



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:20 pm GMT

PDB ID : 3FL8  
Title : Crystal structure of B. anthracis dihydrofolate reductase (DHFR) with RAB1, a TMP-dihydrophthalazine derivative  
Authors : Bourne, C.R.; Barrow, W.W.  
Deposited on : 2008-12-18  
Resolution : 2.29 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

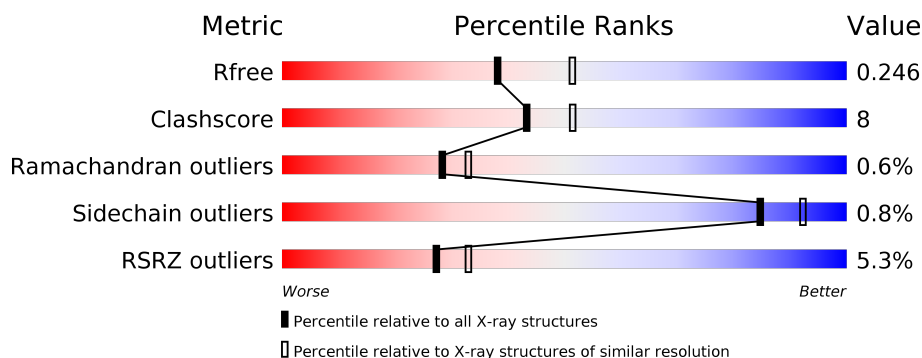
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (2.30-2.26)

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. 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	166	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	B	166	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	C	166	<div> <div>2%</div> <div>86%</div> <div>14%</div> </div>
1	D	166	<div> <div>8%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	E	166	<div> <div>5%</div> <div>85%</div> <div>15%</div> </div>
1	F	166	<div> <div>5%</div> <div>83%</div> <div>17%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	166	<div><div></div><div>5%</div><div>84%</div><div>15%</div><div></div></div>
1	H	166	<div><div></div><div>10%</div><div>81%</div><div>13%</div><div>5%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12608 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 Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1374	889	225	251	9			
1	B	166	Total	C	N	O	S	0	0	0
			1363	883	224	248	8			
1	C	166	Total	C	N	O	S	0	0	0
			1371	888	224	250	9			
1	D	166	Total	C	N	O	S	0	0	0
			1348	874	221	244	9			
1	E	166	Total	C	N	O	S	0	0	0
			1367	886	224	248	9			
1	F	166	Total	C	N	O	S	0	0	0
			1355	878	224	244	9			
1	G	166	Total	C	N	O	S	0	0	0
			1359	882	223	245	9			
1	H	157	Total	C	N	O	S	0	0	0
			1254	818	200	227	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LEU	-	EXPRESSION TAG	UNP Q81R22
A	164	VAL	-	EXPRESSION TAG	UNP Q81R22
A	165	PRO	-	EXPRESSION TAG	UNP Q81R22
A	166	ARG	-	EXPRESSION TAG	UNP Q81R22
B	163	LEU	-	EXPRESSION TAG	UNP Q81R22
B	164	VAL	-	EXPRESSION TAG	UNP Q81R22
B	165	PRO	-	EXPRESSION TAG	UNP Q81R22
B	166	ARG	-	EXPRESSION TAG	UNP Q81R22
C	163	LEU	-	EXPRESSION TAG	UNP Q81R22
C	164	VAL	-	EXPRESSION TAG	UNP Q81R22
C	165	PRO	-	EXPRESSION TAG	UNP Q81R22
C	166	ARG	-	EXPRESSION TAG	UNP Q81R22
D	163	LEU	-	EXPRESSION TAG	UNP Q81R22

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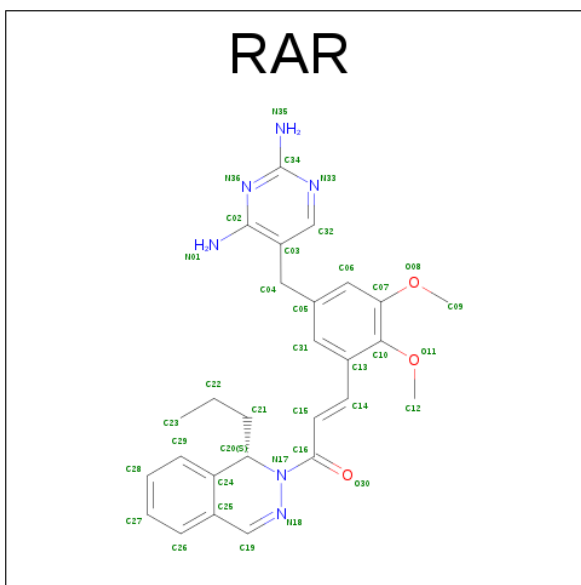
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Chain	Residue	Modelled	Actual	Comment	Reference
D	164	VAL	-	EXPRESSION TAG	UNP Q81R22
D	165	PRO	-	EXPRESSION TAG	UNP Q81R22
D	166	ARG	-	EXPRESSION TAG	UNP Q81R22
E	163	LEU	-	EXPRESSION TAG	UNP Q81R22
E	164	VAL	-	EXPRESSION TAG	UNP Q81R22
E	165	PRO	-	EXPRESSION TAG	UNP Q81R22
E	166	ARG	-	EXPRESSION TAG	UNP Q81R22
F	163	LEU	-	EXPRESSION TAG	UNP Q81R22
F	164	VAL	-	EXPRESSION TAG	UNP Q81R22
F	165	PRO	-	EXPRESSION TAG	UNP Q81R22
F	166	ARG	-	EXPRESSION TAG	UNP Q81R22
G	163	LEU	-	EXPRESSION TAG	UNP Q81R22
G	164	VAL	-	EXPRESSION TAG	UNP Q81R22
G	165	PRO	-	EXPRESSION TAG	UNP Q81R22
G	166	ARG	-	EXPRESSION TAG	UNP Q81R22
H	163	LEU	-	EXPRESSION TAG	UNP Q81R22
H	164	VAL	-	EXPRESSION TAG	UNP Q81R22
H	165	PRO	-	EXPRESSION TAG	UNP Q81R22
H	166	ARG	-	EXPRESSION TAG	UNP Q81R22

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is 5-(3,4-DIMETHOXY-5-{(1E)-3-OXO-3-[(1S)-1-PROPYLPHTHALAZIN-2(1H)-YL]PROP-1-EN-1-YL}BENZYL)PYRIMIDINE-2,4-DIAMINE (three-letter code: RAR) (formula: C<sub>27</sub>H<sub>30</sub>N<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			36	27	6	3		
3	B	1	Total	C	N	O	0	0
			36	27	6	3		
3	C	1	Total	C	N	O	0	0
			36	27	6	3		
3	D	1	Total	C	N	O	0	0
			36	27	6	3		
3	E	1	Total	C	N	O	0	0
			36	27	6	3		
3	F	1	Total	C	N	O	0	0
			36	27	6	3		
3	G	1	Total	C	N	O	0	0
			36	27	6	3		
3	H	1	Total	C	N	O	0	0
			36	27	6	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	210	Total	O	0	0
			210	210		
4	B	188	Total	O	0	0
			188	188		
4	C	232	Total	O	0	0
			232	232		
4	D	187	Total	O	0	0
			187	187		

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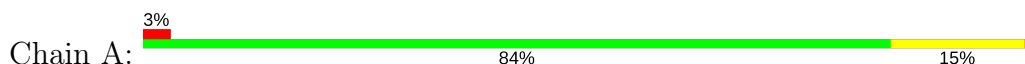
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	199	Total 199	O 199	0	0
4	F	155	Total 155	O 155	0	0
4	G	186	Total 186	O 186	0	0
4	H	164	Total 164	O 164	0	0

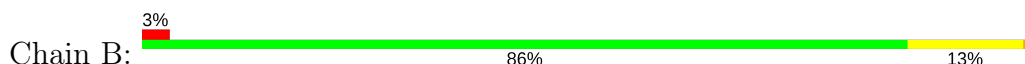
### 3 Residue-property plots [i](#)

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.

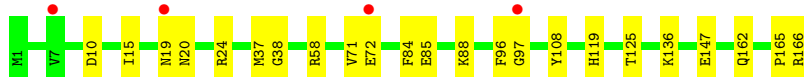
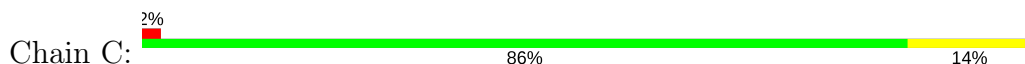
- Molecule 1: Dihydrofolate reductase



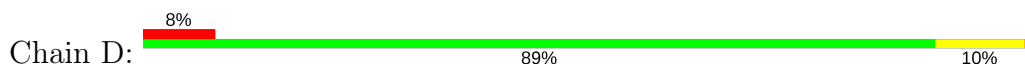
- Molecule 1: Dihydrofolate reductase



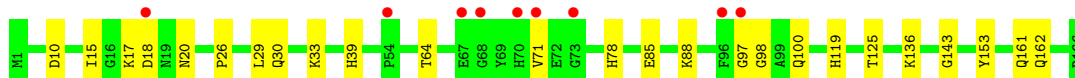
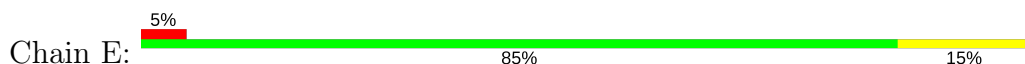
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase

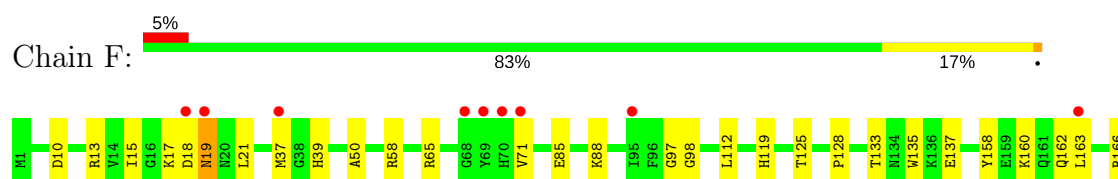


- Molecule 1: Dihydrofolate reductase

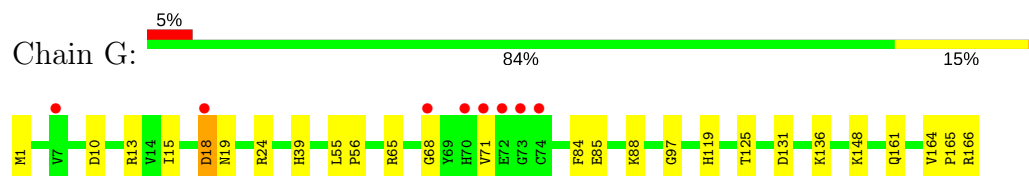


- Molecule 1: Dihydrofolate reductase

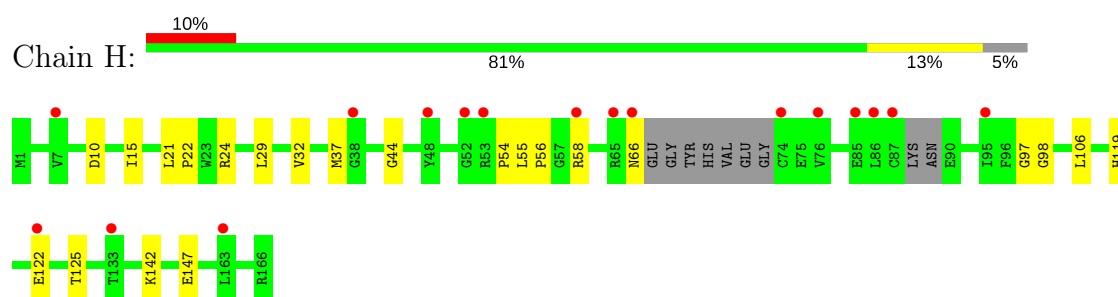




- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.18Å 135.92Å 168.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.97 – 2.29 24.97 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.97-2.29) 97.9 (24.97-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.206 , 0.254 0.198 , 0.246	Depositor DCC
$R_{free}$ test set	3529 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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 21.74 % 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 6.5836e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.41	0/1412	0.54	0/1911
1	B	0.39	0/1401	0.54	1/1898 (0.1%)
1	C	0.43	0/1409	0.56	0/1907
1	D	0.42	0/1386	0.53	1/1879 (0.1%)
1	E	0.42	0/1405	0.53	1/1902 (0.1%)
1	F	2.05	1/1393 (0.1%)	0.55	1/1887 (0.1%)
1	G	1.93	1/1397 (0.1%)	0.54	0/1892
1	H	0.42	0/1286	0.56	2/1742 (0.1%)
All	All	1.06	2/11089 (0.0%)	0.54	6/15018 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	ARG	CA-CB	74.97	3.18	1.53
1	G	166	ARG	CA-CB	70.61	3.09	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	54	PRO	N-CA-CB	6.56	111.17	103.30
1	H	56	PRO	N-CA-CB	5.88	110.36	103.30
1	E	98	GLY	N-CA-C	-5.33	99.78	113.10
1	B	98	GLY	N-CA-C	-5.19	100.13	113.10
1	F	98	GLY	N-CA-C	-5.17	100.18	113.10
1	D	98	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	GLY	Peptide
1	B	97	GLY	Peptide
1	C	165	PRO	Peptide
1	C	97	GLY	Peptide
1	D	97	GLY	Peptide
1	E	97	GLY	Peptide
1	F	97	GLY	Peptide
1	G	97	GLY	Peptide
1	H	97	GLY	Peptide

## 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	1374	0	1335	23	1
1	B	1363	0	1318	19	0
1	C	1371	0	1331	26	0
1	D	1348	0	1291	17	0
1	E	1367	0	1327	14	0
1	F	1355	0	1308	22	0
1	G	1359	0	1317	16	1
1	H	1254	0	1185	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	36	0	30	5	0
3	B	36	0	30	7	0
3	C	36	0	30	9	0
3	D	36	0	30	7	0
3	E	36	0	30	4	0
3	F	36	0	30	6	0
3	G	36	0	30	4	0
3	H	36	0	30	3	0
4	A	210	0	0	8	0
4	B	188	0	0	6	0
4	C	232	0	0	11	0
4	D	187	0	0	5	0
4	E	199	0	0	8	0
4	F	155	0	0	6	0
4	G	186	0	0	5	0
4	H	164	0	0	5	0
All	All	12608	0	10652	167	1

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 8.

All (167) 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:F:162:GLN:CB	1:F:163:LEU:HA	1.71	1.17
1:A:18:ASP:O	1:A:19:ASN:HB2	1.46	1.15
3:E:200:RAR:N18	3:E:200:RAR:H14	1.74	1.02
1:A:18:ASP:OD2	4:A:913:HOH:O	1.80	0.98
3:C:200:RAR:H14	3:C:200:RAR:N18	1.75	0.98
3:B:200:RAR:N18	3:B:200:RAR:H14	1.80	0.96
3:A:200:RAR:H14	3:A:200:RAR:N18	1.82	0.94
1:A:24:ARG:NH2	1:C:88:LYS:HG2	1.86	0.91
3:G:200:RAR:H14	3:G:200:RAR:N18	1.86	0.90
1:C:136:LYS:HE2	4:C:1177:HOH:O	1.71	0.89
1:D:19:ASN:HA	4:D:1123:HOH:O	1.72	0.88
1:F:37:MET:HG3	4:F:934:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG23	4:A:692:HOH:O	1.75	0.84
1:B:88:LYS:HG2	1:H:24:ARG:NH2	1.99	0.78
3:F:200:RAR:N18	3:F:200:RAR:H14	1.98	0.78
1:C:37:MET:SD	1:H:122:GLU:OE2	2.41	0.78
1:F:137:GLU:O	1:H:142:LYS:HE3	1.85	0.76
1:D:70:HIS:HD2	4:D:1387:HOH:O	1.69	0.75
1:F:162:GLN:CB	1:F:163:LEU:CA	2.57	0.75
1:C:136:LYS:HD3	4:C:1140:HOH:O	1.88	0.73
1:C:38:GLY:HA2	4:C:610:HOH:O	1.90	0.70
1:D:29:LEU:HD22	3:D:200:RAR:H14	1.72	0.70
1:F:21:LEU:HG	3:F:200:RAR:H09A	1.73	0.70
1:A:147:GLU:OE2	1:C:108:TYR:HB3	1.92	0.69
1:C:37:MET:SD	1:H:122:GLU:OE1	2.51	0.68
3:D:200:RAR:H12B	3:D:200:RAR:O08	1.96	0.64
3:G:200:RAR:C14	3:G:200:RAR:N18	2.51	0.64
1:B:70:HIS:HB3	4:B:1076:HOH:O	1.96	0.64
1:B:136:LYS:HB2	1:B:161:GLN:OE1	1.98	0.64
1:A:18:ASP:O	1:A:19:ASN:CB	2.31	0.63
1:F:128:PRO:HB2	4:F:963:HOH:O	1.98	0.63
3:A:200:RAR:C14	3:A:200:RAR:N18	2.52	0.63
3:G:200:RAR:H22	3:G:200:RAR:C29	2.29	0.63
1:A:162:GLN:O	1:A:163:LEU:HB2	1.99	0.62
1:C:37:MET:SD	1:H:122:GLU:CD	2.77	0.62
1:A:26:PRO:HG3	4:A:528:HOH:O	2.00	0.62
1:F:162:GLN:CB	1:F:163:LEU:HD23	2.29	0.62
1:E:100:GLN:HG3	4:E:588:HOH:O	1.99	0.61
1:B:163:LEU:HA	4:B:1425:HOH:O	2.00	0.61
1:A:160:LYS:HD2	4:A:602:HOH:O	2.00	0.60
1:B:55:LEU:HD13	3:B:200:RAR:C25	2.32	0.60
1:F:58:ARG:NH1	4:F:934:HOH:O	2.35	0.60
1:D:70:HIS:HB2	4:D:1386:HOH:O	2.02	0.59
1:B:2:ILE:HG12	4:B:1402:HOH:O	2.01	0.59
1:B:39:HIS:HD2	4:B:894:HOH:O	1.85	0.59
1:E:20:ASN:OD1	4:E:931:HOH:O	2.16	0.59
1:D:72:GLU:HB2	4:D:965:HOH:O	2.02	0.59
1:D:58:ARG:CD	3:D:200:RAR:H27	2.32	0.59
1:A:19:ASN:N	4:A:629:HOH:O	2.35	0.59
3:C:200:RAR:H12B	3:C:200:RAR:O08	2.02	0.58
1:D:12:ASN:ND2	4:D:659:HOH:O	2.37	0.57
3:E:200:RAR:N18	3:E:200:RAR:C14	2.52	0.57
1:C:20:ASN:CG	4:C:1093:HOH:O	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:LYS:HB2	3:D:200:RAR:H21	1.87	0.56
1:A:39:HIS:HD2	4:A:190:HOH:O	1.88	0.56
1:E:136:LYS:HB2	1:E:161:GLN:OE1	2.05	0.56
1:H:66:ASN:HA	4:H:1159:HOH:O	2.05	0.56
1:C:72:GLU:HB2	4:C:660:HOH:O	2.04	0.55
1:E:33:LYS:HE2	4:E:1405:HOH:O	2.06	0.55
1:F:88:LYS:HG2	1:G:24:ARG:NH2	2.22	0.55
1:E:30:GLN:HG3	4:E:382:HOH:O	2.07	0.54
3:C:200:RAR:C14	3:C:200:RAR:N18	2.53	0.54
1:C:24:ARG:HD3	4:C:1144:HOH:O	2.07	0.54
1:H:29:LEU:HB3	3:H:200:RAR:H22A	1.90	0.54
1:C:58:ARG:NE	3:C:200:RAR:H27	2.23	0.53
3:F:200:RAR:N18	3:F:200:RAR:C14	2.63	0.53
1:B:108:TYR:HB3	1:H:147:GLU:OE2	2.08	0.53
1:B:55:LEU:HD13	3:B:200:RAR:C19	2.39	0.53
1:G:148:LYS:HE3	4:G:857:HOH:O	2.08	0.53
1:G:39:HIS:HE1	4:G:1090:HOH:O	1.92	0.52
1:C:96:PHE:CZ	3:C:200:RAR:H31	2.44	0.52
1:E:39:HIS:HD2	4:E:1385:HOH:O	1.92	0.52
1:A:147:GLU:HG3	1:C:84:PHE:CZ	2.45	0.51
1:A:24:ARG:CZ	1:C:88:LYS:HG2	2.40	0.51
1:F:39:HIS:HD2	4:F:883:HOH:O	1.93	0.50
1:E:29:LEU:HB3	3:E:200:RAR:H21A	1.92	0.50
1:E:26:PRO:HG3	4:E:1361:HOH:O	2.11	0.50
1:F:85:GLU:O	1:F:88:LYS:HB2	2.11	0.50
1:D:21:LEU:HG	3:D:200:RAR:H09A	1.93	0.50
1:A:17:LYS:C	1:A:19:ASN:H	2.15	0.50
1:H:44:GLY:HA3	4:H:1100:HOH:O	2.12	0.49
1:F:112:LEU:HB2	1:F:158:TYR:HB2	1.94	0.49
1:C:20:ASN:ND2	4:C:1093:HOH:O	2.44	0.49
1:B:88:LYS:HG2	1:H:24:ARG:CZ	2.42	0.49
1:A:109:VAL:O	1:A:160:LYS:HE2	2.12	0.49
1:B:89:ASN:OD1	1:H:24:ARG:NH2	2.43	0.49
1:C:162:GLN:HG2	4:C:989:HOH:O	2.13	0.49
1:G:65:ARG:HG2	4:G:1373:HOH:O	2.13	0.48
3:B:200:RAR:N18	3:B:200:RAR:C14	2.56	0.48
1:H:32:VAL:HG12	3:H:200:RAR:H19	1.95	0.48
1:F:13:ARG:NH2	4:F:247:HOH:O	2.46	0.47
3:F:200:RAR:H15	3:F:200:RAR:O11	2.14	0.47
1:G:85:GLU:O	1:G:88:LYS:HB2	2.15	0.47
1:D:58:ARG:HD2	3:D:200:RAR:H27	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LYS:O	1:F:18:ASP:HB2	2.14	0.47
1:D:18:ASP:N	1:D:124:ASP:OD2	2.47	0.47
1:D:85:GLU:O	1:D:88:LYS:HB2	2.15	0.47
1:H:58:ARG:CZ	3:H:200:RAR:H27	2.44	0.46
1:E:143:GLY:HA3	1:E:153:TYR:CE1	2.50	0.46
1:B:96:PHE:CZ	3:B:200:RAR:H31	2.51	0.46
1:A:136:LYS:HE2	4:A:1023:HOH:O	2.16	0.46
1:C:85:GLU:O	1:C:88:LYS:HB2	2.15	0.46
1:D:147:GLU:HG2	4:E:167:HOH:O	2.14	0.46
1:B:88:LYS:HG3	4:H:902:HOH:O	2.16	0.46
1:D:18:ASP:OD1	1:D:19:ASN:N	2.47	0.45
3:A:200:RAR:H23B	3:A:200:RAR:H20	1.63	0.45
1:E:85:GLU:O	1:E:88:LYS:HB2	2.16	0.45
3:F:200:RAR:O30	3:F:200:RAR:H23B	2.16	0.45
1:F:15:ILE:HG13	1:F:125:THR:HG23	1.99	0.45
1:A:37:MET:HE2	4:A:430:HOH:O	2.17	0.45
1:F:58:ARG:NE	3:F:200:RAR:H27	2.32	0.44
1:A:85:GLU:O	1:A:88:LYS:HB2	2.17	0.44
1:F:88:LYS:HB2	1:F:88:LYS:HE3	1.69	0.44
3:D:200:RAR:H20	3:D:200:RAR:H23B	1.62	0.44
1:C:15:ILE:HG13	1:C:125:THR:HG23	1.99	0.44
1:F:10:ASP:HB2	1:F:119:HIS:O	2.18	0.44
1:G:1:MET:HE1	1:G:84:PHE:CD1	2.53	0.43
3:B:200:RAR:H06	3:B:200:RAR:H09A	1.69	0.43
3:C:200:RAR:H23B	3:C:200:RAR:H20	1.37	0.43
3:E:200:RAR:H20	3:E:200:RAR:H23B	1.57	0.43
1:H:106:LEU:HD21	4:H:1501:HOH:O	2.18	0.43
1:G:1:MET:HE3	1:G:84:PHE:CE1	2.52	0.43
1:G:88:LYS:HB2	1:G:88:LYS:HE3	1.69	0.43
1:H:98:GLY:HA3	4:H:1127:HOH:O	2.18	0.43
1:B:15:ILE:HG13	1:B:125:THR:HG23	2.00	0.42
1:C:147:GLU:HB2	4:C:639:HOH:O	2.19	0.42
1:G:10:ASP:HB2	1:G:119:HIS:O	2.19	0.42
3:G:200:RAR:C12	3:G:200:RAR:O08	2.67	0.42
1:A:55:LEU:HB3	3:A:200:RAR:C27	2.49	0.42
1:C:96:PHE:HZ	3:C:200:RAR:H31	1.85	0.42
1:D:97:GLY:HA2	1:D:102:TYR:CZ	2.55	0.42
1:A:164:VAL:HA	1:A:165:PRO:HD2	1.85	0.42
1:C:58:ARG:CD	3:C:200:RAR:H27	2.50	0.42
1:D:88:LYS:HE3	1:D:88:LYS:HB2	1.71	0.42
1:F:135:TRP:CH2	1:F:160:LYS:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ARG:NH2	4:F:537:HOH:O	2.53	0.42
1:G:164:VAL:HA	1:G:165:PRO:HD3	1.90	0.42
1:F:19:ASN:O	1:F:50:ALA:HB1	2.20	0.41
1:G:1:MET:CE	1:G:84:PHE:CD1	3.03	0.41
4:E:600:HOH:O	1:H:37:MET:HE1	2.20	0.41
1:A:10:ASP:HB2	1:A:119:HIS:O	2.20	0.41
1:B:85:GLU:O	1:B:88:LYS:HB2	2.20	0.41
1:C:166:ARG:CB	4:C:1182:HOH:O	2.68	0.41
1:G:15:ILE:HG13	1:G:125:THR:HG23	2.02	0.41
1:G:55:LEU:HA	1:G:56:PRO:HD3	1.90	0.41
1:H:10:ASP:HB2	1:H:119:HIS:O	2.20	0.41
1:B:10:ASP:HB2	1:B:119:HIS:O	2.20	0.41
1:D:1:MET:HE1	1:D:84:PHE:CD1	2.56	0.41
1:H:15:ILE:HG13	1:H:125:THR:HG23	2.03	0.41
1:A:96:PHE:CZ	3:A:200:RAR:H31	2.56	0.41
1:E:10:ASP:HB2	1:E:119:HIS:O	2.21	0.41
1:E:17:LYS:O	1:E:18:ASP:HB2	2.21	0.41
1:G:136:LYS:HB2	1:G:161:GLN:OE1	2.20	0.41
1:G:13:ARG:NH2	4:G:391:HOH:O	2.53	0.41
1:H:21:LEU:HA	1:H:22:PRO:HD3	1.94	0.41
1:A:55:LEU:HA	1:A:56:PRO:HD3	1.89	0.41
1:C:10:ASP:HB2	1:C:119:HIS:O	2.21	0.41
3:C:200:RAR:C12	3:C:200:RAR:O08	2.67	0.41
1:G:68:GLY:HA2	4:G:917:HOH:O	2.21	0.41
1:B:163:LEU:HD12	1:B:163:LEU:H	1.86	0.40
1:B:17:LYS:HG2	4:B:1204:HOH:O	2.21	0.40
3:B:200:RAR:H12B	4:B:904:HOH:O	2.20	0.40
1:C:19:ASN:CB	4:C:1093:HOH:O	2.70	0.40
1:E:15:ILE:HG13	1:E:125:THR:HG23	2.04	0.40
1:E:64:THR:O	1:E:78:HIS:HA	2.22	0.40
1:B:19:ASN:O	1:B:50:ALA:HB1	2.20	0.40
1:C:72:GLU:OE2	1:F:133:THR:HG21	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE2	1:G:131:ASP:OD1[1_655]	1.89	0.31

## 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	164/166 (99%)	158 (96%)	5 (3%)	1 (1%)	28	33
1	B	164/166 (99%)	158 (96%)	4 (2%)	2 (1%)	15	15
1	C	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	D	164/166 (99%)	160 (98%)	3 (2%)	1 (1%)	28	33
1	E	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
1	F	164/166 (99%)	157 (96%)	6 (4%)	1 (1%)	28	33
1	G	164/166 (99%)	158 (96%)	4 (2%)	2 (1%)	15	15
1	H	151/166 (91%)	144 (95%)	6 (4%)	1 (1%)	25	29
All	All	1299/1328 (98%)	1253 (96%)	38 (3%)	8 (1%)	28	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	19	ASN
1	A	19	ASN
1	B	18	ASP
1	D	18	ASP
1	G	18	ASP
1	B	19	ASN
1	H	55	LEU
1	G	19	ASN

### 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	149/150 (99%)	148 (99%)	1 (1%)	87	93
1	B	146/150 (97%)	145 (99%)	1 (1%)	87	93
1	C	148/150 (99%)	147 (99%)	1 (1%)	87	93
1	D	142/150 (95%)	141 (99%)	1 (1%)	87	93
1	E	147/150 (98%)	145 (99%)	2 (1%)	71	83
1	F	144/150 (96%)	143 (99%)	1 (1%)	87	93
1	G	145/150 (97%)	143 (99%)	2 (1%)	71	83
1	H	129/150 (86%)	129 (100%)	0	100	100
All	All	1150/1200 (96%)	1141 (99%)	9 (1%)	85	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	B	71	VAL
1	C	71	VAL
1	D	71	VAL
1	E	71	VAL
1	E	162	GLN
1	F	71	VAL
1	G	18	ASP
1	G	71	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	B	39	HIS
1	C	39	HIS
1	C	70	HIS
1	D	39	HIS
1	E	20	ASN
1	E	30	GLN
1	E	39	HIS
1	F	30	GLN
1	F	39	HIS
1	G	39	HIS

### 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 ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	RAR	A	200	-	38,39,39	5.24	28 (73%)	46,54,54	3.03	16 (34%)
3	RAR	B	200	-	38,39,39	5.24	28 (73%)	46,54,54	2.80	22 (47%)
3	RAR	C	200	-	38,39,39	5.26	28 (73%)	46,54,54	2.88	18 (39%)
3	RAR	D	200	-	38,39,39	5.36	28 (73%)	46,54,54	2.73	22 (47%)
3	RAR	E	200	-	38,39,39	5.20	28 (73%)	46,54,54	3.23	21 (45%)
3	RAR	F	200	-	38,39,39	5.22	27 (71%)	46,54,54	2.69	15 (32%)
3	RAR	G	200	-	38,39,39	5.24	28 (73%)	46,54,54	2.85	17 (36%)
3	RAR	H	200	-	38,39,39	5.17	28 (73%)	46,54,54	2.77	21 (45%)

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	RAR	A	200	-	-	0/19/33/33	0/3/4/4
3	RAR	B	200	-	-	0/19/33/33	0/3/4/4
3	RAR	C	200	-	-	0/19/33/33	0/3/4/4
3	RAR	D	200	-	-	0/19/33/33	0/3/4/4
3	RAR	E	200	-	-	0/19/33/33	0/3/4/4
3	RAR	F	200	-	-	0/19/33/33	0/3/4/4
3	RAR	G	200	-	-	0/19/33/33	0/3/4/4
3	RAR	H	200	-	-	0/19/33/33	0/3/4/4

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	RAR	O30-C16	-3.69	1.15	1.23
3	F	200	RAR	O30-C16	-3.69	1.15	1.23
3	H	200	RAR	O30-C16	-3.68	1.15	1.23
3	B	200	RAR	O30-C16	-3.68	1.15	1.23
3	E	200	RAR	O30-C16	-3.67	1.15	1.23
3	G	200	RAR	O30-C16	-3.44	1.16	1.23
3	D	200	RAR	O30-C16	-3.37	1.16	1.23
3	A	200	RAR	O30-C16	-3.34	1.16	1.23
3	H	200	RAR	O08-C09	-2.13	1.36	1.42
3	D	200	RAR	C15-C16	2.03	1.51	1.48
3	C	200	RAR	C15-C16	2.10	1.51	1.48
3	A	200	RAR	C15-C16	2.13	1.51	1.48
3	E	200	RAR	C15-C16	2.18	1.51	1.48
3	E	200	RAR	C25-C19	2.29	1.48	1.44
3	G	200	RAR	C15-C16	2.30	1.52	1.48
3	H	200	RAR	C16-N17	2.42	1.40	1.35
3	E	200	RAR	C03-C02	2.46	1.48	1.42
3	B	200	RAR	C15-C16	2.49	1.52	1.48
3	D	200	RAR	C03-C02	2.54	1.48	1.42
3	B	200	RAR	C03-C02	2.62	1.49	1.42
3	A	200	RAR	C25-C19	2.62	1.48	1.44
3	G	200	RAR	C25-C19	2.66	1.48	1.44
3	C	200	RAR	C03-C02	2.73	1.49	1.42
3	H	200	RAR	C34-N35	2.73	1.39	1.34
3	F	200	RAR	C34-N35	2.76	1.39	1.34
3	H	200	RAR	C25-C19	2.76	1.48	1.44
3	F	200	RAR	C03-C02	2.79	1.49	1.42
3	E	200	RAR	C34-N35	2.80	1.39	1.34
3	C	200	RAR	C34-N35	2.85	1.39	1.34
3	A	200	RAR	C34-N35	2.87	1.39	1.34
3	H	200	RAR	C13-C14	2.90	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	200	RAR	C03-C02	2.92	1.49	1.42
3	B	200	RAR	C25-C19	2.93	1.49	1.44
3	G	200	RAR	C03-C02	2.94	1.49	1.42
3	F	200	RAR	C32-N33	2.96	1.40	1.34
3	H	200	RAR	C03-C02	2.98	1.49	1.42
3	F	200	RAR	C25-C19	2.99	1.49	1.44
3	D	200	RAR	C34-N35	3.09	1.40	1.34
3	C	200	RAR	C25-C19	3.14	1.49	1.44
3	E	200	RAR	C32-N33	3.15	1.41	1.34
3	C	200	RAR	C32-N33	3.24	1.41	1.34
3	A	200	RAR	C32-N33	3.24	1.41	1.34
3	G	200	RAR	C34-N35	3.27	1.40	1.34
3	B	200	RAR	C32-N33	3.28	1.41	1.34
3	D	200	RAR	C25-C19	3.31	1.49	1.44
3	B	200	RAR	C34-N35	3.33	1.40	1.34
3	F	200	RAR	C13-C14	3.43	1.52	1.47
3	E	200	RAR	C13-C14	3.45	1.52	1.47
3	D	200	RAR	C32-N33	3.48	1.41	1.34
3	H	200	RAR	C32-N33	3.52	1.42	1.34
3	G	200	RAR	C32-N33	3.53	1.42	1.34
3	D	200	RAR	C16-N17	3.62	1.42	1.35
3	D	200	RAR	N17-N18	3.66	1.43	1.37
3	G	200	RAR	N17-N18	3.71	1.43	1.37
3	C	200	RAR	N17-N18	3.71	1.43	1.37
3	G	200	RAR	C13-C14	3.80	1.53	1.47
3	A	200	RAR	C16-N17	3.81	1.42	1.35
3	B	200	RAR	N17-N18	3.89	1.43	1.37
3	B	200	RAR	C13-C14	3.97	1.53	1.47
3	A	200	RAR	N17-N18	3.98	1.43	1.37
3	G	200	RAR	C16-N17	4.08	1.42	1.35
3	F	200	RAR	N17-N18	4.10	1.43	1.37
3	F	200	RAR	C16-N17	4.11	1.42	1.35
3	H	200	RAR	N17-N18	4.13	1.43	1.37
3	A	200	RAR	C13-C14	4.17	1.53	1.47
3	C	200	RAR	C13-C14	4.17	1.53	1.47
3	B	200	RAR	C16-N17	4.19	1.43	1.35
3	F	200	RAR	C21-C20	4.27	1.58	1.53
3	E	200	RAR	C02-N36	4.27	1.41	1.35
3	C	200	RAR	C16-N17	4.32	1.43	1.35
3	E	200	RAR	N17-N18	4.33	1.44	1.37
3	B	200	RAR	C21-C20	4.35	1.58	1.53
3	F	200	RAR	C02-N36	4.38	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	RAR	C32-C03	4.40	1.47	1.37
3	E	200	RAR	C32-C03	4.47	1.47	1.37
3	E	200	RAR	C16-N17	4.49	1.43	1.35
3	A	200	RAR	C27-C28	4.51	1.48	1.38
3	H	200	RAR	C21-C20	4.51	1.59	1.53
3	A	200	RAR	C24-C20	4.53	1.57	1.52
3	G	200	RAR	C27-C28	4.53	1.49	1.38
3	A	200	RAR	C32-C03	4.53	1.47	1.37
3	H	200	RAR	C32-C03	4.54	1.47	1.37
3	E	200	RAR	C34-N36	4.57	1.43	1.35
3	H	200	RAR	C27-C28	4.61	1.49	1.38
3	B	200	RAR	C32-C03	4.63	1.47	1.37
3	B	200	RAR	C27-C28	4.67	1.49	1.38
3	D	200	RAR	C13-C14	4.73	1.54	1.47
3	G	200	RAR	C02-N36	4.73	1.42	1.35
3	C	200	RAR	C27-C28	4.75	1.49	1.38
3	G	200	RAR	C25-C24	4.75	1.46	1.40
3	C	200	RAR	C34-N36	4.77	1.44	1.35
3	F	200	RAR	C32-C03	4.77	1.47	1.37
3	F	200	RAR	C34-N36	4.78	1.44	1.35
3	F	200	RAR	C27-C28	4.78	1.49	1.38
3	G	200	RAR	C32-C03	4.78	1.47	1.37
3	D	200	RAR	C27-C28	4.80	1.49	1.38
3	A	200	RAR	C25-C24	4.80	1.46	1.40
3	C	200	RAR	C02-N36	4.81	1.42	1.35
3	G	200	RAR	C21-C20	4.83	1.59	1.53
3	D	200	RAR	C32-C03	4.83	1.48	1.37
3	E	200	RAR	C27-C28	4.84	1.49	1.38
3	F	200	RAR	C24-C20	4.85	1.57	1.52
3	D	200	RAR	C02-N36	4.85	1.42	1.35
3	H	200	RAR	C34-N36	4.85	1.44	1.35
3	A	200	RAR	C34-N36	4.87	1.44	1.35
3	H	200	RAR	C02-N36	4.95	1.42	1.35
3	C	200	RAR	C25-C24	4.98	1.46	1.40
3	D	200	RAR	C21-C20	5.01	1.59	1.53
3	C	200	RAR	C21-C20	5.08	1.59	1.53
3	B	200	RAR	C24-C20	5.11	1.58	1.52
3	G	200	RAR	C24-C20	5.12	1.58	1.52
3	D	200	RAR	C24-C20	5.12	1.58	1.52
3	G	200	RAR	C34-N36	5.13	1.44	1.35
3	E	200	RAR	C21-C20	5.14	1.59	1.53
3	D	200	RAR	C34-N36	5.14	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	200	RAR	C02-N36	5.18	1.42	1.35
3	E	200	RAR	C25-C24	5.18	1.46	1.40
3	A	200	RAR	C21-C20	5.18	1.59	1.53
3	H	200	RAR	C07-C10	5.38	1.52	1.40
3	E	200	RAR	C24-C20	5.39	1.58	1.52
3	A	200	RAR	C28-C29	5.40	1.49	1.38
3	B	200	RAR	C34-N36	5.43	1.45	1.35
3	C	200	RAR	C24-C20	5.43	1.58	1.52
3	F	200	RAR	C25-C24	5.50	1.47	1.40
3	D	200	RAR	C25-C24	5.53	1.47	1.40
3	B	200	RAR	C25-C24	5.57	1.47	1.40
3	H	200	RAR	C28-C29	5.61	1.49	1.38
3	H	200	RAR	C24-C20	5.62	1.58	1.52
3	A	200	RAR	C02-N36	5.63	1.43	1.35
3	G	200	RAR	C28-C29	5.66	1.49	1.38
3	C	200	RAR	C28-C29	5.79	1.50	1.38
3	B	200	RAR	C28-C29	5.82	1.50	1.38
3	E	200	RAR	C07-C10	5.82	1.53	1.40
3	C	200	RAR	C06-C07	5.87	1.49	1.38
3	E	200	RAR	C06-C07	5.89	1.49	1.38
3	D	200	RAR	C06-C07	5.92	1.49	1.38
3	D	200	RAR	C28-C29	5.94	1.50	1.38
3	E	200	RAR	C28-C29	5.94	1.50	1.38
3	H	200	RAR	C25-C24	5.95	1.47	1.40
3	D	200	RAR	C07-C10	5.98	1.53	1.40
3	A	200	RAR	C07-C10	6.01	1.53	1.40
3	H	200	RAR	C06-C07	6.06	1.50	1.38
3	F	200	RAR	C28-C29	6.06	1.50	1.38
3	B	200	RAR	C06-C07	6.06	1.50	1.38
3	A	200	RAR	C27-C26	6.08	1.50	1.38
3	G	200	RAR	C07-C10	6.14	1.53	1.40
3	B	200	RAR	C07-C10	6.14	1.53	1.40
3	G	200	RAR	C27-C26	6.15	1.50	1.38
3	F	200	RAR	C06-C07	6.26	1.50	1.38
3	G	200	RAR	C06-C07	6.30	1.50	1.38
3	C	200	RAR	C07-C10	6.31	1.54	1.40
3	H	200	RAR	C13-C10	6.31	1.53	1.41
3	C	200	RAR	C27-C26	6.35	1.51	1.38
3	B	200	RAR	C27-C26	6.35	1.51	1.38
3	F	200	RAR	C07-C10	6.37	1.54	1.40
3	B	200	RAR	C31-C13	6.38	1.52	1.40
3	D	200	RAR	C27-C26	6.44	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	200	RAR	C27-C26	6.45	1.51	1.38
3	E	200	RAR	C27-C26	6.46	1.51	1.38
3	F	200	RAR	C31-C13	6.48	1.52	1.40
3	F	200	RAR	C27-C26	6.49	1.51	1.38
3	A	200	RAR	C06-C07	6.55	1.51	1.38
3	H	200	RAR	C31-C13	6.59	1.52	1.40
3	C	200	RAR	C31-C13	6.72	1.52	1.40
3	F	200	RAR	C13-C10	6.75	1.54	1.41
3	G	200	RAR	C31-C13	6.77	1.52	1.40
3	E	200	RAR	C31-C13	6.78	1.52	1.40
3	A	200	RAR	C26-C25	6.80	1.53	1.41
3	C	200	RAR	C26-C25	6.86	1.53	1.41
3	G	200	RAR	C26-C25	6.86	1.53	1.41
3	D	200	RAR	C31-C13	6.90	1.52	1.40
3	H	200	RAR	C26-C25	6.94	1.53	1.41
3	E	200	RAR	C26-C25	6.98	1.54	1.41
3	A	200	RAR	C31-C13	6.98	1.53	1.40
3	B	200	RAR	C13-C10	6.99	1.54	1.41
3	B	200	RAR	C26-C25	7.09	1.54	1.41
3	E	200	RAR	C13-C10	7.11	1.55	1.41
3	G	200	RAR	C13-C10	7.27	1.55	1.41
3	F	200	RAR	C26-C25	7.37	1.54	1.41
3	C	200	RAR	C13-C10	7.38	1.55	1.41
3	D	200	RAR	C13-C10	7.38	1.55	1.41
3	A	200	RAR	C13-C10	7.39	1.55	1.41
3	D	200	RAR	C26-C25	7.49	1.54	1.41
3	C	200	RAR	C06-C05	7.91	1.53	1.39
3	G	200	RAR	C31-C05	7.97	1.53	1.39
3	E	200	RAR	C06-C05	8.00	1.53	1.39
3	B	200	RAR	C31-C05	8.04	1.53	1.39
3	C	200	RAR	C31-C05	8.04	1.53	1.39
3	E	200	RAR	C31-C05	8.13	1.53	1.39
3	H	200	RAR	C31-C05	8.14	1.53	1.39
3	F	200	RAR	C31-C05	8.15	1.53	1.39
3	B	200	RAR	C06-C05	8.20	1.53	1.39
3	D	200	RAR	C06-C05	8.21	1.53	1.39
3	D	200	RAR	C31-C05	8.38	1.54	1.39
3	F	200	RAR	C06-C05	8.42	1.54	1.39
3	A	200	RAR	C31-C05	8.47	1.54	1.39
3	G	200	RAR	C06-C05	8.51	1.54	1.39
3	H	200	RAR	C06-C05	8.59	1.54	1.39
3	A	200	RAR	C06-C05	8.77	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	200	RAR	C34-N33	9.92	1.49	1.35
3	B	200	RAR	C34-N33	10.00	1.49	1.35
3	E	200	RAR	C34-N33	10.07	1.49	1.35
3	C	200	RAR	C34-N33	10.11	1.49	1.35
3	H	200	RAR	C34-N33	10.18	1.49	1.35
3	A	200	RAR	C29-C24	10.40	1.53	1.39
3	A	200	RAR	C19-N18	10.41	1.41	1.29
3	G	200	RAR	C34-N33	10.52	1.50	1.35
3	H	200	RAR	C19-N18	10.56	1.41	1.29
3	A	200	RAR	C34-N33	10.59	1.50	1.35
3	B	200	RAR	C19-N18	10.67	1.41	1.29
3	G	200	RAR	C19-N18	10.71	1.41	1.29
3	E	200	RAR	C19-N18	10.72	1.41	1.29
3	D	200	RAR	C34-N33	10.73	1.50	1.35
3	F	200	RAR	C29-C24	10.79	1.53	1.39
3	E	200	RAR	C29-C24	10.89	1.53	1.39
3	B	200	RAR	C29-C24	10.90	1.53	1.39
3	C	200	RAR	C19-N18	10.91	1.41	1.29
3	G	200	RAR	C29-C24	10.93	1.53	1.39
3	D	200	RAR	C29-C24	10.97	1.54	1.39
3	F	200	RAR	C19-N18	10.99	1.41	1.29
3	H	200	RAR	C29-C24	11.01	1.54	1.39
3	D	200	RAR	C19-N18	11.09	1.42	1.29
3	C	200	RAR	C29-C24	11.29	1.54	1.39

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	200	RAR	C25-C19-N18	-11.98	111.02	125.75
3	E	200	RAR	C25-C19-N18	-11.02	112.21	125.75
3	G	200	RAR	C25-C19-N18	-9.04	114.64	125.75
3	C	200	RAR	C25-C19-N18	-8.23	115.63	125.75
3	F	200	RAR	C25-C19-N18	-8.08	115.82	125.75
3	B	200	RAR	N33-C34-N36	-7.75	117.69	125.82
3	G	200	RAR	N33-C34-N36	-7.67	117.78	125.82
3	A	200	RAR	N33-C34-N36	-7.62	117.83	125.82
3	E	200	RAR	N33-C34-N36	-7.52	117.94	125.82
3	H	200	RAR	C25-C19-N18	-7.51	116.52	125.75
3	C	200	RAR	N33-C34-N36	-7.31	118.16	125.82
3	F	200	RAR	N33-C34-N36	-7.25	118.22	125.82
3	H	200	RAR	N33-C34-N36	-7.23	118.24	125.82
3	D	200	RAR	N33-C34-N36	-6.93	118.55	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	200	RAR	C25-C19-N18	-6.63	117.60	125.75
3	C	200	RAR	O08-C07-C06	-6.21	113.69	124.17
3	B	200	RAR	O08-C07-C06	-6.04	113.98	124.17
3	B	200	RAR	C25-C19-N18	-5.86	118.54	125.75
3	F	200	RAR	O08-C07-C06	-5.70	114.56	124.17
3	E	200	RAR	O08-C07-C06	-5.48	114.93	124.17
3	G	200	RAR	O08-C07-C06	-5.45	114.98	124.17
3	D	200	RAR	O08-C07-C06	-5.23	115.36	124.17
3	E	200	RAR	C04-C03-C02	-4.91	116.05	122.28
3	D	200	RAR	C04-C03-C02	-4.43	116.67	122.28
3	E	200	RAR	C03-C32-N33	-4.31	116.58	123.87
3	B	200	RAR	C04-C03-C02	-4.28	116.86	122.28
3	A	200	RAR	O08-C07-C06	-4.27	116.98	124.17
3	A	200	RAR	C28-C29-C24	-4.18	115.64	121.01
3	H	200	RAR	O08-C07-C06	-4.07	117.30	124.17
3	C	200	RAR	C04-C03-C02	-4.05	117.15	122.28
3	E	200	RAR	C28-C29-C24	-3.97	115.92	121.01
3	H	200	RAR	C04-C03-C02	-3.95	117.27	122.28
3	E	200	RAR	C09-O08-C07	-3.95	111.85	117.54
3	C	200	RAR	C03-C32-N33	-3.93	117.22	123.87
3	F	200	RAR	C28-C29-C24	-3.58	116.42	121.01
3	D	200	RAR	C03-C32-N33	-3.57	117.83	123.87
3	A	200	RAR	C03-C32-N33	-3.53	117.90	123.87
3	H	200	RAR	C03-C32-N33	-3.52	117.91	123.87
3	G	200	RAR	C04-C03-C02	-3.51	117.84	122.28
3	H	200	RAR	C16-N17-N18	-3.48	112.75	117.70
3	H	200	RAR	C09-O08-C07	-3.45	112.57	117.54
3	D	200	RAR	C28-C29-C24	-3.37	116.69	121.01
3	A	200	RAR	C03-C02-N01	-3.31	117.41	122.22
3	C	200	RAR	C28-C29-C24	-3.23	116.86	121.01
3	A	200	RAR	C27-C26-C25	-3.18	116.09	121.00
3	D	200	RAR	C03-C02-N01	-3.15	117.64	122.22
3	B	200	RAR	C28-C29-C24	-3.13	117.00	121.01
3	F	200	RAR	C09-O08-C07	-3.11	113.06	117.54
3	B	200	RAR	C09-O08-C07	-3.09	113.08	117.54
3	E	200	RAR	C27-C26-C25	-3.05	116.30	121.00
3	G	200	RAR	C28-C29-C24	-3.04	117.11	121.01
3	G	200	RAR	C03-C32-N33	-2.98	118.83	123.87
3	B	200	RAR	C03-C02-N01	-2.97	117.90	122.22
3	D	200	RAR	O11-C10-C07	-2.96	115.91	120.12
3	G	200	RAR	C09-O08-C07	-2.93	113.32	117.54
3	A	200	RAR	O11-C10-C07	-2.92	115.97	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	200	RAR	C13-C31-C05	-2.90	118.89	122.29
3	H	200	RAR	C28-C29-C24	-2.89	117.30	121.01
3	E	200	RAR	O11-C10-C07	-2.88	116.03	120.12
3	F	200	RAR	C13-C14-C15	-2.85	121.32	126.90
3	E	200	RAR	C03-C02-N01	-2.83	118.10	122.22
3	B	200	RAR	C03-C32-N33	-2.77	119.18	123.87
3	C	200	RAR	C09-O08-C07	-2.71	113.64	117.54
3	F	200	RAR	C03-C32-N33	-2.70	119.31	123.87
3	E	200	RAR	C13-C31-C05	-2.66	119.17	122.29
3	F	200	RAR	C04-C03-C02	-2.66	118.91	122.28
3	H	200	RAR	C13-C14-C15	-2.65	121.71	126.90
3	H	200	RAR	C27-C26-C25	-2.58	117.02	121.00
3	D	200	RAR	C04-C05-C06	-2.52	115.59	120.69
3	C	200	RAR	C27-C26-C25	-2.51	117.13	121.00
3	F	200	RAR	C27-C26-C25	-2.51	117.14	121.00
3	G	200	RAR	C27-C26-C25	-2.44	117.24	121.00
3	G	200	RAR	C16-N17-N18	-2.43	114.25	117.70
3	D	200	RAR	C09-O08-C07	-2.43	114.04	117.54
3	D	200	RAR	C31-C13-C10	-2.42	117.06	120.24
3	B	200	RAR	C31-C13-C10	-2.41	117.07	120.24
3	B	200	RAR	C27-C26-C25	-2.39	117.31	121.00
3	G	200	RAR	C03-C02-N01	-2.35	118.80	122.22
3	C	200	RAR	C03-C02-N01	-2.34	118.82	122.22
3	D	200	RAR	C27-C26-C25	-2.34	117.40	121.00
3	A	200	RAR	C04-C03-C02	-2.32	119.35	122.28
3	A	200	RAR	C09-O08-C07	-2.32	114.20	117.54
3	E	200	RAR	C04-C05-C06	-2.30	116.03	120.69
3	H	200	RAR	C03-C02-N01	-2.29	118.89	122.22
3	D	200	RAR	C13-C31-C05	-2.29	119.61	122.29
3	C	200	RAR	C04-C05-C06	-2.24	116.17	120.69
3	H	200	RAR	C14-C15-C16	-2.13	115.81	120.48
3	B	200	RAR	O11-C10-C07	-2.08	117.16	120.12
3	C	200	RAR	C13-C31-C05	-2.05	119.89	122.29
3	E	200	RAR	C31-C05-C06	2.01	121.85	118.96
3	D	200	RAR	N01-C02-N36	2.03	120.00	117.00
3	D	200	RAR	C34-N36-C02	2.08	119.30	116.99
3	D	200	RAR	C31-C05-C06	2.11	122.00	118.96
3	C	200	RAR	C34-N36-C02	2.13	119.36	116.99
3	B	200	RAR	C25-C24-C20	2.15	118.94	116.88
3	H	200	RAR	C04-C03-C32	2.15	124.70	121.73
3	G	200	RAR	C04-C03-C32	2.23	124.81	121.73
3	G	200	RAR	C13-C10-C07	2.27	121.36	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	200	RAR	C04-C03-C32	2.28	124.88	121.73
3	B	200	RAR	N35-C34-N36	2.30	120.91	117.24
3	B	200	RAR	N01-C02-N36	2.35	120.48	117.00
3	B	200	RAR	C24-C25-C19	2.39	119.70	117.70
3	H	200	RAR	C13-C10-C07	2.39	121.54	117.82
3	E	200	RAR	C32-C03-C02	2.39	118.86	115.68
3	E	200	RAR	C04-C03-C32	2.39	125.03	121.73
3	F	200	RAR	C13-C10-C07	2.40	121.56	117.82
3	G	200	RAR	C34-N36-C02	2.43	119.69	116.99
3	A	200	RAR	N35-C34-N36	2.49	121.21	117.24
3	H	200	RAR	C24-C25-C19	2.50	119.80	117.70
3	E	200	RAR	C13-C10-C07	2.50	121.72	117.82
3	E	200	RAR	C26-C25-C24	2.51	121.04	118.64
3	D	200	RAR	C32-C03-C02	2.52	119.03	115.68
3	C	200	RAR	C13-C10-C07	2.52	121.75	117.82
3	A	200	RAR	C13-C10-C07	2.62	121.90	117.82
3	C	200	RAR	C32-C03-C02	2.64	119.19	115.68
3	B	200	RAR	C13-C10-C07	2.77	122.14	117.82
3	G	200	RAR	C29-C24-C25	2.94	122.17	119.43
3	H	200	RAR	C25-C24-C20	2.95	119.72	116.88
3	H	200	RAR	C29-C24-C25	3.03	122.24	119.43
3	B	200	RAR	C34-N36-C02	3.07	120.40	116.99
3	B	200	RAR	C29-C24-C25	3.16	122.36	119.43
3	D	200	RAR	C13-C10-C07	3.25	122.88	117.82
3	F	200	RAR	C34-N36-C02	3.33	120.68	116.99
3	F	200	RAR	C32-N33-C34	3.47	122.32	116.27
3	D	200	RAR	C29-C24-C25	3.50	122.68	119.43
3	C	200	RAR	C29-C24-C25	3.54	122.72	119.43
3	F	200	RAR	C29-C24-C25	3.56	122.74	119.43
3	E	200	RAR	C29-C24-C25	3.61	122.79	119.43
3	A	200	RAR	N35-C34-N33	3.67	120.92	117.39
3	B	200	RAR	C32-N33-C34	3.77	122.85	116.27
3	D	200	RAR	C32-N33-C34	3.82	122.94	116.27
3	D	200	RAR	N35-C34-N33	3.94	121.17	117.39
3	G	200	RAR	C32-N33-C34	3.99	123.23	116.27
3	B	200	RAR	N35-C34-N33	4.17	121.39	117.39
3	F	200	RAR	N35-C34-N33	4.22	121.44	117.39
3	C	200	RAR	N35-C34-N33	4.29	121.50	117.39
3	H	200	RAR	C32-N33-C34	4.29	123.75	116.27
3	A	200	RAR	C29-C24-C25	4.35	123.47	119.43
3	C	200	RAR	C32-N33-C34	4.40	123.95	116.27
3	A	200	RAR	O08-C07-C10	4.59	123.29	115.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	200	RAR	C32-N33-C34	4.74	124.54	116.27
3	H	200	RAR	O08-C07-C10	4.77	123.61	115.22
3	E	200	RAR	C32-N33-C34	4.77	124.60	116.27
3	H	200	RAR	N35-C34-N33	5.06	122.25	117.39
3	G	200	RAR	N35-C34-N33	5.53	122.69	117.39
3	E	200	RAR	N35-C34-N33	5.59	122.75	117.39
3	E	200	RAR	O08-C07-C10	5.73	125.30	115.22
3	D	200	RAR	O08-C07-C10	5.80	125.42	115.22
3	B	200	RAR	O08-C07-C10	6.06	125.89	115.22
3	F	200	RAR	O08-C07-C10	6.12	126.00	115.22
3	G	200	RAR	O08-C07-C10	6.45	126.57	115.22
3	C	200	RAR	O08-C07-C10	6.64	126.91	115.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	200	RAR	5	0
3	B	200	RAR	7	0
3	C	200	RAR	9	0
3	D	200	RAR	7	0
3	E	200	RAR	4	0
3	F	200	RAR	6	0
3	G	200	RAR	4	0
3	H	200	RAR	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 ⓘ

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	166/166 (100%)	0.11	5 (3%)	51	57	11, 26, 52, 68	0
1	B	166/166 (100%)	-0.00	5 (3%)	51	57	11, 25, 49, 67	0
1	C	166/166 (100%)	0.08	4 (2%)	59	66	12, 25, 51, 61	0
1	D	166/166 (100%)	0.25	13 (7%)	14	18	12, 27, 57, 73	0
1	E	166/166 (100%)	0.16	9 (5%)	26	32	12, 27, 53, 65	0
1	F	166/166 (100%)	0.13	9 (5%)	26	32	12, 27, 50, 69	0
1	G	166/166 (100%)	0.12	8 (4%)	31	37	13, 27, 51, 64	0
1	H	157/166 (94%)	0.43	17 (10%)	6	8	12, 28, 54, 76	0
All	All	1319/1328 (99%)	0.16	70 (5%)	27	33	11, 26, 53, 76	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	74	CYS	9.2
1	H	66	ASN	5.4
1	D	166	ARG	5.4
1	H	52	GLY	4.7
1	A	18	ASP	4.6
1	E	54	PRO	3.8
1	H	163	LEU	3.8
1	H	48	TYR	3.7
1	E	18	ASP	3.5
1	G	73	GLY	3.4
1	F	71	VAL	3.4
1	F	18	ASP	3.3
1	F	37	MET	3.2
1	E	73	GLY	3.1
1	G	68	GLY	3.1
1	G	74	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	71	VAL	3.0
1	H	133	THR	2.9
1	A	37	MET	2.9
1	D	163	LEU	2.9
1	D	165	PRO	2.8
1	D	123	GLY	2.8
1	H	86	LEU	2.7
1	H	53	ARG	2.7
1	H	95	ILE	2.7
1	D	19	ASN	2.6
1	H	65	ARG	2.6
1	H	7	VAL	2.6
1	H	58	ARG	2.6
1	F	163	LEU	2.5
1	E	71	VAL	2.5
1	C	72	GLU	2.5
1	E	97	GLY	2.5
1	C	7	VAL	2.5
1	B	95	ILE	2.5
1	H	122	GLU	2.4
1	D	52	GLY	2.4
1	C	19	ASN	2.4
1	F	70	HIS	2.4
1	D	164	VAL	2.4
1	D	37	MET	2.4
1	H	76	VAL	2.4
1	D	7	VAL	2.3
1	F	19	ASN	2.3
1	E	96	PHE	2.3
1	E	70	HIS	2.3
1	G	18	ASP	2.3
1	A	162	GLN	2.3
1	D	97	GLY	2.2
1	E	67	GLU	2.2
1	G	72	GLU	2.2
1	H	85	GLU	2.2
1	B	163	LEU	2.2
1	G	70	HIS	2.2
1	A	19	ASN	2.2
1	B	122	GLU	2.2
1	B	42	ILE	2.2
1	H	38	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	7	VAL	2.2
1	E	68	GLY	2.2
1	F	95	ILE	2.2
1	D	42	ILE	2.2
1	A	97	GLY	2.2
1	C	97	GLY	2.2
1	H	87	CYS	2.1
1	D	54	PRO	2.1
1	B	18	ASP	2.1
1	F	68	GLY	2.1
1	F	69	TYR	2.1
1	D	72	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	RAR	G	200	36/36	0.86	0.20	0.70	15,35,63,66	0
3	RAR	H	200	36/36	0.88	0.19	0.23	9,37,56,64	0
3	RAR	D	200	36/36	0.87	0.21	0.14	9,35,52,64	0
3	RAR	B	200	36/36	0.91	0.17	-0.18	10,35,59,69	0
3	RAR	F	200	36/36	0.89	0.17	-0.20	12,41,56,61	0
3	RAR	C	200	36/36	0.90	0.17	-0.23	6,34,48,53	0
3	RAR	E	200	36/36	0.90	0.18	-0.26	9,34,52,54	0
3	RAR	A	200	36/36	0.90	0.17	-0.36	5,35,49,52	0
2	CA	G	300	1/1	0.99	0.08	-1.64	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	E	300	1/1	0.99	0.06	-2.30	26,26,26,26	0
2	CA	D	300	1/1	0.99	0.05	-2.34	25,25,25,25	0
2	CA	B	300	1/1	0.98	0.05	-2.68	22,22,22,22	0
2	CA	F	300	1/1	0.97	0.05	-2.98	27,27,27,27	0
2	CA	C	300	1/1	1.00	0.06	-3.43	16,16,16,16	0
2	CA	H	300	1/1	0.91	0.07	-	40,40,40,40	0
2	CA	A	300	1/1	0.97	0.05	-	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.