



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:36 PM EDT

PDB ID : 2O78  
Title : Tyrosine ammonia-lyase from *Rhodobacter sphaeroides* (His89Phe variant) complexed with cinnamic acid  
Authors : Louie, G.V.; Bowman, M.E.; Moffitt, M.C.; Baiga, T.J.; Moore, B.S.; Noel, J.P.  
Deposited on : 2006-12-10  
Resolution : 1.90 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	:	2.23.2
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)	:	2.23.2

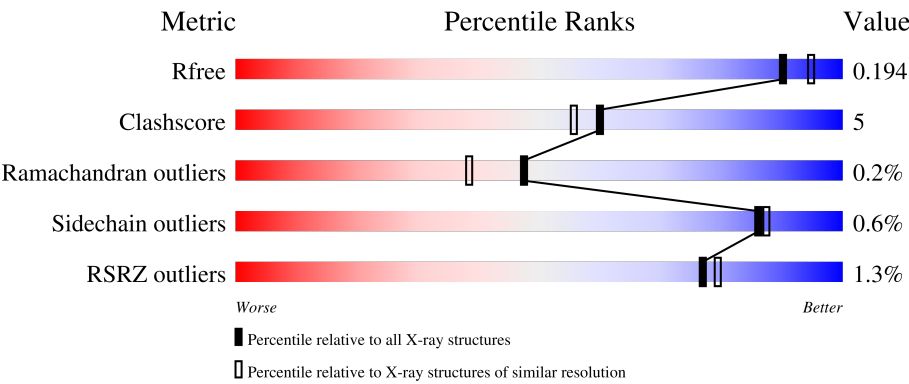
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of 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	521	<div><div>2%</div><div><div></div><div>88%</div><div>10%</div><div>.</div></div></div>
1	B	521	<div><div>%</div><div><div></div><div>88%</div><div>11%</div><div>.</div></div></div>
1	C	521	<div><div>%</div><div><div></div><div>88%</div><div>11%</div><div>.</div></div></div>
1	D	521	<div><div>2%</div><div><div></div><div>86%</div><div>12%</div><div>.</div></div></div>
1	E	521	<div><div>%</div><div><div></div><div>89%</div><div>9%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	521	<div><div></div><div>89%</div><div>9%</div><div></div></div>
1	G	521	<div><div></div><div>89%</div><div>9%</div><div></div></div>
1	H	521	<div><div>2%</div><div></div><div>86%</div><div>12%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33846 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 Putative histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			3814	2366	729	705	14			
1	B	515	Total	C	N	O	S	0	0	0
			3814	2366	729	705	14			
1	C	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	D	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	E	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	F	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	G	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	H	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			

There are 32 discrepancies between the modelled and reference sequences:

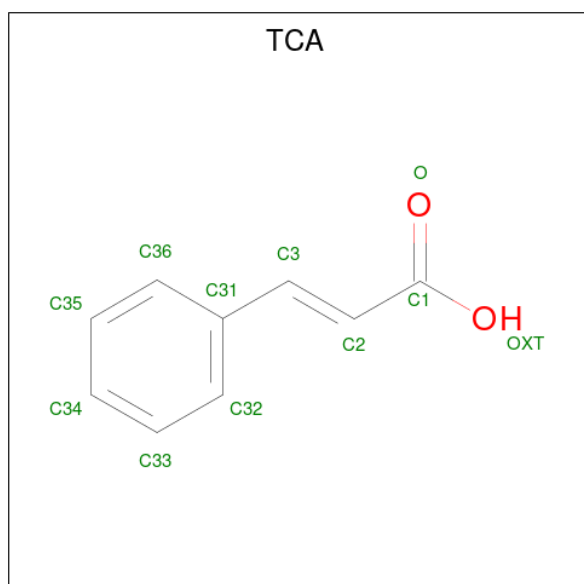
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PHE	HIS	engineered mutation	UNP Q3IWB0
A	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
B	89	PHE	HIS	engineered mutation	UNP Q3IWB0
B	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
C	89	PHE	HIS	engineered mutation	UNP Q3IWB0
C	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
D	89	PHE	HIS	engineered mutation	UNP Q3IWB0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
E	89	PHE	HIS	engineered mutation	UNP Q3IWB0
E	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
F	89	PHE	HIS	engineered mutation	UNP Q3IWB0
F	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
G	89	PHE	HIS	engineered mutation	UNP Q3IWB0
G	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
H	89	PHE	HIS	engineered mutation	UNP Q3IWB0
H	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0

- Molecule 2 is PHENYLETHYLENECARBOXYLIC ACID (three-letter code: TCA) (formula:  $C_9H_8O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	9	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 11 9 2	0	0
2	C	1	Total C O 11 9 2	0	0
2	D	1	Total C O 11 9 2	0	0
2	E	1	Total C O 11 9 2	0	0
2	F	1	Total C O 11 9 2	0	0
2	G	1	Total C O 11 9 2	0	0
2	H	1	Total C O 11 9 2	0	0

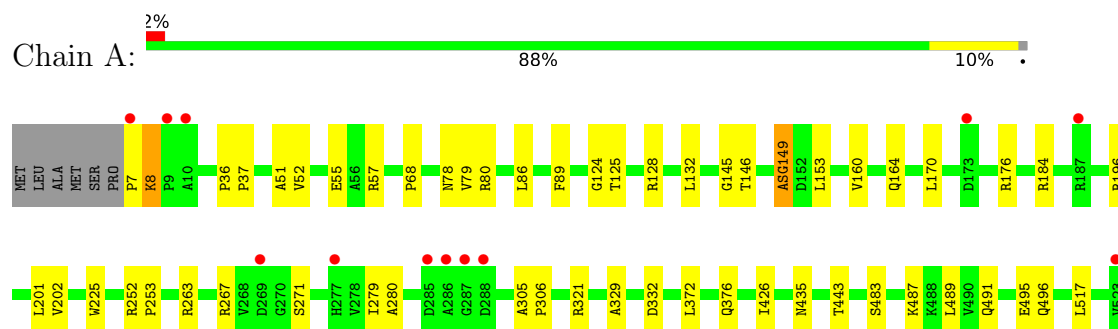
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	374	Total O 374 374	0	0
3	B	394	Total O 394 394	0	0
3	C	415	Total O 415 415	0	0
3	D	400	Total O 400 400	0	0
3	E	392	Total O 392 392	0	0
3	F	486	Total O 486 486	0	0
3	G	435	Total O 435 435	0	0
3	H	392	Total O 392 392	0	0

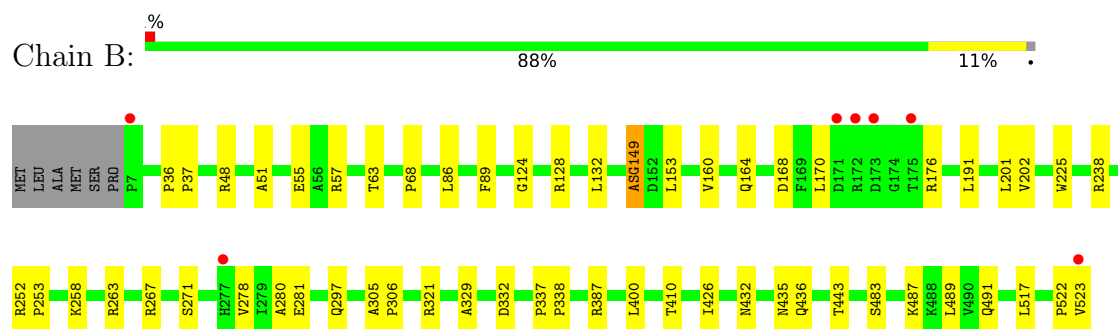
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

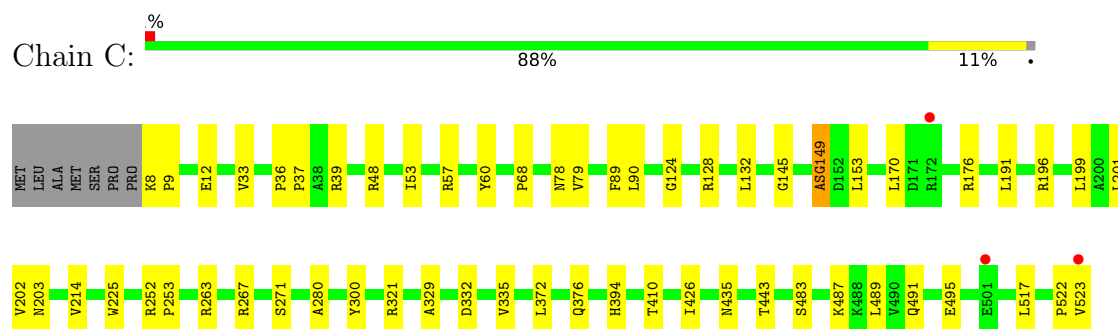
#### • Molecule 1: Putative histidine ammonia-lyase



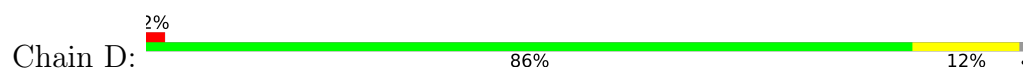
#### • Molecule 1: Putative histidine ammonia-lyase

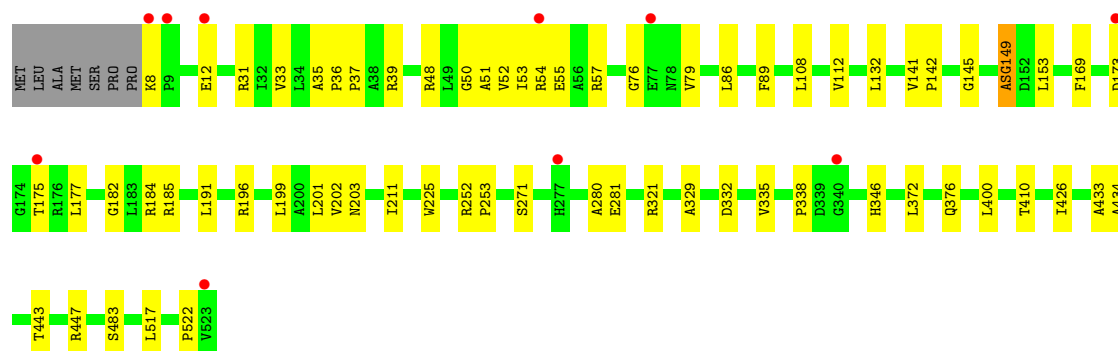


#### • Molecule 1: Putative histidine ammonia-lyase

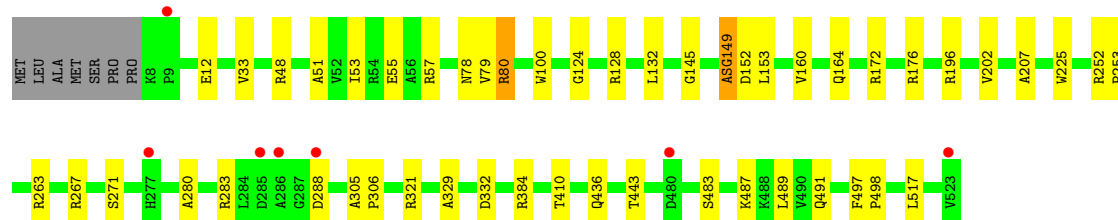
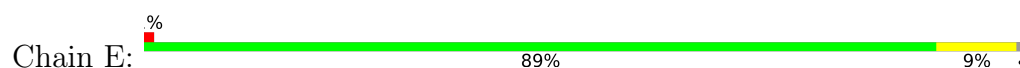


#### • Molecule 1: Putative histidine ammonia-lyase

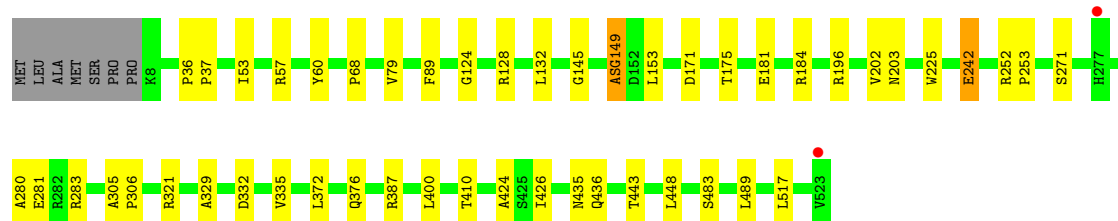




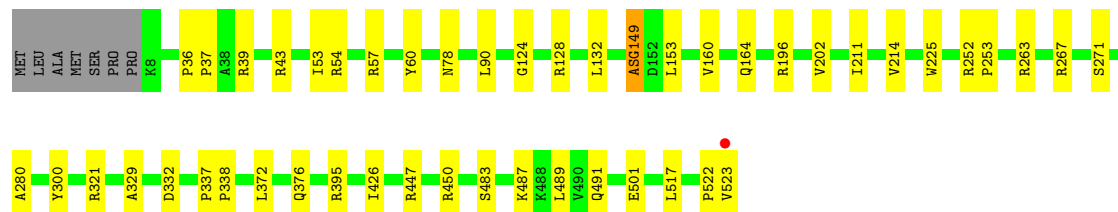
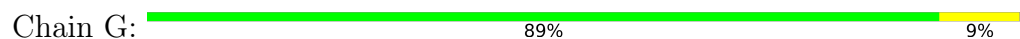
- Molecule 1: Putative histidine ammonia-lyase



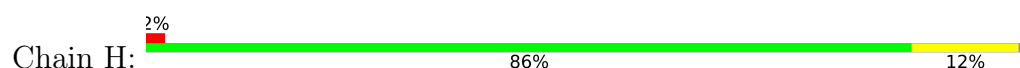
- Molecule 1: Putative histidine ammonia-lyase

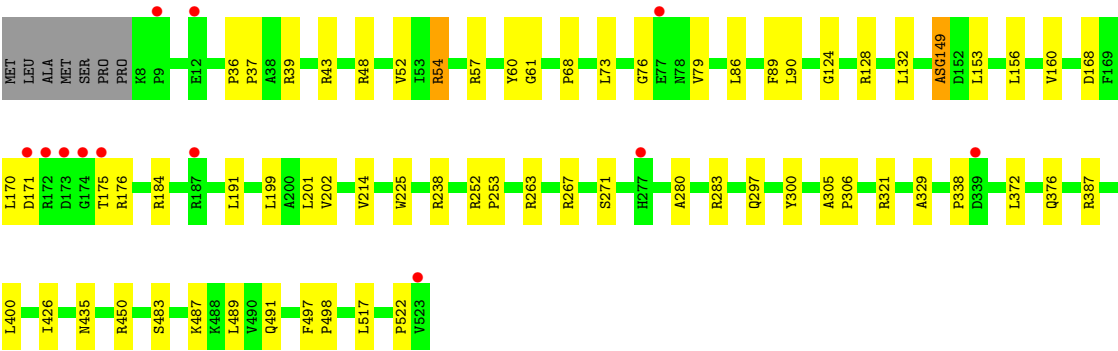


- Molecule 1: Putative histidine ammonia-lyase



- Molecule 1: Putative histidine ammonia-lyase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.59Å 155.05Å 164.04Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	500.00 – 1.90 38.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (500.00-1.90) 99.1 (38.79-1.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.172 , 0.196 0.171 , 0.194	Depositor DCC
$R_{free}$ test set	17040 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	33846	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MDO, TCA

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	0.26	0/3863	0.54	0/5254
1	B	0.27	0/3863	0.55	0/5254
1	C	0.27	0/3855	0.55	0/5243
1	D	0.27	0/3855	0.55	0/5243
1	E	0.27	0/3855	0.55	0/5243
1	F	0.28	0/3855	0.56	0/5243
1	G	0.27	0/3855	0.56	0/5243
1	H	0.27	0/3855	0.54	0/5243
All	All	0.27	0/30856	0.55	0/41966

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	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	MDO	Mainchain,Peptide
1	B	149	MDO	Mainchain,Peptide
1	C	149	MDO	Mainchain,Peptide
1	D	149	MDO	Mainchain,Peptide
1	E	149	MDO	Mainchain,Peptide
1	F	149	MDO	Mainchain,Peptide
1	G	149	MDO	Mainchain,Peptide
1	H	149	MDO	Mainchain,Peptide

## 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	3814	0	3866	39	0
1	B	3814	0	3866	39	0
1	C	3807	0	3858	41	0
1	D	3807	0	3858	43	0
1	E	3807	0	3858	36	0
1	F	3807	0	3858	34	0
1	G	3807	0	3858	31	0
1	H	3807	0	3858	52	0
2	A	11	0	7	0	0
2	B	11	0	7	0	0
2	C	11	0	7	1	0
2	D	11	0	7	0	0
2	E	11	0	7	0	0
2	F	11	0	7	1	0
2	G	11	0	7	1	0
2	H	11	0	7	1	0
3	A	374	0	0	3	0
3	B	394	0	0	4	0
3	C	415	0	0	6	0
3	D	400	0	0	4	0
3	E	392	0	0	5	0
3	F	486	0	0	5	0
3	G	435	0	0	2	0
3	H	392	0	0	4	0
All	All	33846	0	30936	280	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 5.

All (280) 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:153:LEU:HD22	1:F:202:VAL:HG12	1.60	0.82
1:D:153:LEU:HD22	1:D:202:VAL:HG12	1.67	0.77
1:B:153:LEU:HD22	1:B:202:VAL:HG12	1.67	0.77
1:A:153:LEU:HD22	1:A:202:VAL:HG12	1.71	0.72
1:B:487:LYS:O	1:B:491:GLN:HG3	1.93	0.68
1:C:153:LEU:HD22	1:C:202:VAL:HG12	1.74	0.68
1:H:153:LEU:HD22	1:H:202:VAL:HG12	1.76	0.68
1:H:61:GLY:HA3	1:H:199:LEU:HD21	1.76	0.68
1:F:171:ASP:OD2	1:F:175:THR:HB	1.95	0.67
1:H:214:VAL:HB	1:H:450:ARG:NH2	2.09	0.67
1:A:68:PRO:HG3	1:A:435:ASN:HB2	1.77	0.67
1:B:51:ALA:O	1:B:55:GLU:HG3	1.95	0.66
1:H:36:PRO:HB2	1:H:37:PRO:HD3	1.77	0.66
1:A:495:GLU:HG3	1:A:496:GLN:HE21	1.60	0.66
1:C:487:LYS:O	1:C:491:GLN:HG3	1.96	0.65
1:B:258:LYS:HD2	3:B:3514:HOH:O	1.97	0.64
1:E:153:LEU:HD22	1:E:202:VAL:HG12	1.78	0.64
1:F:68:PRO:HG3	1:F:435:ASN:HB2	1.81	0.62
1:F:283:ARG:HD3	3:F:5119:HOH:O	2.00	0.61
1:A:280:ALA:O	1:D:57:ARG:HD2	2.00	0.60
1:C:176:ARG:HD2	3:C:3285:HOH:O	1.99	0.60
1:A:271:SER:HB2	1:A:483:SER:HB3	1.84	0.60
1:G:214:VAL:HB	1:G:450:ARG:NH2	2.16	0.60
1:F:426:ILE:HD13	3:G:3571:HOH:O	2.01	0.60
1:G:271:SER:HB2	1:G:483:SER:HB3	1.83	0.60
1:E:51:ALA:O	1:E:55:GLU:HG3	2.02	0.60
1:A:80:ARG:NH1	1:A:80:ARG:HG3	2.17	0.59
1:D:173:ASP:HB2	1:D:175:THR:HG23	1.85	0.59
1:G:487:LYS:O	1:G:491:GLN:HG3	2.01	0.59
1:B:124:GLY:O	1:B:128:ARG:HG2	2.03	0.59
1:G:39:ARG:HD2	1:G:43:ARG:NH2	2.17	0.59
1:G:53:ILE:HD13	1:G:196:ARG:HD2	1.85	0.58
1:G:153:LEU:HD22	1:G:202:VAL:HG12	1.84	0.58
1:B:238:ARG:HH21	1:B:387:ARG:HH21	1.50	0.58
1:D:50:GLY:O	1:D:54:ARG:HG3	2.04	0.58
1:C:68:PRO:HG3	1:C:435:ASN:HB2	1.85	0.57
1:A:426:ILE:HD13	3:D:3398:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ASN:HB2	1:B:436:GLN:HE21	1.69	0.57
1:H:487:LYS:O	1:H:491:GLN:HG3	2.05	0.57
1:A:80:ARG:HG3	1:A:80:ARG:HH11	1.70	0.57
1:H:271:SER:HB2	1:H:483:SER:HB3	1.86	0.56
1:C:124:GLY:O	1:C:128:ARG:HG2	2.05	0.56
1:H:171:ASP:OD2	1:H:175:THR:HB	2.06	0.56
1:H:176:ARG:HD2	3:H:3379:HOH:O	2.05	0.55
1:B:57:ARG:HD2	1:C:280:ALA:O	2.07	0.55
1:F:36:PRO:HB2	1:F:37:PRO:HD3	1.89	0.55
1:F:225:TRP:CE2	1:F:517:LEU:HD22	2.42	0.55
1:H:297:GLN:HG3	3:H:2410:HOH:O	2.06	0.55
1:A:51:ALA:O	1:A:55:GLU:HG3	2.08	0.54
1:D:225:TRP:CE2	1:D:517:LEU:HD22	2.42	0.54
1:A:225:TRP:CE2	1:A:517:LEU:HD22	2.43	0.54
1:B:68:PRO:HG3	1:B:435:ASN:HB2	1.89	0.54
1:H:39:ARG:HG3	1:H:39:ARG:HH11	1.73	0.54
1:F:387:ARG:HD3	3:F:5133:HOH:O	2.06	0.54
3:A:3436:HOH:O	1:D:426:ILE:HD13	2.08	0.54
1:D:52:VAL:HG13	1:D:57:ARG:HB2	1.88	0.54
1:H:225:TRP:CE2	1:H:517:LEU:HD22	2.43	0.54
1:F:271:SER:HB2	1:F:483:SER:HB3	1.90	0.53
1:C:271:SER:HB2	1:C:483:SER:HB3	1.90	0.53
1:E:225:TRP:CE2	1:E:517:LEU:HD22	2.44	0.53
1:A:252:ARG:HA	1:D:329:ALA:HB1	1.90	0.53
1:B:191:LEU:HD21	1:B:201:LEU:CD1	2.39	0.52
1:D:36:PRO:HB2	1:D:37:PRO:HD3	1.90	0.52
1:E:487:LYS:O	1:E:491:GLN:HG3	2.10	0.52
1:E:132:LEU:C	1:E:132:LEU:HD13	2.29	0.52
1:G:372:LEU:O	1:G:376:GLN:HG3	2.09	0.52
3:F:3660:HOH:O	1:G:426:ILE:HD13	2.09	0.52
1:A:57:ARG:HD2	1:D:280:ALA:O	2.10	0.51
1:G:225:TRP:CE2	1:G:522:PRO:HD3	2.45	0.51
1:A:78:ASN:HB3	1:B:400:LEU:HD11	1.92	0.51
1:B:321:ARG:HH21	1:C:321:ARG:HH21	1.58	0.51
1:C:36:PRO:HB2	1:C:37:PRO:HD3	1.91	0.51
1:E:280:ALA:O	1:H:57:ARG:HD2	2.09	0.51
1:E:283:ARG:HD3	3:H:5485:HOH:O	2.10	0.51
1:H:214:VAL:HB	1:H:450:ARG:HH21	1.74	0.51
1:D:39:ARG:HG3	3:D:5784:HOH:O	2.10	0.51
1:B:271:SER:HB2	1:B:483:SER:HB3	1.93	0.51
1:D:12:GLU:HG2	1:D:35:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:SER:HB2	1:D:483:SER:HB3	1.93	0.51
1:E:57:ARG:HD2	1:H:280:ALA:O	2.11	0.51
1:A:372:LEU:O	1:A:376:GLN:HG3	2.10	0.51
1:C:523:VAL:OXT	1:C:523:VAL:HG12	2.11	0.51
1:E:271:SER:HB2	1:E:483:SER:HB3	1.93	0.51
1:E:263:ARG:O	1:E:267:ARG:HG2	2.10	0.51
1:A:52:VAL:HG13	1:A:57:ARG:HB2	1.92	0.51
1:E:329:ALA:HB1	1:H:252:ARG:HA	1.93	0.51
1:A:80:ARG:HH11	1:A:80:ARG:CG	2.24	0.51
1:G:124:GLY:O	1:G:128:ARG:HG2	2.11	0.51
1:G:132:LEU:HD13	1:G:132:LEU:C	2.32	0.51
1:H:283:ARG:HD3	3:H:5169:HOH:O	2.11	0.50
1:A:495:GLU:HG3	1:A:496:GLN:NE2	2.26	0.50
1:G:523:VAL:OXT	1:G:523:VAL:HG12	2.10	0.50
1:H:170:LEU:HD23	1:H:176:ARG:HG2	1.94	0.50
1:C:225:TRP:CE2	1:C:517:LEU:HD22	2.46	0.50
1:E:176:ARG:HD2	3:E:3308:HOH:O	2.11	0.50
1:H:68:PRO:HG3	1:H:435:ASN:HB2	1.94	0.50
1:F:124:GLY:O	1:F:128:ARG:HG2	2.12	0.50
1:B:329:ALA:HB1	1:C:252:ARG:HA	1.94	0.49
1:C:48:ARG:HH11	1:C:48:ARG:HG2	1.77	0.49
1:H:132:LEU:C	1:H:132:LEU:HD13	2.32	0.49
1:E:53:ILE:HD13	1:E:196:ARG:HD2	1.94	0.49
1:E:124:GLY:O	1:E:128:ARG:HG2	2.12	0.49
1:G:54:ARG:HD2	3:G:2686:HOH:O	2.12	0.49
1:H:124:GLY:O	1:H:128:ARG:HG2	2.12	0.49
1:B:280:ALA:O	1:C:57:ARG:HD2	2.13	0.49
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.78	0.49
1:B:426:ILE:HD13	3:C:3493:HOH:O	2.12	0.49
1:D:132:LEU:HD13	1:D:132:LEU:C	2.32	0.49
1:B:86:LEU:HA	1:B:89:PHE:CE2	2.47	0.49
1:B:170:LEU:CD2	1:B:176:ARG:HG2	2.43	0.49
1:A:321:ARG:HH21	1:D:321:ARG:HH21	1.59	0.49
1:B:225:TRP:CE2	1:B:517:LEU:HD22	2.48	0.49
1:G:160:VAL:O	1:G:164:GLN:HG3	2.13	0.49
1:B:523:VAL:OXT	1:B:523:VAL:HG12	2.13	0.49
1:G:36:PRO:N	1:G:37:PRO:HD2	2.28	0.49
1:F:53:ILE:HD13	1:F:196:ARG:HD2	1.95	0.48
1:A:329:ALA:HB1	1:D:252:ARG:HA	1.95	0.48
1:A:487:LYS:O	1:A:491:GLN:HG3	2.13	0.48
1:C:225:TRP:CD2	1:C:522:PRO:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:TYR:OH	2:G:701:TCA:H2	2.14	0.48
1:A:170:LEU:HD23	1:A:176:ARG:HG2	1.95	0.48
3:B:3548:HOH:O	1:C:426:ILE:HD13	2.13	0.48
1:D:169:PHE:CD2	1:D:182:GLY:HA3	2.48	0.48
1:A:132:LEU:C	1:A:132:LEU:HD13	2.34	0.48
1:F:181:GLU:OE1	1:F:184:ARG:NH1	2.47	0.48
1:A:176:ARG:HD2	3:A:3332:HOH:O	2.14	0.48
1:B:170:LEU:HD23	1:B:176:ARG:HG2	1.96	0.48
1:F:57:ARG:HD2	1:G:280:ALA:O	2.14	0.48
1:C:60:TYR:OH	2:C:701:TCA:H2	2.14	0.47
1:C:263:ARG:O	1:C:267:ARG:HG2	2.13	0.47
1:A:124:GLY:O	1:A:128:ARG:HG2	2.14	0.47
1:D:48:ARG:NH2	1:D:338:PRO:O	2.47	0.47
1:B:489:LEU:HD23	1:B:489:LEU:C	2.35	0.47
1:D:191:LEU:HD21	1:D:201:LEU:CD1	2.45	0.47
1:E:12:GLU:HA	1:E:33:VAL:HG13	1.96	0.47
1:E:489:LEU:HD23	1:E:489:LEU:C	2.34	0.47
1:C:132:LEU:C	1:C:132:LEU:HD13	2.34	0.47
1:E:384:ARG:HD2	3:E:3602:HOH:O	2.15	0.47
1:H:372:LEU:O	1:H:376:GLN:HG3	2.15	0.47
1:B:168:ASP:HB2	1:B:176:ARG:HH21	1.80	0.47
1:H:54:ARG:HG2	1:H:54:ARG:HH11	1.80	0.47
1:E:80:ARG:HG2	3:E:4938:HOH:O	2.15	0.47
1:A:36:PRO:N	1:A:37:PRO:HD2	2.29	0.47
1:B:36:PRO:HB2	1:B:37:PRO:HD3	1.96	0.46
1:B:160:VAL:O	1:B:164:GLN:HG3	2.15	0.46
1:D:51:ALA:O	1:D:55:GLU:HG3	2.15	0.46
1:F:436:GLN:HG2	1:G:300:TYR:CZ	2.51	0.46
1:B:132:LEU:HD13	1:B:132:LEU:C	2.36	0.46
1:B:252:ARG:HA	1:C:329:ALA:HB1	1.96	0.46
1:H:156:LEU:O	1:H:160:VAL:HG23	2.15	0.46
1:B:436:GLN:HG2	1:C:300:TYR:CZ	2.51	0.46
1:E:145:GLY:HA2	1:F:410:THR:HG23	1.97	0.46
1:H:489:LEU:C	1:H:489:LEU:HD23	2.36	0.46
1:A:263:ARG:O	1:A:267:ARG:HG2	2.16	0.46
1:F:252:ARG:HA	1:G:329:ALA:HB1	1.97	0.46
1:F:329:ALA:HB1	1:G:252:ARG:HA	1.98	0.46
1:E:152:ASP:CG	1:E:207:ALA:HB3	2.37	0.46
1:H:168:ASP:HB2	1:H:176:ARG:HH21	1.81	0.46
1:B:297:GLN:HG3	3:B:3097:HOH:O	2.16	0.45
1:H:86:LEU:HA	1:H:89:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:O	1:A:164:GLN:HG3	2.16	0.45
1:C:225:TRP:CE2	1:C:522:PRO:HG3	2.51	0.45
3:E:3348:HOH:O	1:H:426:ILE:HD13	2.17	0.45
1:H:238:ARG:HH11	1:H:387:ARG:NH2	2.15	0.45
1:C:53:ILE:HD13	1:C:196:ARG:HD2	1.98	0.45
1:H:76:GLY:HA2	1:H:79:VAL:HG23	1.97	0.45
1:C:170:LEU:HD23	1:C:176:ARG:HG2	1.98	0.45
1:D:211:ILE:HD13	1:D:447:ARG:HG3	1.98	0.45
1:G:225:TRP:CE2	1:G:517:LEU:HD22	2.52	0.45
1:H:199:LEU:HD12	1:H:199:LEU:N	2.32	0.45
1:G:90:LEU:HD13	1:G:153:LEU:HB3	1.99	0.45
1:A:146:THR:HG22	3:A:2274:HOH:O	2.16	0.45
1:B:225:TRP:CE2	1:B:522:PRO:HD3	2.52	0.45
1:D:199:LEU:O	1:D:203:ASN:HB2	2.17	0.45
1:E:79:VAL:HG11	1:E:196:ARG:HD3	1.99	0.45
1:H:184:ARG:HG2	1:H:184:ARG:HH11	1.82	0.44
1:C:410:THR:HG23	1:D:145:GLY:HA2	1.99	0.44
1:C:491:GLN:O	1:C:495:GLU:HG3	2.17	0.44
1:E:436:GLN:HG2	1:H:300:TYR:CZ	2.52	0.44
1:A:86:LEU:HA	1:A:89:PHE:CE2	2.53	0.44
1:D:12:GLU:CG	1:D:35:ALA:HB2	2.47	0.44
1:D:433:ALA:O	1:D:434:ALA:HB3	2.17	0.44
1:E:78:ASN:HB3	1:F:400:LEU:HD21	1.99	0.44
1:D:12:GLU:HA	1:D:33:VAL:HG13	1.99	0.44
1:B:238:ARG:HH21	1:B:387:ARG:NH2	2.15	0.44
1:F:321:ARG:HH21	1:G:321:ARG:HH21	1.64	0.44
1:G:395:ARG:CZ	1:G:501:GLU:HG2	2.48	0.44
1:H:225:TRP:CE2	1:H:522:PRO:HD3	2.53	0.44
1:D:372:LEU:O	1:D:376:GLN:HG3	2.17	0.44
1:E:497:PHE:HA	1:E:498:PRO:HD3	1.85	0.44
1:F:242:GLU:HB3	3:F:1183:HOH:O	2.18	0.44
1:C:78:ASN:HB3	1:D:400:LEU:HD21	2.00	0.43
1:C:90:LEU:HD13	1:C:153:LEU:HB3	2.00	0.43
1:C:489:LEU:C	1:C:489:LEU:HD23	2.38	0.43
1:A:125:THR:HG23	1:A:201:LEU:HD11	2.01	0.43
1:C:48:ARG:HG2	1:C:48:ARG:NH1	2.33	0.43
1:C:214:VAL:HG13	3:C:4020:HOH:O	2.18	0.43
1:A:170:LEU:CD2	1:A:176:ARG:HG2	2.49	0.43
1:C:12:GLU:HA	1:C:33:VAL:HG13	2.00	0.43
1:C:191:LEU:HD21	1:C:201:LEU:CD1	2.48	0.43
1:D:335:VAL:HG11	3:D:2240:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:LEU:C	1:F:489:LEU:HD23	2.39	0.43
1:G:337:PRO:HA	1:G:338:PRO:HD3	1.92	0.43
1:H:60:TYR:OH	2:H:701:TCA:H2	2.19	0.43
1:D:79:VAL:HG21	3:D:5014:HOH:O	2.19	0.43
1:E:80:ARG:HB3	1:E:80:ARG:HH11	1.84	0.43
1:F:60:TYR:OH	2:F:701:TCA:H2	2.17	0.43
1:A:184:ARG:HG2	1:A:184:ARG:NH1	2.33	0.43
1:D:53:ILE:HD13	1:D:196:ARG:HD2	2.00	0.43
1:D:177:LEU:HD21	1:D:185:ARG:NH1	2.33	0.43
1:F:305:ALA:N	1:F:306:PRO:CD	2.82	0.43
1:H:52:VAL:HG13	1:H:57:ARG:HB2	2.01	0.43
1:C:145:GLY:HA2	1:D:410:THR:HG23	2.01	0.42
1:D:225:TRP:CD2	1:D:517:LEU:HD22	2.53	0.42
1:F:225:TRP:CD2	1:F:517:LEU:HD22	2.54	0.42
1:E:321:ARG:HH21	1:H:321:ARG:HH21	1.67	0.42
1:E:48:ARG:HH11	1:E:48:ARG:HG2	1.84	0.42
1:E:305:ALA:HB3	1:E:306:PRO:HD3	2.02	0.42
1:H:497:PHE:HA	1:H:498:PRO:HD3	1.88	0.42
1:C:79:VAL:HG11	1:C:196:ARG:HD3	2.02	0.42
1:G:214:VAL:HB	1:G:450:ARG:HH21	1.82	0.42
1:H:238:ARG:NH1	1:H:387:ARG:NH2	2.67	0.42
1:H:191:LEU:HD21	1:H:201:LEU:CD1	2.50	0.42
1:D:184:ARG:HG2	1:D:184:ARG:HH11	1.84	0.42
1:H:90:LEU:HD13	1:H:153:LEU:HB3	2.01	0.42
1:F:171:ASP:OD1	1:F:171:ASP:C	2.58	0.42
1:G:489:LEU:HD23	1:G:489:LEU:C	2.40	0.42
1:H:48:ARG:O	1:H:52:VAL:HG23	2.20	0.42
1:H:184:ARG:HG2	1:H:184:ARG:NH1	2.35	0.42
1:H:263:ARG:O	1:H:267:ARG:HG2	2.20	0.42
1:C:394:HIS:HE1	3:C:2881:HOH:O	2.02	0.41
1:D:141:VAL:HA	1:D:142:PRO:HD3	1.97	0.41
1:E:252:ARG:HA	1:H:329:ALA:HB1	2.02	0.41
1:F:372:LEU:O	1:F:376:GLN:HG3	2.20	0.41
1:B:48:ARG:NH2	1:B:338:PRO:O	2.53	0.41
1:B:68:PRO:HG3	1:B:435:ASN:CB	2.50	0.41
1:H:48:ARG:NH2	1:H:338:PRO:O	2.52	0.41
1:A:7:PRO:O	1:A:8:LYS:C	2.59	0.41
1:G:263:ARG:O	1:G:267:ARG:HG2	2.20	0.41
1:A:279:ILE:HD11	1:D:346:HIS:CE1	2.55	0.41
1:E:79:VAL:HG21	3:E:2045:HOH:O	2.20	0.41
1:H:170:LEU:CD2	1:H:176:ARG:HG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:C	1:A:489:LEU:HD23	2.40	0.41
1:C:8:LYS:HA	1:C:9:PRO:HD3	1.94	0.41
1:C:335:VAL:HG11	3:C:1256:HOH:O	2.20	0.41
1:E:410:THR:HG23	1:F:145:GLY:HA2	2.02	0.41
1:H:39:ARG:HD3	1:H:43:ARG:HH21	1.86	0.41
1:A:305:ALA:N	1:A:306:PRO:CD	2.84	0.41
1:H:305:ALA:N	1:H:306:PRO:CD	2.84	0.41
1:C:199:LEU:O	1:C:203:ASN:HB2	2.21	0.41
1:G:211:ILE:HD13	1:G:447:ARG:HG3	2.03	0.41
1:H:39:ARG:O	1:H:43:ARG:HG3	2.20	0.41
1:A:79:VAL:HG11	1:A:196:ARG:HD3	2.03	0.41
1:A:145:GLY:HA2	1:B:410:THR:HG23	2.03	0.41
1:B:63:THR:HG22	3:B:5022:HOH:O	2.20	0.41
1:B:278:VAL:HB	1:B:281:GLU:HG3	2.02	0.41
1:B:337:PRO:HA	1:B:338:PRO:HD3	1.93	0.41
1:D:225:TRP:CE2	1:D:522:PRO:HD3	2.56	0.41
1:E:288:ASP:O	1:H:73:LEU:HD12	2.21	0.41
1:F:79:VAL:HG11	1:F:196:ARG:HD3	2.02	0.41
1:F:280:ALA:O	1:G:57:ARG:HD2	2.20	0.41
1:G:78:ASN:HB3	1:H:400:LEU:HD21	2.03	0.41
1:B:305:ALA:N	1:B:306:PRO:CD	2.84	0.41
1:F:68:PRO:HG3	1:F:435:ASN:CB	2.50	0.41
1:F:335:VAL:HG11	3:F:1411:HOH:O	2.22	0.40
1:B:263:ARG:O	1:B:267:ARG:HG2	2.21	0.40
1:D:86:LEU:HA	1:D:89:PHE:CE2	2.56	0.40
1:D:281:GLU:OE1	1:D:281:GLU:HA	2.22	0.40
1:E:100:TRP:CZ2	1:E:172:ARG:HG2	2.55	0.40
1:C:39:ARG:NH1	3:C:5446:HOH:O	2.54	0.40
1:E:48:ARG:HG2	1:E:48:ARG:NH1	2.37	0.40
1:E:160:VAL:O	1:E:164:GLN:HG3	2.22	0.40
1:C:372:LEU:O	1:C:376:GLN:HG3	2.21	0.40
1:E:436:GLN:HG2	1:H:300:TYR:CE2	2.57	0.40
1:F:132:LEU:C	1:F:132:LEU:HD13	2.42	0.40
1:F:281:GLU:OE1	1:F:281:GLU:HA	2.22	0.40
1:D:8:LYS:CG	1:D:31:ARG:HG3	2.51	0.40
1:D:76:GLY:HA2	1:D:79:VAL:HG23	2.04	0.40
1:D:108:LEU:O	1:D:112:VAL:HG23	2.21	0.40
1:F:424:ALA:HB2	1:F:448:LEU:HD12	2.02	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	512/521 (98%)	501 (98%)	9 (2%)	2 (0%)	34	24
1	B	512/521 (98%)	506 (99%)	5 (1%)	1 (0%)	47	38
1	C	511/521 (98%)	505 (99%)	5 (1%)	1 (0%)	47	38
1	D	511/521 (98%)	501 (98%)	9 (2%)	1 (0%)	47	38
1	E	511/521 (98%)	505 (99%)	5 (1%)	1 (0%)	47	38
1	F	511/521 (98%)	503 (98%)	7 (1%)	1 (0%)	47	38
1	G	511/521 (98%)	504 (99%)	6 (1%)	1 (0%)	47	38
1	H	511/521 (98%)	502 (98%)	8 (2%)	1 (0%)	47	38
All	All	4090/4168 (98%)	4027 (98%)	54 (1%)	9 (0%)	47	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	253	PRO
1	E	253	PRO
1	A	253	PRO
1	C	253	PRO
1	G	253	PRO
1	H	253	PRO
1	A	8	LYS
1	B	253	PRO
1	D	253	PRO

### 5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/389 (99%)	382 (100%)	2 (0%)	88	89
1	B	384/389 (99%)	382 (100%)	2 (0%)	88	89
1	C	383/389 (98%)	380 (99%)	3 (1%)	81	82
1	D	383/389 (98%)	381 (100%)	2 (0%)	88	89
1	E	383/389 (98%)	380 (99%)	3 (1%)	81	82
1	F	383/389 (98%)	378 (99%)	5 (1%)	69	68
1	G	383/389 (98%)	382 (100%)	1 (0%)	92	93
1	H	383/389 (98%)	382 (100%)	1 (0%)	92	93
All	All	3066/3112 (98%)	3047 (99%)	19 (1%)	86	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ASP
1	A	443	THR
1	B	332	ASP
1	B	443	THR
1	C	89	PHE
1	C	332	ASP
1	C	443	THR
1	D	332	ASP
1	D	443	THR
1	E	80	ARG
1	E	332	ASP
1	E	443	THR
1	F	89	PHE
1	F	203	ASN
1	F	242	GLU
1	F	332	ASP
1	F	443	THR
1	G	332	ASP
1	H	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	HIS

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Mol	Chain	Res	Type
1	A	491	GLN
1	A	496	GLN
1	B	394	HIS
1	B	436	GLN
1	C	394	HIS
1	D	189	GLN
1	D	394	HIS
1	D	491	GLN
1	D	496	GLN
1	E	394	HIS
1	F	394	HIS
1	F	491	GLN
1	G	164	GLN
1	G	189	GLN
1	G	394	HIS
1	H	189	GLN
1	H	394	HIS
1	H	508	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	MDO	C	149	1	12,13,14	2.25	4 (33%)	15,18,20	3.86	6 (40%)
1	MDO	H	149	1	12,13,14	2.27	4 (33%)	15,18,20	3.89	6 (40%)
1	MDO	E	149	1	12,13,14	2.24	4 (33%)	15,18,20	3.89	6 (40%)
1	MDO	D	149	1	12,13,14	2.28	4 (33%)	15,18,20	3.92	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MDO	G	149	1	12,13,14	2.24	4 (33%)	15,18,20	3.91	6 (40%)
1	MDO	F	149	1	12,13,14	2.25	4 (33%)	15,18,20	3.94	6 (40%)
1	MDO	A	149	1	12,13,14	2.25	4 (33%)	15,18,20	3.84	6 (40%)
1	MDO	B	149	1	12,13,14	2.39	5 (41%)	15,18,20	3.78	6 (40%)

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	MDO	C	149	1	-	1/4/23/24	0/1/1/1
1	MDO	H	149	1	-	1/4/23/24	0/1/1/1
1	MDO	E	149	1	-	1/4/23/24	0/1/1/1
1	MDO	D	149	1	-	0/4/23/24	0/1/1/1
1	MDO	G	149	1	-	1/4/23/24	0/1/1/1
1	MDO	F	149	1	-	1/4/23/24	0/1/1/1
1	MDO	A	149	1	-	0/4/23/24	0/1/1/1
1	MDO	B	149	1	-	0/4/23/24	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	MDO	O2-C2	5.23	1.34	1.23
1	H	149	MDO	O2-C2	5.08	1.33	1.23
1	D	149	MDO	O2-C2	5.06	1.33	1.23
1	C	149	MDO	O2-C2	5.04	1.33	1.23
1	F	149	MDO	O2-C2	5.00	1.33	1.23
1	E	149	MDO	O2-C2	4.95	1.33	1.23
1	A	149	MDO	O2-C2	4.95	1.33	1.23
1	G	149	MDO	O2-C2	4.90	1.33	1.23
1	B	149	MDO	C2-N3	-3.83	1.30	1.39
1	A	149	MDO	C2-N3	-3.71	1.31	1.39
1	E	149	MDO	C2-N3	-3.68	1.31	1.39
1	D	149	MDO	C2-N3	-3.59	1.31	1.39
1	G	149	MDO	C2-N3	-3.58	1.31	1.39
1	C	149	MDO	C2-N3	-3.56	1.31	1.39
1	H	149	MDO	C2-N3	-3.53	1.31	1.39
1	F	149	MDO	C2-N3	-3.53	1.31	1.39
1	C	149	MDO	CA2-N2	-2.81	1.33	1.39
1	F	149	MDO	CA2-C2	-2.77	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	149	MDO	CA2-N2	-2.76	1.34	1.39
1	B	149	MDO	CA2-N2	-2.74	1.34	1.39
1	E	149	MDO	CA2-N2	-2.73	1.34	1.39
1	A	149	MDO	CA2-N2	-2.71	1.34	1.39
1	H	149	MDO	CA2-C2	-2.65	1.37	1.43
1	D	149	MDO	CA2-C2	-2.61	1.38	1.43
1	E	149	MDO	CA2-C2	-2.57	1.38	1.43
1	G	149	MDO	CA2-C2	-2.54	1.38	1.43
1	B	149	MDO	CA2-C2	-2.49	1.38	1.43
1	H	149	MDO	CA2-N2	-2.47	1.34	1.39
1	A	149	MDO	CA2-C2	-2.40	1.38	1.43
1	F	149	MDO	CA2-N2	-2.39	1.34	1.39
1	D	149	MDO	CA2-N2	-2.34	1.34	1.39
1	C	149	MDO	CA2-C2	-2.32	1.38	1.43
1	B	149	MDO	C1-N3	-2.16	1.33	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	MDO	CA2-C2-N3	12.44	109.25	103.37
1	F	149	MDO	CA2-C2-N3	12.41	109.24	103.37
1	G	149	MDO	CA2-C2-N3	12.39	109.23	103.37
1	E	149	MDO	CA2-C2-N3	12.39	109.23	103.37
1	H	149	MDO	CA2-C2-N3	12.33	109.20	103.37
1	B	149	MDO	CA2-C2-N3	12.25	109.16	103.37
1	C	149	MDO	CA2-C2-N3	12.25	109.16	103.37
1	A	149	MDO	CA2-C2-N3	12.23	109.15	103.37
1	F	149	MDO	O2-C2-CA2	-5.19	128.04	130.96
1	G	149	MDO	O2-C2-CA2	-5.02	128.14	130.96
1	D	149	MDO	O2-C2-CA2	-4.88	128.22	130.96
1	H	149	MDO	O2-C2-CA2	-4.87	128.22	130.96
1	E	149	MDO	O2-C2-CA2	-4.78	128.28	130.96
1	C	149	MDO	O2-C2-CA2	-4.62	128.37	130.96
1	A	149	MDO	O2-C2-CA2	-4.54	128.41	130.96
1	B	149	MDO	O2-C2-CA2	-3.95	128.74	130.96
1	D	149	MDO	C2-CA2-N2	-3.75	106.31	108.93
1	B	149	MDO	C2-CA2-N2	-3.72	106.33	108.93
1	A	149	MDO	C2-CA2-N2	-3.66	106.37	108.93
1	C	149	MDO	C2-CA2-N2	-3.56	106.44	108.93
1	H	149	MDO	C2-CA2-N2	-3.55	106.45	108.93
1	A	149	MDO	CB2-CA2-C2	3.52	129.20	122.76
1	F	149	MDO	C2-CA2-N2	-3.49	106.49	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	MDO	CB2-CA2-C2	3.47	129.12	122.76
1	E	149	MDO	C2-CA2-N2	-3.47	106.50	108.93
1	E	149	MDO	CB2-CA2-C2	3.42	129.03	122.76
1	C	149	MDO	CB2-CA2-C2	3.42	129.02	122.76
1	G	149	MDO	C2-CA2-N2	-3.41	106.55	108.93
1	G	149	MDO	CB2-CA2-C2	3.37	128.92	122.76
1	D	149	MDO	CB2-CA2-C2	3.34	128.88	122.76
1	F	149	MDO	N3-C1-N2	-3.28	109.18	111.45
1	F	149	MDO	CB2-CA2-C2	3.28	128.76	122.76
1	H	149	MDO	CB2-CA2-C2	3.27	128.75	122.76
1	H	149	MDO	N3-C1-N2	-3.10	109.31	111.45
1	D	149	MDO	N3-C1-N2	-3.05	109.34	111.45
1	G	149	MDO	N3-C1-N2	-2.98	109.39	111.45
1	C	149	MDO	N3-C1-N2	-2.97	109.40	111.45
1	E	149	MDO	N3-C1-N2	-2.96	109.41	111.45
1	A	149	MDO	N3-C1-N2	-2.67	109.61	111.45
1	C	149	MDO	CA2-N2-C1	2.62	107.77	105.40
1	B	149	MDO	N3-C1-N2	-2.59	109.66	111.45
1	E	149	MDO	CA2-N2-C1	2.49	107.65	105.40
1	F	149	MDO	CA2-N2-C1	2.49	107.65	105.40
1	G	149	MDO	CA2-N2-C1	2.47	107.63	105.40
1	H	149	MDO	CA2-N2-C1	2.41	107.58	105.40
1	A	149	MDO	CA2-N2-C1	2.41	107.58	105.40
1	D	149	MDO	CA2-N2-C1	2.36	107.53	105.40
1	B	149	MDO	CA2-N2-C1	2.17	107.37	105.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	149	MDO	N2-C1-CA-CB
1	E	149	MDO	N2-C1-CA-CB
1	F	149	MDO	N2-C1-CA-CB
1	G	149	MDO	N2-C1-CA-CB
1	H	149	MDO	N2-C1-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 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
2	TCA	F	701	-	8,11,11	2.50	6 (75%)	10,13,13	0.36	0
2	TCA	D	701	-	8,11,11	2.52	6 (75%)	10,13,13	0.25	0
2	TCA	A	701	-	8,11,11	2.46	6 (75%)	10,13,13	0.35	0
2	TCA	B	701	-	8,11,11	2.51	6 (75%)	10,13,13	0.29	0
2	TCA	H	701	-	8,11,11	2.49	6 (75%)	10,13,13	0.36	0
2	TCA	G	701	-	8,11,11	2.49	6 (75%)	10,13,13	0.34	0
2	TCA	C	701	-	8,11,11	2.46	6 (75%)	10,13,13	0.39	0
2	TCA	E	701	-	8,11,11	2.49	6 (75%)	10,13,13	0.39	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
2	TCA	F	701	-	-	0/3/5/5	0/1/1/1
2	TCA	D	701	-	-	0/3/5/5	0/1/1/1
2	TCA	A	701	-	-	0/3/5/5	0/1/1/1
2	TCA	B	701	-	-	0/3/5/5	0/1/1/1
2	TCA	H	701	-	-	0/3/5/5	0/1/1/1
2	TCA	G	701	-	-	0/3/5/5	0/1/1/1
2	TCA	C	701	-	-	0/3/5/5	0/1/1/1
2	TCA	E	701	-	-	0/3/5/5	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	701	TCA	C32-C31	3.51	1.46	1.39
2	D	701	TCA	C32-C31	3.46	1.46	1.39
2	E	701	TCA	C32-C31	3.44	1.46	1.39
2	B	701	TCA	C32-C31	3.44	1.46	1.39
2	A	701	TCA	C32-C31	3.42	1.46	1.39
2	F	701	TCA	C32-C31	3.40	1.46	1.39
2	G	701	TCA	C32-C31	3.36	1.46	1.39
2	C	701	TCA	C32-C31	3.28	1.45	1.39
2	D	701	TCA	C36-C31	3.13	1.45	1.39
2	B	701	TCA	C36-C31	3.13	1.45	1.39
2	F	701	TCA	C36-C31	3.10	1.45	1.39
2	G	701	TCA	C36-C31	3.05	1.45	1.39
2	C	701	TCA	C36-C31	3.03	1.45	1.39
2	E	701	TCA	C36-C31	3.01	1.45	1.39
2	A	701	TCA	C36-C31	2.95	1.45	1.39
2	H	701	TCA	C36-C31	2.91	1.45	1.39
2	E	701	TCA	C33-C32	2.85	1.44	1.38
2	H	701	TCA	C33-C32	2.83	1.44	1.38
2	C	701	TCA	C33-C32	2.80	1.44	1.38
2	G	701	TCA	C33-C32	2.79	1.44	1.38
2	F	701	TCA	C33-C32	2.77	1.44	1.38
2	D	701	TCA	C33-C32	2.76	1.44	1.38
2	B	701	TCA	C33-C32	2.73	1.44	1.38
2	A	701	TCA	C33-C32	2.73	1.44	1.38
2	B	701	TCA	C35-C34	2.57	1.44	1.38
2	G	701	TCA	C35-C36	2.57	1.44	1.38
2	C	701	TCA	C35-C34	2.56	1.44	1.38
2	D	701	TCA	C35-C34	2.55	1.44	1.38
2	H	701	TCA	C35-C34	2.52	1.44	1.38
2	B	701	TCA	C35-C36	2.51	1.44	1.38
2	F	701	TCA	C35-C34	2.50	1.44	1.38
2	C	701	TCA	C35-C36	2.48	1.44	1.38
2	A	701	TCA	C35-C34	2.48	1.44	1.38
2	E	701	TCA	C35-C34	2.48	1.44	1.38
2	E	701	TCA	C35-C36	2.47	1.44	1.38
2	D	701	TCA	C35-C36	2.47	1.44	1.38
2	F	701	TCA	C35-C36	2.44	1.44	1.38
2	G	701	TCA	C34-C33	2.41	1.44	1.38
2	G	701	TCA	C35-C34	2.40	1.44	1.38
2	A	701	TCA	C35-C36	2.40	1.44	1.38
2	H	701	TCA	C35-C36	2.40	1.44	1.38
2	B	701	TCA	C34-C33	2.39	1.44	1.38
2	H	701	TCA	C34-C33	2.36	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	TCA	C34-C33	2.34	1.44	1.38
2	F	701	TCA	C34-C33	2.34	1.44	1.38
2	A	701	TCA	C34-C33	2.31	1.44	1.38
2	C	701	TCA	C34-C33	2.28	1.44	1.38
2	E	701	TCA	C34-C33	2.26	1.44	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	TCA	1	0
2	H	701	TCA	1	0
2	G	701	TCA	1	0
2	C	701	TCA	1	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	514/521 (98%)	0.02	12 (2%) 60 63	6, 14, 34, 54	0
1	B	514/521 (98%)	-0.20	7 (1%) 75 77	5, 13, 31, 49	0
1	C	513/521 (98%)	-0.24	3 (0%) 89 90	6, 12, 27, 48	0
1	D	513/521 (98%)	-0.09	10 (1%) 66 69	3, 14, 32, 50	0
1	E	513/521 (98%)	-0.05	7 (1%) 75 77	4, 13, 31, 50	0
1	F	513/521 (98%)	-0.32	2 (0%) 92 93	3, 11, 24, 43	0
1	G	513/521 (98%)	-0.26	1 (0%) 95 95	4, 11, 26, 46	0
1	H	513/521 (98%)	0.03	12 (2%) 60 63	5, 14, 32, 49	0
All	All	4106/4168 (98%)	-0.14	54 (1%) 77 79	3, 13, 30, 54	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	523	VAL	8.9
1	A	523	VAL	8.7
1	B	523	VAL	8.0
1	G	523	VAL	7.6
1	F	523	VAL	7.4
1	A	7	PRO	7.4
1	E	523	VAL	7.3
1	C	523	VAL	7.0
1	H	523	VAL	6.2
1	D	277	HIS	5.4
1	A	285	ASP	5.2
1	H	277	HIS	4.8
1	B	277	HIS	4.6
1	B	7	PRO	4.6
1	E	277	HIS	3.8
1	A	277	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	9	PRO	3.5
1	D	9	PRO	3.4
1	A	286	ALA	3.4
1	A	187	ARG	3.3
1	A	9	PRO	3.2
1	B	173	ASP	3.2
1	H	173	ASP	3.1
1	H	174	GLY	3.1
1	E	286	ALA	3.0
1	F	277	HIS	3.0
1	A	10	ALA	3.0
1	E	9	PRO	2.8
1	D	340	GLY	2.8
1	E	285	ASP	2.7
1	A	173	ASP	2.6
1	B	172	ARG	2.6
1	A	288	ASP	2.5
1	H	175	THR	2.5
1	B	175	THR	2.5
1	E	288	ASP	2.5
1	D	54	ARG	2.5
1	D	77	GLU	2.4
1	D	175	THR	2.3
1	H	12	GLU	2.2
1	D	12	GLU	2.2
1	A	269	ASP	2.2
1	H	172	ARG	2.2
1	E	480	ASP	2.2
1	H	171	ASP	2.1
1	A	287	GLY	2.1
1	C	172	ARG	2.1
1	C	501	GLU	2.1
1	D	8	LYS	2.1
1	H	187	ARG	2.1
1	H	339	ASP	2.1
1	H	77	GLU	2.1
1	B	171	ASP	2.0
1	D	173	ASP	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( $\text{\AA}^2$ )	Q<0.9
1	MDO	H	149	13/14	0.92	0.15	13,16,20,21	0
1	MDO	F	149	13/14	0.94	0.13	9,14,18,19	0
1	MDO	G	149	13/14	0.94	0.13	8,12,14,17	0
1	MDO	A	149	13/14	0.94	0.16	11,15,18,19	0
1	MDO	B	149	13/14	0.95	0.10	11,14,17,18	0
1	MDO	D	149	13/14	0.95	0.14	14,16,18,20	0
1	MDO	E	149	13/14	0.95	0.15	9,12,16,19	0
1	MDO	C	149	13/14	0.96	0.12	9,10,14,15	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
2	TCA	H	701	11/11	0.86	0.23	34,35,38,39	0
2	TCA	B	701	11/11	0.89	0.15	22,23,29,29	0
2	TCA	D	701	11/11	0.90	0.17	24,30,31,31	0
2	TCA	E	701	11/11	0.92	0.15	21,23,24,25	0
2	TCA	G	701	11/11	0.92	0.12	19,22,24,25	0
2	TCA	C	701	11/11	0.92	0.11	20,21,23,23	0
2	TCA	A	701	11/11	0.93	0.18	22,23,26,26	0
2	TCA	F	701	11/11	0.94	0.10	21,24,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.