



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:06 AM GMT

PDB ID : 2O7B  
Title : Tyrosine ammonia-lyase from Rhodobacter sphaeroides, complexed with coumarate  
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 : 1.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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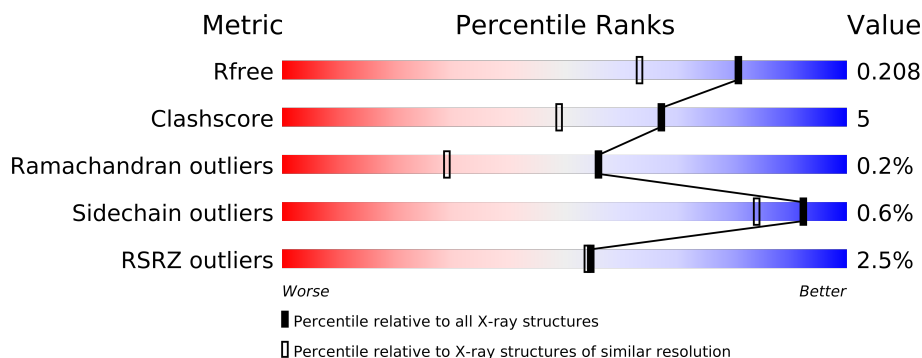
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **FAILED**  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.60 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))
$R_{free}$	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	521	
1	B	521	
1	C	521	
1	D	521	
1	E	521	
1	F	521	
1	G	521	
1	H	521	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	HC4	A	701	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	HC4	B	701	-	X
2	HC4	C	701	-	X
2	HC4	D	701	-	X
2	HC4	E	701	-	X
2	HC4	G	701	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34040 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			3813	2363	731	705	14			
1	B	515	Total	C	N	O	S	0	0	0
			3813	2363	731	705	14			
1	C	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	D	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	E	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	F	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	G	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	H	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			

There are 24 discrepancies between the modelled and reference sequences:

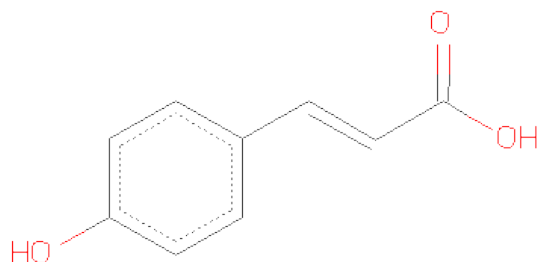
Chain	Residue	Modelled	Actual	Comment	Reference
A	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	ALA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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	GLY	SEE REMARK 999	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	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	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 4'-HYDROXYCINNAMIC ACID (three-letter code: HC4) (formula: C<sub>9</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	9	3		
2	B	1	Total	C	O	0	0
			12	9	3		
2	C	1	Total	C	O	0	0
			12	9	3		
2	D	1	Total	C	O	0	0
			12	9	3		
2	E	1	Total	C	O	0	0
			12	9	3		
2	F	1	Total	C	O	0	0
			12	9	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			12	9	3		
2	H	1	Total	C	O	0	0
			12	9	3		

- Molecule 3 is water.

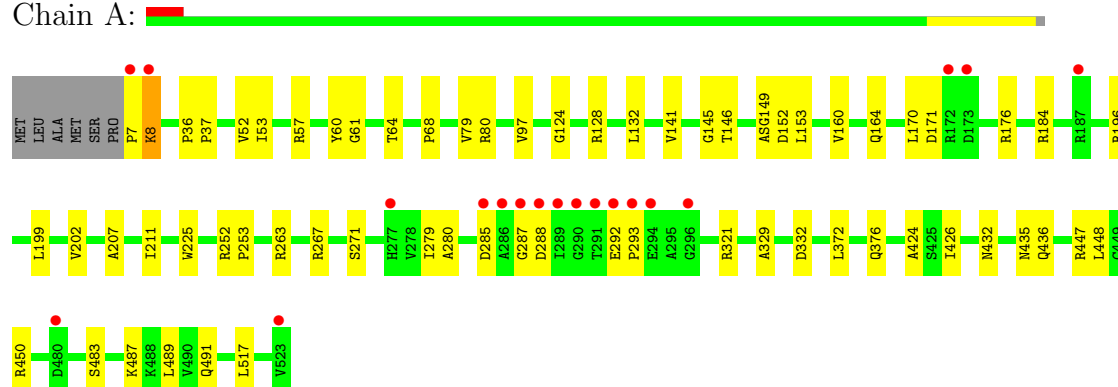
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	397	Total	O		0	0
			397	397			
3	B	416	Total	O		0	0
			416	416			
3	C	451	Total	O		0	0
			451	451			
3	D	408	Total	O		0	0
			408	408			
3	E	428	Total	O		0	0
			428	428			
3	F	522	Total	O		0	0
			522	522			
3	G	464	Total	O		0	0
			464	464			
3	H	396	Total	O		0	0
			396	396			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

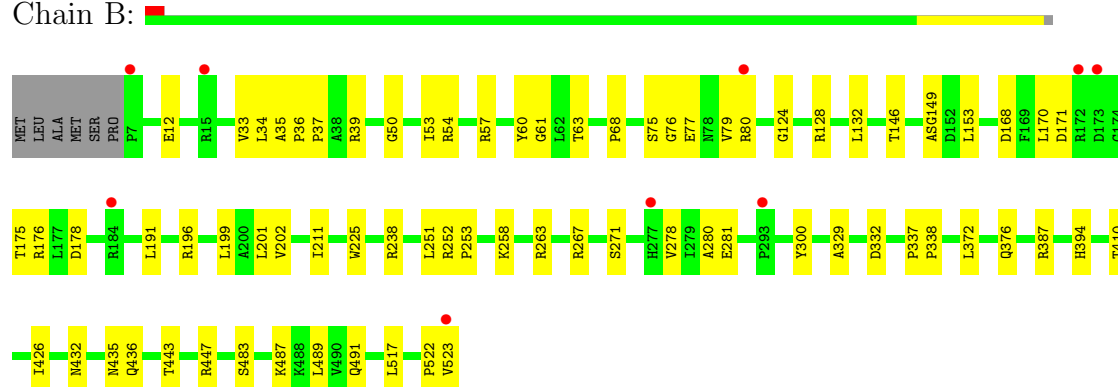
#### • Molecule 1: Putative histidine ammonia-lyase

Chain A:



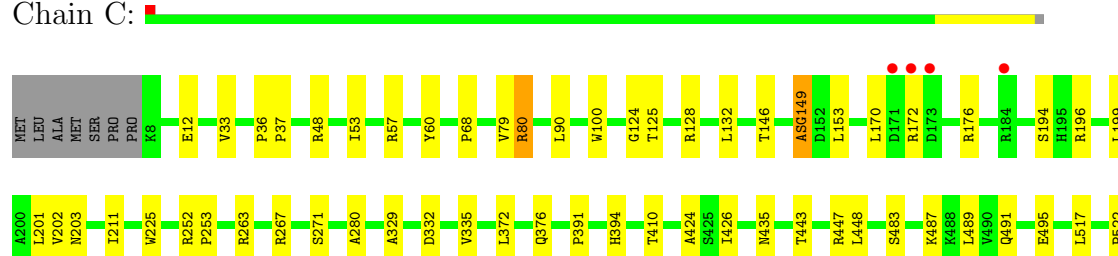
#### • Molecule 1: Putative histidine ammonia-lyase

Chain B:



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

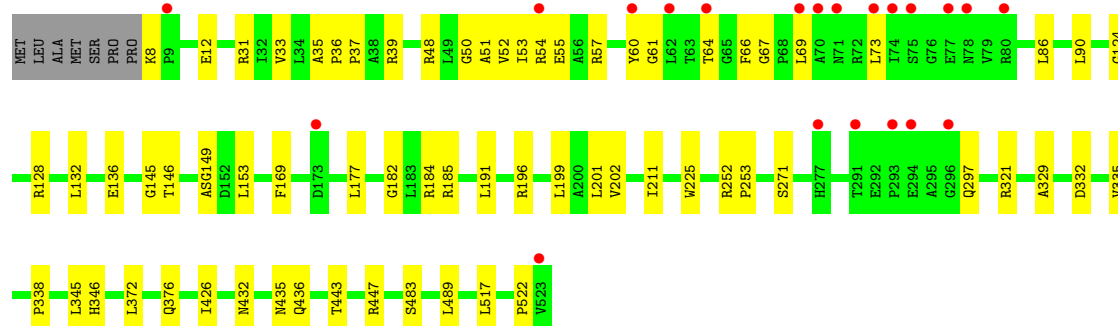
Chain C:



V523

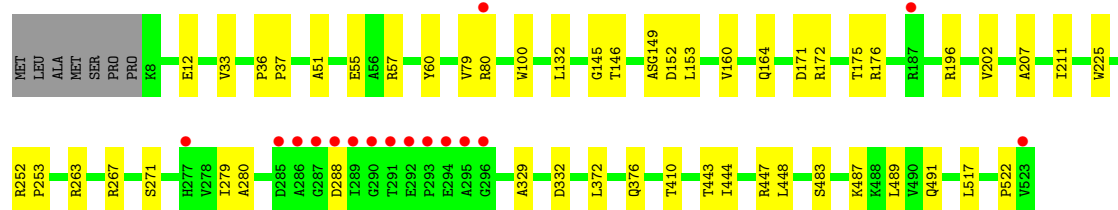
- Molecule 1: Putative histidine ammonia-lyase

Chain D:



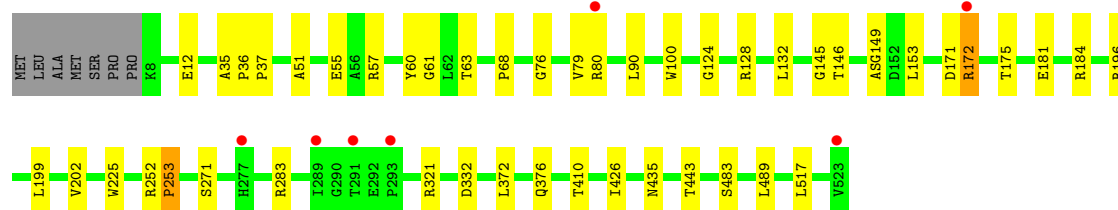
- Molecule 1: Putative histidine ammonia-lyase

Chain E:



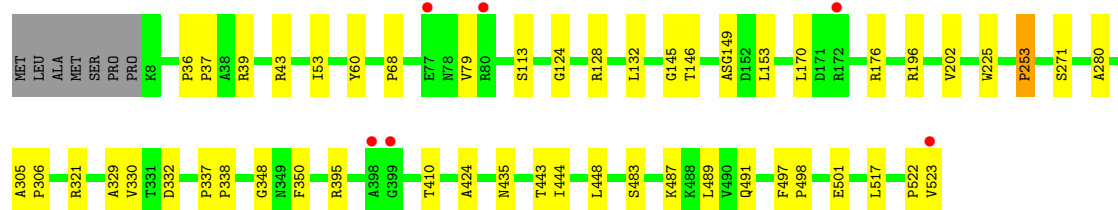
- Molecule 1: Putative histidine ammonia-lyase

Chain F:



- Molecule 1: Putative histidine ammonia-lyase

Chain G:

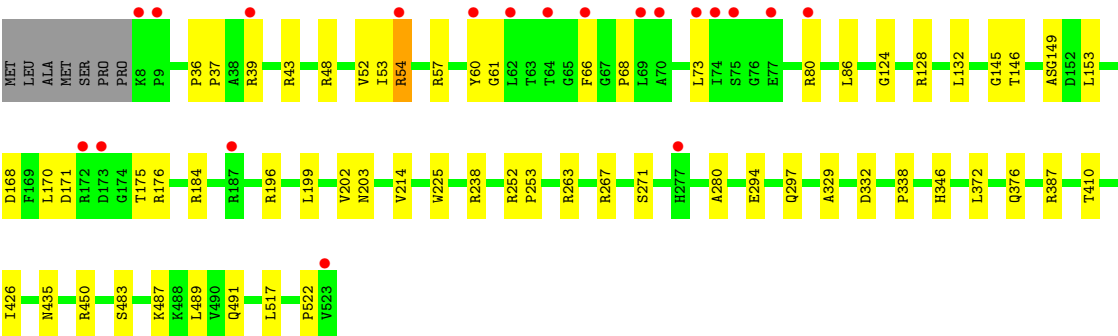


- Molecule 1: Putative histidine ammonia-lyase

Chain H:







## 4 Data and refinement statistics

Xtrriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.41Å 154.82Å 164.06Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	500.00 – 1.60 19.85 – 1.58	Depositor EDS
% Data completeness (in resolution range)	88.1 (500.00-1.60) 87.7 (19.85-1.58)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.192 , 0.208 0.192 , 0.208	Depositor DCC
$R_{free}$ test set	25650 reflections (5.04%)	DCC
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MDO, HC4

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	0.29	1/3862 (0.0%)	0.57	1/5253 (0.0%)
1	B	0.27	0/3862	0.56	0/5253
1	C	0.28	0/3854	0.56	0/5242
1	D	0.27	0/3854	0.56	0/5242
1	E	0.27	0/3854	0.56	0/5242
1	F	0.29	0/3854	0.57	1/5242 (0.0%)
1	G	0.28	0/3854	0.57	1/5242 (0.0%)
1	H	0.27	0/3854	0.54	0/5242
All	All	0.28	1/30848 (0.0%)	0.56	3/41958 (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	3
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	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	PRO	C-N	-6.01	1.20	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	GLY	O-C-N	5.33	131.22	122.70
1	F	253	PRO	N-CA-C	5.10	125.36	112.10
1	G	253	PRO	N-CA-C	5.02	125.16	112.10

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	MDO	Mainchain,Peptide
1	A	450	ARG	Sidechain
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3813	0	3864	41	0
1	B	3813	0	3864	52	0
1	C	3806	0	3856	43	0
1	D	3806	0	3856	46	0
1	E	3806	0	3856	38	0
1	F	3806	0	3856	31	0
1	G	3806	0	3856	30	0
1	H	3806	0	3856	57	0
2	A	12	0	6	1	0
2	B	12	0	6	1	0
2	C	12	0	6	1	0
2	D	12	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	12	0	6	2	0
2	F	12	0	6	1	0
2	G	12	0	6	1	0
2	H	12	0	6	1	0
3	A	397	0	0	4	0
3	B	416	0	0	8	0
3	C	451	0	0	5	0
3	D	408	0	0	5	0
3	E	428	0	0	5	0
3	F	522	0	0	4	0
3	G	464	0	0	2	0
3	H	396	0	0	4	0
All	All	34040	0	30912	309	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (309) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:153:LEU:HD22	1:D:202:VAL:HG12	1.63	0.80
1:B:487:LYS:O	1:B:491:GLN:HG3	1.82	0.78
1:A:153:LEU:HD22	1:A:202:VAL:HG12	1.66	0.78
1:E:487:LYS:O	1:E:491:GLN:HG3	1.85	0.77
1:H:153:LEU:HD22	1:H:202:VAL:HG12	1.69	0.74
1:H:53:ILE:HG21	1:H:196:ARG:HH11	1.51	0.74
1:B:153:LEU:HD22	1:B:202:VAL:HG12	1.70	0.74
1:A:285:ASP:OD1	1:A:288:ASP:OD2	2.06	0.74
1:B:171:ASP:OD2	1:B:175:THR:OG1	2.08	0.72
1:D:61:GLY:HA3	1:D:199:LEU:HD11	1.70	0.71
1:F:153:LEU:HD22	1:F:202:VAL:HG12	1.72	0.71
1:A:184:ARG:HH11	1:A:184:ARG:HG2	1.55	0.70
1:A:146:THR:HG22	3:A:2274:HOH:O	1.91	0.70
1:E:153:LEU:HD22	1:E:202:VAL:HG12	1.74	0.69
1:C:487:LYS:O	1:C:491:GLN:HG3	1.92	0.69
1:F:146:THR:HG22	3:F:2088:HOH:O	1.93	0.68
1:C:149:MDO:C1	3:C:3568:HOH:O	2.40	0.68
1:B:53:ILE:HG21	1:B:196:ARG:HH11	1.56	0.68
1:B:61:GLY:HA3	1:B:199:LEU:HD11	1.74	0.68
1:H:238:ARG:HH11	1:H:387:ARG:NH2	1.92	0.67
1:F:79:VAL:HG11	1:F:196:ARG:HD3	1.76	0.67
1:D:435:ASN:ND2	2:D:701:HC4:O1	2.24	0.66
1:D:50:GLY:O	1:D:54:ARG:HG3	1.96	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:60:TYR:OH	2:E:701:HC4:H2	1.97	0.65
1:C:153:LEU:HD22	1:C:202:VAL:HG12	1.79	0.64
1:G:53:ILE:HD13	1:G:196:ARG:HD2	1.81	0.63
1:H:214:VAL:HB	1:H:450:ARG:NH2	2.13	0.63
1:B:251:LEU:HD13	1:C:335:VAL:HG21	1.80	0.62
1:G:487:LYS:O	1:G:491:GLN:HG3	1.98	0.62
1:H:238:ARG:NH1	1:H:387:ARG:NH2	2.48	0.62
1:D:53:ILE:HD13	1:D:196:ARG:HD2	1.81	0.61
1:H:61:GLY:HA3	1:H:199:LEU:HD21	1.82	0.60
1:B:146:THR:HG22	3:B:2492:HOH:O	2.02	0.60
1:H:146:THR:HG22	3:H:2163:HOH:O	2.01	0.60
1:G:271:SER:HB2	1:G:483:SER:HB3	1.85	0.59
1:D:52:VAL:HG13	1:D:57:ARG:HB2	1.84	0.58
1:H:53:ILE:HG21	1:H:196:ARG:NH1	2.17	0.58
1:C:60:TYR:OH	2:C:701:HC4:H2	2.03	0.58
1:C:271:SER:HB2	1:C:483:SER:HB3	1.87	0.57
1:E:372:LEU:O	1:E:376:GLN:HG3	2.04	0.57
1:F:283:ARG:HD3	3:F:4975:HOH:O	2.04	0.57
1:F:426:ILE:HD13	3:G:3571:HOH:O	2.05	0.57
1:D:51:ALA:O	1:D:55:GLU:HG3	2.05	0.57
3:B:3548:HOH:O	1:C:426:ILE:HD13	2.06	0.56
1:B:124:GLY:O	1:B:128:ARG:HG2	2.05	0.56
1:F:36:PRO:HB2	1:F:37:PRO:HD3	1.88	0.56
1:C:124:GLY:O	1:C:128:ARG:HG2	2.06	0.56
1:H:54:ARG:HG2	1:H:54:ARG:HH11	1.71	0.55
1:D:67:GLY:HA2	2:D:701:HC4:C2	2.37	0.55
1:B:39:ARG:NH2	3:B:5291:HOH:O	2.39	0.55
1:H:39:ARG:HG3	1:H:39:ARG:HH11	1.72	0.55
3:A:3436:HOH:O	1:D:426:ILE:HD13	2.07	0.54
1:F:60:TYR:OH	2:F:701:HC4:H2	2.08	0.54
1:B:12:GLU:HA	1:B:33:VAL:HG23	1.89	0.54
1:B:60:TYR:OH	2:B:701:HC4:H2	2.08	0.54
1:B:63:THR:HG22	3:B:5312:HOH:O	2.08	0.54
1:A:279:ILE:HD11	1:D:346:HIS:CE1	2.43	0.54
1:C:146:THR:HG22	3:C:1832:HOH:O	2.08	0.53
1:F:68:PRO:HG3	1:F:435:ASN:HB2	1.89	0.53
1:D:36:PRO:HB2	1:D:37:PRO:HD3	1.89	0.53
1:E:145:GLY:HA2	1:F:410:THR:HG23	1.91	0.53
1:A:280:ALA:O	1:D:57:ARG:HD2	2.07	0.53
1:F:124:GLY:O	1:F:128:ARG:HG2	2.09	0.53
1:E:176:ARG:HD2	3:E:3308:HOH:O	2.07	0.53
1:G:153:LEU:HD22	1:G:202:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:12:GLU:HG2	1:D:35:ALA:HB2	1.91	0.53
1:A:184:ARG:NH1	1:A:184:ARG:HG2	2.15	0.53
1:D:12:GLU:HA	1:D:33:VAL:HG13	1.90	0.53
1:F:171:ASP:OD2	1:F:175:THR:HB	2.09	0.53
1:B:252:ARG:HA	1:C:329:ALA:HB1	1.90	0.52
1:H:176:ARG:HD2	3:H:3379:HOH:O	2.08	0.52
1:C:225:TRP:CE2	1:C:517:LEU:HD22	2.43	0.52
1:G:60:TYR:OH	2:G:701:HC4:H2	2.09	0.52
1:H:60:TYR:OH	2:H:701:HC4:H2	2.08	0.52
1:A:487:LYS:O	1:A:491:GLN:HG3	2.10	0.52
1:H:225:TRP:CE2	1:H:517:LEU:HD22	2.45	0.52
1:A:170:LEU:HD23	1:A:176:ARG:HG2	1.91	0.52
1:C:12:GLU:HA	1:C:33:VAL:HG13	1.92	0.52
1:H:271:SER:HB2	1:H:483:SER:HB3	1.91	0.52
1:A:271:SER:HB2	1:A:483:SER:HB3	1.92	0.51
1:B:225:TRP:CE2	1:B:522:PRO:HD3	2.45	0.51
1:H:52:VAL:HG13	1:H:57:ARG:HB2	1.92	0.51
1:G:146:THR:HG22	3:G:1967:HOH:O	2.10	0.51
1:A:225:TRP:CE2	1:A:517:LEU:HD22	2.45	0.51
1:H:132:LEU:C	1:H:132:LEU:HD13	2.31	0.51
1:B:168:ASP:HB2	1:B:176:ARG:HH21	1.76	0.51
1:E:12:GLU:HA	1:E:33:VAL:HG13	1.91	0.51
1:A:263:ARG:O	1:A:267:ARG:HG2	2.11	0.51
1:E:79:VAL:HG21	3:E:2045:HOH:O	2.10	0.51
1:C:36:PRO:HB2	1:C:37:PRO:HD3	1.92	0.51
1:H:487:LYS:O	1:H:491:GLN:HG3	2.11	0.51
1:B:191:LEU:HD21	1:B:201:LEU:CD1	2.41	0.51
1:E:280:ALA:O	1:H:57:ARG:HD2	2.11	0.51
1:C:263:ARG:O	1:C:267:ARG:HG2	2.10	0.51
1:C:176:ARG:HD2	3:C:3285:HOH:O	2.11	0.51
1:D:90:LEU:HD13	1:D:153:LEU:HB3	1.93	0.50
1:G:225:TRP:CE2	1:G:522:PRO:HD3	2.47	0.50
1:F:225:TRP:CE2	1:F:517:LEU:HD22	2.46	0.50
1:A:52:VAL:HG13	1:A:57:ARG:HB2	1.93	0.50
1:B:523:VAL:OXT	1:B:523:VAL:HG12	2.11	0.50
1:B:225:TRP:CE2	1:B:517:LEU:HD22	2.46	0.50
1:C:80:ARG:HE	1:C:194:SER:HA	1.77	0.50
1:D:225:TRP:CE2	1:D:517:LEU:HD22	2.46	0.50
1:E:132:LEU:C	1:E:132:LEU:HD13	2.31	0.50
1:B:258:LYS:HD2	3:B:3514:HOH:O	2.12	0.50
1:F:271:SER:HB2	1:F:483:SER:HB3	1.94	0.50
1:G:523:VAL:OXT	1:G:523:VAL:HG12	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:53:ILE:CG2	1:B:196:ARG:HH11	2.23	0.50
1:H:225:TRP:CE2	1:H:522:PRO:HD3	2.47	0.50
1:D:39:ARG:HG3	3:D:5495:HOH:O	2.12	0.50
1:B:432:ASN:HB2	1:B:436:GLN:HE21	1.76	0.49
1:F:80:ARG:HG2	3:F:2717:HOH:O	2.12	0.49
1:C:80:ARG:NE	1:C:194:SER:HA	2.27	0.49
1:E:271:SER:HB2	1:E:483:SER:HB3	1.94	0.49
1:H:184:ARG:HG2	1:H:184:ARG:HH11	1.78	0.49
1:F:252:ARG:HA	1:G:329:ALA:HB1	1.94	0.49
1:H:66:PHE:CZ	1:H:86:LEU:HD22	2.48	0.49
1:C:211:ILE:HD13	1:C:447:ARG:HG3	1.93	0.49
1:B:34:LEU:HD23	1:B:39:ARG:HG2	1.95	0.49
1:B:132:LEU:HD13	1:B:132:LEU:C	2.33	0.49
1:G:79:VAL:HG11	1:G:196:ARG:HD3	1.94	0.49
1:F:79:VAL:CG1	1:F:196:ARG:HD3	2.42	0.48
1:B:36:PRO:HB2	1:B:37:PRO:HD3	1.94	0.48
1:A:53:ILE:HD13	1:A:196:ARG:HD2	1.95	0.48
1:D:184:ARG:HG2	1:D:184:ARG:HH11	1.77	0.48
1:D:146:THR:HG22	3:D:2324:HOH:O	2.14	0.48
1:A:68:PRO:HG3	1:A:435:ASN:HB2	1.94	0.48
1:H:199:LEU:HD12	1:H:199:LEU:N	2.29	0.48
1:A:252:ARG:HA	1:D:329:ALA:HB1	1.95	0.48
1:G:132:LEU:C	1:G:132:LEU:HD13	2.34	0.48
1:B:68:PRO:HG3	1:B:435:ASN:HB2	1.96	0.48
1:E:288:ASP:O	1:H:73:LEU:HD12	2.13	0.48
1:H:170:LEU:HD23	1:H:176:ARG:HG2	1.96	0.48
1:A:176:ARG:HD2	3:A:3332:HOH:O	2.14	0.48
1:A:170:LEU:CD2	1:A:176:ARG:HG2	2.44	0.48
1:A:132:LEU:HD13	1:A:132:LEU:C	2.34	0.48
1:B:171:ASP:OD1	1:B:171:ASP:C	2.53	0.47
1:D:489:LEU:HD23	1:D:489:LEU:C	2.34	0.47
1:C:523:VAL:OXT	1:C:523:VAL:HG12	2.15	0.47
1:B:489:LEU:C	1:B:489:LEU:HD23	2.35	0.47
1:H:168:ASP:HB2	1:H:176:ARG:HH21	1.80	0.47
1:E:146:THR:HG22	3:E:1932:HOH:O	2.15	0.47
1:B:57:ARG:HD2	1:C:280:ALA:O	2.14	0.47
1:B:271:SER:HB2	1:B:483:SER:HB3	1.97	0.47
1:B:263:ARG:O	1:B:267:ARG:HG2	2.14	0.47
1:A:372:LEU:O	1:A:376:GLN:HG3	2.14	0.47
1:E:225:TRP:CE2	1:E:522:PRO:HD3	2.50	0.47
1:E:171:ASP:OD2	1:E:175:THR:HB	2.14	0.47
1:C:90:LEU:HD13	1:C:153:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:214:VAL:HB	1:H:450:ARG:HH21	1.78	0.47
1:B:426:ILE:HD13	3:C:3493:HOH:O	2.15	0.47
1:E:196:ARG:HH11	1:E:196:ARG:HG3	1.79	0.47
1:G:225:TRP:CE2	1:G:517:LEU:HD22	2.50	0.46
1:E:329:ALA:HB1	1:H:252:ARG:HA	1.97	0.46
1:E:263:ARG:O	1:E:267:ARG:HG2	2.15	0.46
1:A:426:ILE:HD13	3:D:3398:HOH:O	2.14	0.46
1:E:279:ILE:HD11	1:H:346:HIS:CE1	2.50	0.46
1:D:12:GLU:CG	1:D:35:ALA:HB2	2.44	0.46
1:C:80:ARG:HH21	1:C:194:SER:CB	2.29	0.46
1:A:61:GLY:HA3	1:A:199:LEU:HD21	1.98	0.46
1:A:329:ALA:HB1	1:D:252:ARG:HA	1.98	0.46
1:H:297:GLN:HG3	3:H:2410:HOH:O	2.16	0.46
1:A:60:TYR:OH	2:A:701:HC4:H2	2.16	0.46
1:A:124:GLY:O	1:A:128:ARG:HG2	2.16	0.46
1:H:36:PRO:N	1:H:37:PRO:HD2	2.29	0.46
1:E:279:ILE:HD11	1:H:346:HIS:CG	2.51	0.46
1:A:292:GLU:OE1	1:D:73:LEU:HD21	2.15	0.46
1:G:305:ALA:HB3	1:G:306:PRO:HD3	1.98	0.46
1:C:394:HIS:HE1	3:C:2881:HOH:O	1.98	0.46
1:B:12:GLU:HA	1:B:33:VAL:CG2	2.45	0.46
1:G:489:LEU:HD23	1:G:489:LEU:C	2.35	0.46
1:B:12:GLU:HG2	1:B:35:ALA:HB2	1.98	0.45
1:D:124:GLY:O	1:D:128:ARG:HG2	2.16	0.45
1:C:489:LEU:HD23	1:C:489:LEU:C	2.36	0.45
1:H:68:PRO:HG3	1:H:435:ASN:HB2	1.98	0.45
1:D:132:LEU:C	1:D:132:LEU:HD13	2.36	0.45
1:E:100:TRP:CZ2	1:E:172:ARG:HG2	2.51	0.45
1:G:68:PRO:HG3	1:G:435:ASN:HB2	1.99	0.45
1:C:132:LEU:HD13	1:C:132:LEU:C	2.37	0.45
1:B:280:ALA:O	1:C:57:ARG:HD2	2.15	0.45
1:H:124:GLY:O	1:H:128:ARG:HG2	2.16	0.45
1:B:329:ALA:HB1	1:C:252:ARG:HA	1.97	0.45
1:H:53:ILE:HD13	1:H:196:ARG:HD2	1.98	0.45
3:E:3348:HOH:O	1:H:426:ILE:HD13	2.15	0.45
1:B:211:ILE:HD13	1:B:447:ARG:HG3	1.98	0.45
1:E:489:LEU:C	1:E:489:LEU:HD23	2.35	0.45
1:C:225:TRP:CE2	1:C:522:PRO:HG3	2.52	0.45
1:H:184:ARG:NH1	1:H:184:ARG:HG2	2.32	0.45
1:F:12:GLU:CG	1:F:35:ALA:HB2	2.47	0.45
1:B:75:SER:OG	1:B:77:GLU:HG2	2.16	0.45
1:D:48:ARG:NH2	1:D:338:PRO:O	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:170:LEU:HD23	1:C:176:ARG:HG2	1.99	0.45
1:B:372:LEU:O	1:B:376:GLN:HG3	2.16	0.45
1:B:80:ARG:HG2	3:B:5409:HOH:O	2.17	0.45
1:E:225:TRP:CE2	1:E:517:LEU:HD22	2.53	0.44
1:F:90:LEU:HD13	1:F:153:LEU:HB3	1.99	0.44
1:B:53:ILE:HD13	1:B:196:ARG:HD2	1.99	0.44
1:F:321:ARG:HH21	1:G:321:ARG:HH21	1.63	0.44
1:G:36:PRO:N	1:G:37:PRO:HD2	2.33	0.44
1:H:263:ARG:O	1:H:267:ARG:HG2	2.18	0.44
1:D:372:LEU:O	1:D:376:GLN:HG3	2.17	0.44
1:F:51:ALA:O	1:F:55:GLU:HG3	2.17	0.44
1:E:410:THR:HG23	1:F:145:GLY:HA2	1.98	0.44
1:H:66:PHE:CE2	1:H:86:LEU:HB2	2.53	0.44
1:F:181:GLU:OE1	1:F:184:ARG:NH1	2.50	0.44
1:G:124:GLY:O	1:G:128:ARG:HG2	2.17	0.44
1:C:12:GLU:HA	1:C:33:VAL:CG1	2.47	0.44
1:D:225:TRP:CE2	1:D:522:PRO:HD3	2.53	0.44
1:D:66:PHE:CE2	1:D:86:LEU:HB2	2.53	0.44
1:D:211:ILE:HD13	1:D:447:ARG:HG3	1.99	0.44
1:C:79:VAL:HG11	1:C:196:ARG:HD3	2.00	0.44
1:D:297:GLN:HG3	3:D:3086:HOH:O	2.17	0.44
1:H:489:LEU:C	1:H:489:LEU:HD23	2.38	0.44
1:G:145:GLY:HA2	1:H:410:THR:HG23	1.99	0.44
1:D:184:ARG:NH1	1:D:184:ARG:HG2	2.32	0.44
1:H:80:ARG:HH11	1:H:80:ARG:HG3	1.82	0.44
1:F:171:ASP:C	1:F:171:ASP:OD1	2.57	0.44
1:D:271:SER:HB2	1:D:483:SER:HB3	2.00	0.43
1:A:79:VAL:HG11	1:A:196:ARG:HD3	1.99	0.43
1:E:51:ALA:O	1:E:55:GLU:HG3	2.19	0.43
1:F:100:TRP:CH2	1:F:172:ARG:HD3	2.53	0.43
1:D:66:PHE:CZ	1:D:86:LEU:HD22	2.52	0.43
1:F:57:ARG:HD2	1:G:280:ALA:O	2.18	0.43
1:E:57:ARG:HD2	1:H:280:ALA:O	2.19	0.43
1:G:410:THR:HG23	1:H:145:GLY:HA2	2.00	0.43
1:E:252:ARG:HA	1:H:329:ALA:HB1	2.00	0.43
1:A:489:LEU:HD23	1:A:489:LEU:C	2.38	0.43
1:G:395:ARG:CZ	1:G:501:GLU:HG2	2.49	0.43
1:F:76:GLY:O	1:F:79:VAL:HG23	2.19	0.43
1:H:170:LEU:CD2	1:H:176:ARG:HG2	2.48	0.43
1:A:152:ASP:CG	1:A:207:ALA:HB3	2.39	0.43
1:G:348:GLY:HA2	1:G:350:PHE:CE2	2.54	0.43
1:D:60:TYR:HA	1:D:64:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:53:ILE:HD13	1:C:196:ARG:HD2	2.00	0.43
1:D:8:LYS:CG	1:D:31:ARG:HG3	2.49	0.43
1:E:12:GLU:HA	1:E:33:VAL:CG1	2.49	0.42
1:E:80:ARG:HG2	3:E:5099:HOH:O	2.19	0.42
1:H:171:ASP:OD2	1:H:175:THR:HB	2.19	0.42
1:C:68:PRO:HG3	1:C:435:ASN:HB2	2.00	0.42
1:B:170:LEU:CD2	1:B:176:ARG:HG2	2.49	0.42
1:E:279:ILE:HD11	1:H:346:HIS:CD2	2.54	0.42
1:D:169:PHE:CD2	1:D:182:GLY:HA3	2.53	0.42
1:E:36:PRO:HB2	1:E:37:PRO:HD3	2.00	0.42
1:H:238:ARG:NH1	1:H:387:ARG:HH22	2.15	0.42
1:E:152:ASP:CG	1:E:207:ALA:HB3	2.40	0.42
1:A:321:ARG:HH21	1:D:321:ARG:HH21	1.65	0.42
1:H:48:ARG:NH2	1:H:338:PRO:O	2.52	0.42
1:A:7:PRO:O	1:A:8:LYS:C	2.58	0.42
1:A:171:ASP:C	1:A:171:ASP:OD1	2.58	0.42
1:F:489:LEU:HD23	1:F:489:LEU:C	2.40	0.42
1:A:60:TYR:HA	1:A:64:THR:OG1	2.19	0.42
1:D:191:LEU:HD21	1:D:201:LEU:CD1	2.50	0.42
1:G:39:ARG:HD2	1:G:43:ARG:NH2	2.35	0.42
1:F:63:THR:HG22	3:F:4949:HOH:O	2.19	0.42
1:B:394:HIS:HE1	3:B:2935:HOH:O	2.02	0.42
1:C:100:TRP:CZ2	1:C:172:ARG:HG2	2.55	0.42
1:C:125:THR:HG23	1:C:201:LEU:HD11	2.02	0.42
1:H:39:ARG:HD3	1:H:43:ARG:HH21	1.85	0.42
1:A:97:VAL:HA	1:A:141:VAL:O	2.20	0.42
1:A:211:ILE:HD13	1:A:447:ARG:HG3	2.02	0.42
1:G:444:ILE:O	1:G:448:LEU:HG	2.20	0.41
1:A:145:GLY:HA2	1:B:410:THR:HG23	2.02	0.41
1:H:450:ARG:HG2	1:H:450:ARG:HH11	1.85	0.41
1:H:39:ARG:O	1:H:43:ARG:HG3	2.20	0.41
1:G:497:PHE:HA	1:G:498:PRO:HD2	1.95	0.41
1:C:372:LEU:O	1:C:376:GLN:HG3	2.20	0.41
1:G:170:LEU:HD23	1:G:176:ARG:HD2	2.02	0.41
1:A:36:PRO:N	1:A:37:PRO:HD2	2.35	0.41
1:H:372:LEU:O	1:H:376:GLN:HG3	2.20	0.41
1:D:432:ASN:HB3	1:D:436:GLN:HG3	2.03	0.41
1:H:80:ARG:HG2	3:H:5265:HOH:O	2.20	0.41
1:F:61:GLY:HA3	1:F:199:LEU:HD21	2.02	0.41
1:E:211:ILE:HD13	1:E:447:ARG:HG3	2.02	0.41
1:B:50:GLY:O	1:B:54:ARG:HG3	2.20	0.41
1:C:48:ARG:HG2	1:C:48:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:177:LEU:HD21	1:D:185:ARG:NH1	2.35	0.41
1:H:48:ARG:O	1:H:52:VAL:HG23	2.19	0.41
1:G:424:ALA:HB2	1:G:448:LEU:HD12	2.03	0.41
1:B:178:ASP:C	1:B:178:ASP:OD2	2.58	0.41
1:B:79:VAL:HG21	3:B:4966:HOH:O	2.20	0.41
1:A:424:ALA:HB2	1:A:448:LEU:HD12	2.01	0.41
1:B:53:ILE:HG21	1:B:196:ARG:NH1	2.30	0.41
1:H:199:LEU:O	1:H:203:ASN:HB2	2.21	0.41
1:E:196:ARG:NH1	1:E:196:ARG:HG3	2.35	0.41
1:B:337:PRO:HA	1:B:338:PRO:HD3	1.94	0.41
1:F:132:LEU:HD13	1:F:132:LEU:C	2.41	0.41
1:D:136:GLU:HG2	3:D:6033:HOH:O	2.21	0.41
1:A:80:ARG:HB2	3:A:2221:HOH:O	2.19	0.41
1:C:199:LEU:O	1:C:203:ASN:HB2	2.21	0.41
1:H:294:GLU:OE1	1:H:387:ARG:NH2	2.54	0.41
1:B:76:GLY:O	1:B:79:VAL:HG23	2.21	0.41
1:B:278:VAL:HB	1:B:281:GLU:HG3	2.03	0.41
1:E:444:ILE:O	1:E:448:LEU:HG	2.21	0.41
1:B:238:ARG:HH21	1:B:387:ARG:HH21	1.67	0.41
1:C:225:TRP:CD2	1:C:522:PRO:HG3	2.55	0.40
1:A:160:VAL:O	1:A:164:GLN:HG3	2.21	0.40
1:B:300:TYR:N	1:B:300:TYR:CD1	2.89	0.40
1:E:171:ASP:OD1	1:E:171:ASP:C	2.59	0.40
1:C:410:THR:HG23	1:D:145:GLY:HA2	2.03	0.40
1:A:432:ASN:HB3	1:A:436:GLN:HG3	2.04	0.40
1:C:391:PRO:HB2	1:D:69:LEU:HD21	2.02	0.40
1:G:113:SER:OG	1:G:330:VAL:HA	2.21	0.40
1:C:491:GLN:O	1:C:495:GLU:HG3	2.21	0.40
1:D:335:VAL:HG23	1:D:345:LEU:HB2	2.03	0.40
1:C:424:ALA:HB2	1:C:448:LEU:HD12	2.04	0.40
1:E:160:VAL:O	1:E:164:GLN:HG3	2.22	0.40
1:G:337:PRO:HA	1:G:338:PRO:HD3	1.97	0.40
1:E:60:TYR:HH	2:E:701:HC4:H2	1.84	0.40
1:F:372:LEU:O	1:F:376:GLN:HG3	2.21	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%)	504 (98%)	6 (1%)	2 (0%)	43	18
1	B	512/521 (98%)	505 (99%)	6 (1%)	1 (0%)	56	29
1	C	511/521 (98%)	506 (99%)	4 (1%)	1 (0%)	56	29
1	D	511/521 (98%)	503 (98%)	7 (1%)	1 (0%)	56	29
1	E	511/521 (98%)	502 (98%)	8 (2%)	1 (0%)	56	29
1	F	511/521 (98%)	506 (99%)	4 (1%)	1 (0%)	56	29
1	G	511/521 (98%)	506 (99%)	4 (1%)	1 (0%)	56	29
1	H	511/521 (98%)	501 (98%)	9 (2%)	1 (0%)	56	29
All	All	4090/4168 (98%)	4033 (99%)	48 (1%)	9 (0%)	56	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	PRO
1	A	8	LYS
1	B	253	PRO
1	C	253	PRO
1	E	253	PRO
1	H	253	PRO
1	D	253	PRO
1	F	253	PRO
1	G	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%)	383 (100%)	1 (0%)	96	91
1	B	384/389 (99%)	382 (100%)	2 (0%)	94	87
1	C	383/389 (98%)	380 (99%)	3 (1%)	89	78
1	D	383/389 (98%)	381 (100%)	2 (0%)	94	87
1	E	383/389 (98%)	381 (100%)	2 (0%)	94	87
1	F	383/389 (98%)	380 (99%)	3 (1%)	89	78
1	G	383/389 (98%)	381 (100%)	2 (0%)	94	87
1	H	383/389 (98%)	381 (100%)	2 (0%)	94	87
All	All	3066/3112 (98%)	3049 (99%)	17 (1%)	92	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ASP
1	B	332	ASP
1	B	443	THR
1	C	80	ARG
1	C	332	ASP
1	C	443	THR
1	D	332	ASP
1	D	443	THR
1	E	332	ASP
1	E	443	THR
1	F	172	ARG
1	F	332	ASP
1	F	443	THR
1	G	332	ASP
1	G	443	THR
1	H	54	ARG
1	H	332	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	HIS
1	A	491	GLN
1	B	394	HIS
1	B	436	GLN
1	B	519	GLN

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Mol	Chain	Res	Type
1	C	394	HIS
1	D	189	GLN
1	D	394	HIS
1	D	491	GLN
1	E	189	GLN
1	E	394	HIS
1	E	520	GLN
1	F	394	HIS
1	F	491	GLN
1	G	394	HIS
1	H	394	HIS
1	H	508	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	A	149	1	13,13,14	6.17	8 (61%)	16,18,20	2.33	6 (37%)
1	MDO	B	149	1	13,13,14	6.08	8 (61%)	16,18,20	2.38	6 (37%)
1	MDO	C	149	1	13,13,14	5.81	8 (61%)	16,18,20	2.30	6 (37%)
1	MDO	D	149	1	13,13,14	6.16	8 (61%)	16,18,20	2.26	6 (37%)
1	MDO	E	149	1	13,13,14	6.03	8 (61%)	16,18,20	2.36	6 (37%)
1	MDO	F	149	1	13,13,14	6.02	8 (61%)	16,18,20	2.39	6 (37%)
1	MDO	G	149	1	13,13,14	6.22	8 (61%)	16,18,20	2.31	6 (37%)
1	MDO	H	149	1	13,13,14	6.16	8 (61%)	16,18,20	2.32	6 (37%)

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

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	149	MDO	O-C	18.44	1.24	1.11
1	D	149	MDO	O-C	18.37	1.24	1.11
1	A	149	MDO	O-C	18.12	1.23	1.11
1	H	149	MDO	O-C	18.12	1.23	1.11
1	B	149	MDO	O-C	17.84	1.23	1.11
1	E	149	MDO	O-C	17.75	1.23	1.11
1	F	149	MDO	O-C	17.62	1.23	1.11
1	C	149	MDO	O-C	16.47	1.22	1.11
1	H	149	MDO	CB2-CA2	7.75	1.52	1.34
1	B	149	MDO	CB2-CA2	7.75	1.52	1.34
1	D	149	MDO	CB2-CA2	7.67	1.52	1.34
1	A	149	MDO	CB2-CA2	7.65	1.52	1.34
1	F	149	MDO	CB2-CA2	7.60	1.52	1.34
1	E	149	MDO	CB2-CA2	7.60	1.52	1.34
1	C	149	MDO	CB2-CA2	7.59	1.52	1.34
1	G	149	MDO	CB2-CA2	7.45	1.51	1.34
1	A	149	MDO	CA2-N2	-5.58	1.33	1.38
1	E	149	MDO	CA2-N2	-5.35	1.33	1.38
1	G	149	MDO	CA2-N2	-5.26	1.33	1.38
1	C	149	MDO	CA2-N2	-5.11	1.34	1.38
1	F	149	MDO	CA2-N2	-5.03	1.34	1.38
1	H	149	MDO	CA3-C	4.97	1.54	1.48
1	A	149	MDO	CA3-C	4.95	1.54	1.48
1	D	149	MDO	O2-C2	4.82	1.33	1.23
1	C	149	MDO	CA3-C	4.82	1.54	1.48
1	H	149	MDO	O2-C2	4.81	1.33	1.23
1	F	149	MDO	CA3-C	4.80	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	MDO	O2-C2	4.70	1.33	1.23
1	H	149	MDO	CA2-N2	-4.69	1.34	1.38
1	G	149	MDO	CA3-C	4.65	1.54	1.48
1	G	149	MDO	O2-C2	4.62	1.33	1.23
1	B	149	MDO	CA2-N2	-4.62	1.34	1.38
1	C	149	MDO	O2-C2	4.62	1.33	1.23
1	E	149	MDO	CA3-C	4.61	1.54	1.48
1	A	149	MDO	O2-C2	4.59	1.33	1.23
1	F	149	MDO	O2-C2	4.54	1.33	1.23
1	E	149	MDO	O2-C2	4.51	1.33	1.23
1	B	149	MDO	CA3-C	4.42	1.54	1.48
1	D	149	MDO	CA3-C	4.34	1.54	1.48
1	D	149	MDO	CA2-N2	-4.29	1.34	1.38
1	C	149	MDO	C2-N3	-4.23	1.30	1.39
1	G	149	MDO	C2-N3	-4.11	1.31	1.39
1	B	149	MDO	C2-N3	-4.11	1.31	1.39
1	F	149	MDO	C2-N3	-4.04	1.31	1.39
1	H	149	MDO	C2-N3	-4.01	1.31	1.39
1	A	149	MDO	C2-N3	-4.00	1.31	1.39
1	D	149	MDO	C2-N3	-3.89	1.31	1.39
1	E	149	MDO	C2-N3	-3.84	1.31	1.39
1	B	149	MDO	CA3-N3	-3.49	1.44	1.47
1	D	149	MDO	CA3-N3	-3.19	1.44	1.47
1	C	149	MDO	CA3-N3	-3.13	1.44	1.47
1	G	149	MDO	CA3-N3	-3.11	1.44	1.47
1	H	149	MDO	CA3-N3	-2.86	1.44	1.47
1	F	149	MDO	CA3-N3	-2.46	1.45	1.47
1	G	149	MDO	CA2-C2	-2.37	1.37	1.43
1	E	149	MDO	CA3-N3	-2.37	1.45	1.47
1	F	149	MDO	CA2-C2	-2.37	1.37	1.43
1	C	149	MDO	CA2-C2	-2.31	1.38	1.43
1	H	149	MDO	CA2-C2	-2.28	1.38	1.43
1	E	149	MDO	CA2-C2	-2.28	1.38	1.43
1	D	149	MDO	CA2-C2	-2.23	1.38	1.43
1	A	149	MDO	CA2-C2	-2.22	1.38	1.43
1	A	149	MDO	CA3-N3	-2.20	1.45	1.47
1	B	149	MDO	CA2-C2	-2.18	1.38	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	149	MDO	O2-C2-CA2	-5.09	128.02	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	149	MDO	O2-C2-CA2	-4.67	128.26	130.96
1	A	149	MDO	O2-C2-CA2	-4.66	128.27	130.96
1	B	149	MDO	O2-C2-CA2	-4.61	128.29	130.96
1	E	149	MDO	O2-C2-CA2	-4.57	128.32	130.96
1	D	149	MDO	O2-C2-CA2	-4.47	128.37	130.96
1	G	149	MDO	O2-C2-CA2	-4.45	128.38	130.96
1	C	149	MDO	O2-C2-CA2	-4.37	128.43	130.96
1	B	149	MDO	CB2-CA2-C2	4.32	129.30	122.29
1	C	149	MDO	CB2-CA2-C2	4.26	129.20	122.29
1	A	149	MDO	CB2-CA2-C2	4.23	129.15	122.29
1	E	149	MDO	CB2-CA2-C2	4.15	129.02	122.29
1	F	149	MDO	CB2-CA2-C2	4.13	128.99	122.29
1	G	149	MDO	CB2-CA2-C2	4.13	128.98	122.29
1	D	149	MDO	CB2-CA2-C2	4.12	128.96	122.29
1	H	149	MDO	CB2-CA2-C2	4.03	128.83	122.29
1	B	149	MDO	C2-CA2-N2	-3.82	106.00	108.96
1	H	149	MDO	C2-CA2-N2	-3.50	106.25	108.96
1	A	149	MDO	C2-CA2-N2	-3.43	106.30	108.96
1	C	149	MDO	C2-CA2-N2	-3.40	106.32	108.96
1	E	149	MDO	C2-CA2-N2	-3.40	106.32	108.96
1	F	149	MDO	C2-CA2-N2	-3.34	106.37	108.96
1	D	149	MDO	C2-CA2-N2	-3.30	106.40	108.96
1	G	149	MDO	C2-CA2-N2	-3.26	106.43	108.96
1	G	149	MDO	N3-C1-N2	-3.20	109.16	111.51
1	F	149	MDO	N3-C1-N2	-3.02	109.30	111.51
1	E	149	MDO	CA2-N2-C1	3.01	107.99	105.36
1	E	149	MDO	N3-C1-N2	-2.98	109.32	111.51
1	C	149	MDO	N3-C1-N2	-2.97	109.33	111.51
1	H	149	MDO	N3-C1-N2	-2.93	109.36	111.51
1	B	149	MDO	N3-C1-N2	-2.90	109.38	111.51
1	B	149	MDO	CA2-N2-C1	2.78	107.79	105.36
1	D	149	MDO	N3-C1-N2	-2.76	109.48	111.51
1	A	149	MDO	N3-C1-N2	-2.72	109.51	111.51
1	G	149	MDO	CA2-N2-C1	2.71	107.72	105.36
1	A	149	MDO	CA2-N2-C1	2.70	107.72	105.36
1	A	149	MDO	CA2-C2-N3	2.65	109.55	104.40
1	F	149	MDO	CA2-N2-C1	2.64	107.66	105.36
1	F	149	MDO	CA2-C2-N3	2.63	109.50	104.40
1	H	149	MDO	CA2-C2-N3	2.61	109.46	104.40
1	H	149	MDO	CA2-N2-C1	2.60	107.62	105.36
1	C	149	MDO	CA2-C2-N3	2.59	109.42	104.40
1	G	149	MDO	CA2-C2-N3	2.57	109.38	104.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	MDO	CA2-C2-N3	2.56	109.37	104.40
1	C	149	MDO	CA2-N2-C1	2.53	107.57	105.36
1	B	149	MDO	CA2-C2-N3	2.52	109.29	104.40
1	D	149	MDO	CA2-C2-N3	2.47	109.19	104.40
1	D	149	MDO	CA2-N2-C1	2.35	107.41	105.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates 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	HC4	A	701	-	12,12,12	1.47	2 (16%)	15,15,15	0.49	0
2	HC4	B	701	-	12,12,12	1.49	3 (25%)	15,15,15	0.50	0
2	HC4	C	701	-	12,12,12	1.51	4 (33%)	15,15,15	0.50	0
2	HC4	D	701	-	12,12,12	1.43	2 (16%)	15,15,15	0.52	0
2	HC4	E	701	-	12,12,12	1.45	3 (25%)	15,15,15	0.51	0
2	HC4	F	701	-	12,12,12	1.52	2 (16%)	15,15,15	0.45	0
2	HC4	G	701	-	12,12,12	1.45	2 (16%)	15,15,15	0.46	0
2	HC4	H	701	-	12,12,12	1.47	3 (25%)	15,15,15	0.51	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	HC4	A	701	-	-	0/5/5/5	0/1/1/1
2	HC4	B	701	-	-	0/5/5/5	0/1/1/1
2	HC4	C	701	-	-	0/5/5/5	0/1/1/1
2	HC4	D	701	-	-	0/5/5/5	0/1/1/1
2	HC4	E	701	-	-	0/5/5/5	0/1/1/1
2	HC4	F	701	-	-	0/5/5/5	0/1/1/1
2	HC4	G	701	-	-	0/5/5/5	0/1/1/1
2	HC4	H	701	-	-	0/5/5/5	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	HC4	C3'-C2'	2.45	1.43	1.38
2	C	701	HC4	C2'-C1'	2.43	1.44	1.39
2	A	701	HC4	C3'-C2'	2.32	1.43	1.38
2	C	701	HC4	C3'-C4'	2.26	1.43	1.38
2	B	701	HC4	C2'-C1'	2.23	1.43	1.39
2	G	701	HC4	C3'-C2'	2.23	1.43	1.38
2	D	701	HC4	C3'-C2'	2.22	1.43	1.38
2	F	701	HC4	C2'-C1'	2.22	1.43	1.39
2	B	701	HC4	C3'-C2'	2.21	1.43	1.38
2	A	701	HC4	C2'-C1'	2.20	1.43	1.39
2	C	701	HC4	C3'-C2'	2.19	1.43	1.38
2	E	701	HC4	C2'-C1'	2.17	1.43	1.39
2	H	701	HC4	C2'-C1'	2.16	1.43	1.39
2	H	701	HC4	C3'-C2'	2.15	1.42	1.38
2	D	701	HC4	C2'-C1'	2.13	1.43	1.39
2	B	701	HC4	C6'-C5'	2.09	1.42	1.38
2	C	701	HC4	C6'-C5'	2.06	1.42	1.38
2	E	701	HC4	C6'-C5'	2.05	1.42	1.38
2	E	701	HC4	C3'-C2'	2.03	1.42	1.38
2	G	701	HC4	C2'-C1'	2.03	1.43	1.39
2	H	701	HC4	C6'-C5'	2.02	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	515/521 (98%)	-0.01	19 (3%) 39 38	9, 18, 37, 55	0
1	B	515/521 (98%)	-0.14	9 (1%) 67 67	8, 17, 33, 49	0
1	C	514/521 (98%)	-0.25	5 (0%) 79 81	7, 15, 30, 43	0
1	D	514/521 (98%)	-0.09	21 (4%) 35 34	7, 16, 35, 50	0
1	E	514/521 (98%)	-0.12	16 (3%) 47 45	8, 15, 32, 61	0
1	F	514/521 (98%)	-0.35	7 (1%) 72 73	7, 13, 27, 38	0
1	G	514/521 (98%)	-0.31	6 (1%) 75 76	7, 14, 28, 42	0
1	H	514/521 (98%)	-0.01	20 (3%) 37 36	8, 17, 37, 54	0
All	All	4114/4168 (98%)	-0.16	103 (2%) 54 54	7, 15, 33, 61	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	523	VAL	8.9
1	A	7	PRO	8.0
1	B	523	VAL	7.5
1	G	523	VAL	7.3
1	H	77	GLU	6.7
1	B	7	PRO	6.6
1	A	293	PRO	6.4
1	A	523	VAL	6.4
1	A	286	ALA	6.4
1	E	293	PRO	6.1
1	E	523	VAL	6.1
1	E	291	THR	6.1
1	E	286	ALA	6.1
1	F	523	VAL	6.0
1	A	289	ILE	5.7
1	D	523	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	288	ASP	5.6
1	F	293	PRO	5.5
1	C	523	VAL	5.5
1	A	285	ASP	5.5
1	H	74	ILE	5.4
1	A	296	GLY	5.2
1	A	291	THR	5.2
1	D	74	ILE	5.0
1	E	289	ILE	5.0
1	E	290	GLY	4.5
1	E	285	ASP	4.5
1	E	287	GLY	4.4
1	D	293	PRO	4.3
1	D	77	GLU	4.2
1	E	294	GLU	4.1
1	B	277	HIS	4.1
1	E	296	GLY	4.0
1	H	277	HIS	3.7
1	A	294	GLU	3.6
1	H	69	LEU	3.6
1	H	75	SER	3.4
1	D	71	ASN	3.4
1	H	9	PRO	3.4
1	A	277	HIS	3.4
1	H	187	ARG	3.3
1	A	288	ASP	3.3
1	E	277	HIS	3.3
1	A	287	GLY	3.2
1	A	187	ARG	3.2
1	B	172	ARG	3.2
1	F	277	HIS	3.2
1	F	291	THR	3.1
1	D	70	ALA	3.1
1	D	80	ARG	3.1
1	B	173	ASP	3.0
1	B	184	ARG	3.0
1	A	173	ASP	3.0
1	H	172	ARG	2.9
1	D	277	HIS	2.8
1	A	172	ARG	2.8
1	C	172	ARG	2.8
1	E	187	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	60	TYR	2.8
1	H	80	ARG	2.8
1	A	290	GLY	2.8
1	D	294	GLU	2.8
1	D	54	ARG	2.7
1	G	399	GLY	2.7
1	H	73	LEU	2.7
1	H	173	ASP	2.7
1	D	296	GLY	2.6
1	E	295	ALA	2.5
1	D	9	PRO	2.5
1	H	54	ARG	2.5
1	C	173	ASP	2.5
1	F	172	ARG	2.4
1	D	69	LEU	2.4
1	B	293	PRO	2.4
1	H	66	PHE	2.4
1	E	292	GLU	2.4
1	F	80	ARG	2.4
1	G	80	ARG	2.4
1	B	80	ARG	2.3
1	D	75	SER	2.3
1	D	62	LEU	2.3
1	D	60	TYR	2.3
1	G	398	ALA	2.2
1	H	62	LEU	2.2
1	A	292	GLU	2.2
1	H	70	ALA	2.2
1	D	173	ASP	2.2
1	H	8	LYS	2.2
1	D	64	THR	2.2
1	C	171	ASP	2.1
1	B	15	ARG	2.1
1	G	77	GLU	2.1
1	A	480	ASP	2.1
1	H	39	ARG	2.1
1	D	73	LEU	2.1
1	C	184	ARG	2.1
1	D	291	THR	2.1
1	E	80	ARG	2.1
1	G	172	ARG	2.1
1	H	64	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	8	LYS	2.0
1	D	78	ASN	2.0
1	F	289	ILE	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	MDO	F	149	13/14	0.12	6.70	12,15,21,26	0
1	MDO	E	149	13/14	0.10	4.21	10,14,20,22	0
1	MDO	D	149	13/14	0.10	2.64	16,18,23,27	0
1	MDO	G	149	13/14	0.09	2.54	11,14,19,22	0
1	MDO	C	149	13/14	0.10	2.42	10,13,19,20	0
1	MDO	H	149	13/14	0.10	2.03	15,18,25,25	0
1	MDO	B	149	13/14	0.09	1.76	15,17,22,24	0
1	MDO	A	149	13/14	0.09	1.74	13,16,20,20	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HC4	E	701	12/12	0.14	6.18	18,27,33,35	0
2	HC4	A	701	12/12	0.14	4.66	21,29,36,40	0
2	HC4	D	701	12/12	0.19	3.06	25,36,43,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HC4	G	701	12/12	0.12	2.80	16,24,37,42	0
2	HC4	B	701	12/12	0.12	2.65	20,25,31,35	0
2	HC4	C	701	12/12	0.10	2.27	14,21,28,32	0
2	HC4	H	701	12/12	0.17	1.98	28,41,50,51	0
2	HC4	F	701	12/12	0.10	1.81	14,18,29,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.