:D:324:THR:HG23	1:D:351:THR:HG22	2.01	0.42
1:B:3:LYS:HG2	1:B:390:ASP:OD1	2.19	0.42
1:D:36:GLU:HG3	1:D:221:LEU:O	2.20	0.42
1:B:159:ASP:OD1	1:B:160:LYS:N	2.52	0.42
1:A:111:LEU:CD2	1:A:112:PRO:O	2.68	0.42
1:C:312:LEU:O	1:C:316:VAL:HG22	2.20	0.42
1:D:127:PHE:O	1:D:130:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD11	1:A:399:TYR:CD1	2.55	0.42
1:A:160:LYS:HZ1	1:A:160:LYS:HB2	1.85	0.42
1:A:320:THR:HA	1:A:354:CYS:O	2.19	0.42
1:C:322:VAL:HG22	1:C:353:ILE:CD1	2.49	0.42
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.85	0.42
1:B:143:VAL:HG13	1:B:143:VAL:O	2.19	0.41
1:C:298:PRO:O	1:C:301:ALA:HB3	2.20	0.41
1:D:208:GLN:HG2	1:D:208:GLN:O	2.20	0.41
1:D:314:ASN:ND2	1:D:323:ILE:HD11	2.35	0.41
1:A:359:LYS:HE3	1:A:384:GLU:HB2	2.02	0.41
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.78	0.41
1:C:362:GLY:HA2	1:C:387:THR:OG1	2.21	0.41
1:C:9:PRO:HB3	1:C:382:ILE:O	2.19	0.41
1:A:138:LEU:HD22	2:A:500:TR9:C2	2.45	0.41
1:C:91:ARG:HG2	1:C:91:ARG:NH1	2.35	0.41
1:D:307:GLN:HG3	1:D:325:GLU:HG2	2.02	0.41
1:D:56:LEU:C	1:D:56:LEU:HD23	2.40	0.41
1:A:111:LEU:HD11	1:A:122:VAL:HG11	2.01	0.41
1:C:41:ILE:HG22	1:C:44:VAL:CG2	2.50	0.41
1:A:329:GLU:HB3	1:A:350:ASN:HB3	2.02	0.41
1:A:329:GLU:HB3	1:A:350:ASN:CB	2.50	0.41
1:A:320:THR:HG23	1:A:354:CYS:O	2.21	0.41
1:A:370:LEU:HD11	1:A:399:TYR:HD1	1.85	0.41
1:A:111:LEU:HD22	1:A:112:PRO:O	2.21	0.41
1:B:119:ALA:C	1:B:120:ARG:HG3	2.41	0.41
1:D:170:MET:O	1:D:174:THR:HG23	2.21	0.41
1:C:4:PHE:CD1	1:C:392:ILE:HG21	2.55	0.40
1:D:63:LYS:HB2	1:D:73:ASP:HB3	2.02	0.40
1:A:297:ALA:HB3	1:A:301:ALA:HB3	2.03	0.40
1:D:25:ALA:O	1:D:29:LEU:HG	2.21	0.40
1:D:108:GLN:CG	1:D:144:LYS:HG2	2.52	0.40
1:A:150:ARG:HD3	1:A:177:GLU:N	2.37	0.40
1:A:138:LEU:CD2	2:A:500:TR9:H2	2.45	0.40
1:D:297:ALA:HB1	1:D:298:PRO:CD	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	415/419 (99%)	408 (98%)	7 (2%)	0	100	100
1	B	415/419 (99%)	409 (99%)	5 (1%)	1 (0%)	47	55
1	C	415/419 (99%)	407 (98%)	6 (1%)	2 (0%)	29	29
1	D	415/419 (99%)	404 (97%)	8 (2%)	3 (1%)	22	21
All	All	1660/1676 (99%)	1628 (98%)	26 (2%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	330	ASN
1	B	418	GLY
1	C	418	GLY
1	D	114	GLY
1	D	417	LYS
1	D	111	LEU

### 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	329/329 (100%)	322 (98%)	7 (2%)	53	62
1	B	329/329 (100%)	318 (97%)	11 (3%)	38	46
1	C	329/329 (100%)	321 (98%)	8 (2%)	49	58
1	D	329/329 (100%)	321 (98%)	8 (2%)	49	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1316/1316 (100%)	1282 (97%)	34 (3%)	46 55

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	85	ASP
1	A	159	ASP
1	A	160	LYS
1	A	307	GLN
1	A	359	LYS
1	A	414	GLU
1	B	7	GLN
1	B	59	GLN
1	B	78	ASN
1	B	85	ASP
1	B	106	GLN
1	B	111	LEU
1	B	158	MET
1	B	229	LEU
1	B	304	THR
1	B	307	GLN
1	B	330	ASN
1	C	1	MET
1	C	3	LYS
1	C	59	GLN
1	C	111	LEU
1	C	159	ASP
1	C	229	LEU
1	C	307	GLN
1	C	361	SER
1	D	85	ASP
1	D	110	SER
1	D	148	ASN
1	D	184	ASN
1	D	229	LEU
1	D	307	GLN
1	D	325	GLU
1	D	419	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	59	GLN
1	A	76	ASN
1	A	148	ASN
1	A	184	ASN
1	B	7	GLN
1	B	43	ASN
1	B	59	GLN
1	B	78	ASN
1	B	106	GLN
1	B	148	ASN
1	B	184	ASN
1	B	330	ASN
1	C	59	GLN
1	C	76	ASN
1	C	148	ASN
1	C	155	HIS
1	C	184	ASN
1	D	59	GLN
1	D	76	ASN
1	D	184	ASN
1	D	344	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z  > 2$
1	IAS	D	67	1	4,7,8	0.64	0	2,8,10	1.41	0
1	IAS	C	67	1	4,7,8	0.67	0	2,8,10	1.29	0
1	IAS	B	67	1	4,7,8	0.73	0	2,8,10	1.68	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	IAS	A	67	1	4,7,8	0.74	0	2,8,10	1.12	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
1	IAS	D	67	1	-	0/3/7/8	-
1	IAS	C	67	1	-	0/3/7/8	-
1	IAS	B	67	1	-	0/3/7/8	-
1	IAS	A	67	1	-	0/3/7/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	67	IAS	OD1-CG-CB	-2.27	118.83	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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
2	TR9	D	500	1,3	10,11,11	6.15	6 (60%)	11,16,16	1.49	1 (9%)
2	TR9	B	500	1,3	10,11,11	6.27	6 (60%)	11,16,16	1.20	1 (9%)
2	TR9	C	500	1,3	10,11,11	5.86	6 (60%)	11,16,16	1.63	2 (18%)
2	TR9	A	500	1,3	10,11,11	6.11	6 (60%)	11,16,16	1.38	2 (18%)

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
2	TR9	D	500	1,3	-	-	0/1/1/1
2	TR9	B	500	1,3	-	-	0/1/1/1
2	TR9	C	500	1,3	-	-	0/1/1/1
2	TR9	A	500	1,3	-	-	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	TR9	C5-C4	14.63	1.54	1.35
2	D	500	TR9	C5-C4	14.20	1.54	1.35
2	A	500	TR9	C5-C4	13.18	1.52	1.35
2	C	500	TR9	C5-C4	12.66	1.52	1.35
2	D	500	TR9	O3-C3	8.78	1.37	1.22
2	A	500	TR9	O3-C3	8.10	1.36	1.22
2	B	500	TR9	O3-C3	8.06	1.36	1.22
2	C	500	TR9	O3-C3	8.01	1.36	1.22
2	A	500	TR9	O4-C6	7.25	1.37	1.23
2	C	500	TR9	O4-C6	6.95	1.37	1.23
2	B	500	TR9	O4-C6	6.82	1.36	1.23
2	C	500	TR9	C7-C4	-6.04	1.38	1.50
2	D	500	TR9	O4-C6	6.01	1.35	1.23
2	D	500	TR9	C7-C4	-5.83	1.38	1.50
2	A	500	TR9	C7-C4	-5.61	1.38	1.50
2	B	500	TR9	C7-C4	-5.42	1.39	1.50
2	A	500	TR9	C5-C6	-4.92	1.38	1.46
2	A	500	TR9	C1-C6	4.55	1.57	1.50
2	B	500	TR9	C5-C6	-4.32	1.39	1.46
2	C	500	TR9	C1-C6	4.00	1.56	1.50
2	D	500	TR9	C5-C6	-3.83	1.40	1.46
2	B	500	TR9	C1-C6	3.80	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	TR9	C5-C6	-3.24	1.41	1.46
2	D	500	TR9	C1-C6	2.89	1.55	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	TR9	O1-C5-C6	4.06	123.23	115.66
2	D	500	TR9	O1-C5-C6	3.50	122.20	115.66
2	A	500	TR9	O1-C5-C6	3.21	121.64	115.66
2	B	500	TR9	O1-C5-C6	3.06	121.38	115.66
2	A	500	TR9	C7-C4-C3	2.31	120.50	116.13
2	C	500	TR9	C7-C4-C3	2.12	120.13	116.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	TR9	1	0
2	B	500	TR9	1	0
2	A	500	TR9	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	67:IAS	C	68:GLY	N	4.45
1	A	67:IAS	C	68:GLY	N	4.44
1	C	67:IAS	C	68:GLY	N	4.43
1	B	67:IAS	C	68:GLY	N	4.33

## 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	418/419 (99%)	-0.46	4 (0%) 82 84	14, 26, 44, 79	0
1	B	418/419 (99%)	-0.50	4 (0%) 82 84	12, 23, 41, 83	0
1	C	418/419 (99%)	-0.32	6 (1%) 75 77	14, 28, 48, 84	0
1	D	418/419 (99%)	-0.12	10 (2%) 59 62	19, 37, 56, 85	0
All	All	1672/1676 (99%)	-0.35	24 (1%) 75 77	12, 28, 50, 85	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	419	GLU	5.7
1	B	419	GLU	5.2
1	A	419	GLU	5.0
1	B	418	GLY	4.8
1	C	418	GLY	4.2
1	D	418	GLY	4.1
1	D	419	GLU	4.0
1	A	418	GLY	3.6
1	C	329	GLU	3.5
1	D	330	ASN	3.3
1	B	329	GLU	3.3
1	D	329	GLU	3.0
1	D	219	GLU	3.0
1	D	328	PHE	2.7
1	D	216	GLU	2.6
1	D	140	GLU	2.6
1	D	277	GLU	2.4
1	A	330	ASN	2.4
1	B	330	ASN	2.4
1	C	348	GLU	2.2
1	C	358	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	148	ASN	2.1
1	D	119	ALA	2.1
1	C	349	SER	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	IAS	D	67	8/9	0.91	0.16	34,36,42,48	0
1	IAS	B	67	8/9	0.92	0.20	22,28,38,38	0
1	IAS	C	67	8/9	0.94	0.18	32,39,41,44	0
1	IAS	A	67	8/9	0.94	0.17	21,31,43,47	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	TR9	C	500	11/11	0.85	0.14	44,50,52,52	0
3	CA	C	421	1/1	0.90	0.07	50,50,50,50	0
2	TR9	A	500	11/11	0.90	0.14	24,26,29,30	0
2	TR9	B	500	11/11	0.94	0.13	19,24,28,28	0
3	CA	B	423	1/1	0.95	0.05	36,36,36,36	0
2	TR9	D	500	11/11	0.96	0.12	34,38,40,41	0
3	CA	A	420	1/1	0.96	0.04	28,28,28,28	0
3	CA	B	421	1/1	0.96	0.05	29,29,29,29	0
3	CA	D	421	1/1	0.96	0.05	34,34,34,34	0
3	CA	D	420	1/1	0.97	0.05	34,34,34,34	0
3	CA	C	420	1/1	0.97	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	420	1/1	0.98	0.08	26,26,26,26	0
3	CA	A	421	1/1	0.99	0.03	27,27,27,27	0
3	CA	B	422	1/1	0.99	0.04	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.