



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 08:15 PM GMT

PDB ID : 1UMF  
Title : crystal structure of chorismate synthase  
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Deposited on : 2003-09-30  
Resolution : 2.25 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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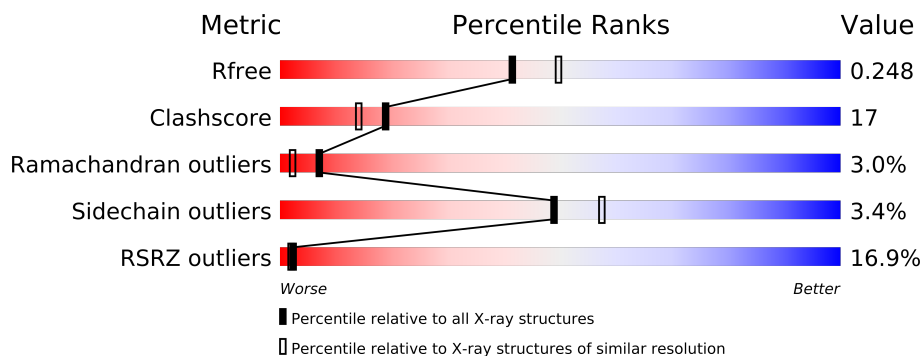
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
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 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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	365	
1	B	365	
1	C	365	
1	D	365	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11756 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	B	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	C	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	D	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			

- Molecule 2 is water.

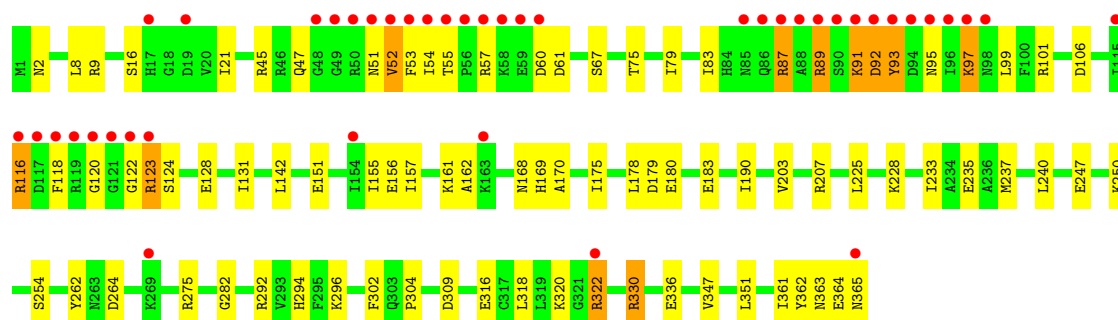
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	173	Total	O	0	0
			173	173		
2	B	82	Total	O	0	0
			82	82		
2	C	90	Total	O	0	0
			90	90		
2	D	147	Total	O	0	0
			147	147		

### 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.

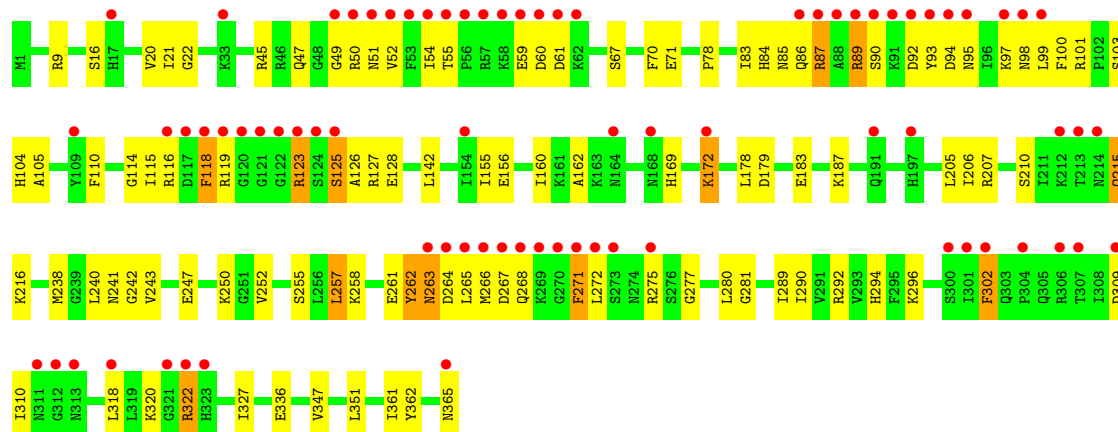
#### • Molecule 1: Chorismate synthase

Chain A: 



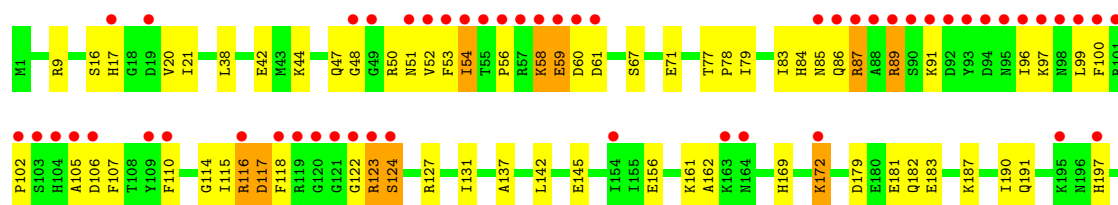
#### • Molecule 1: Chorismate synthase

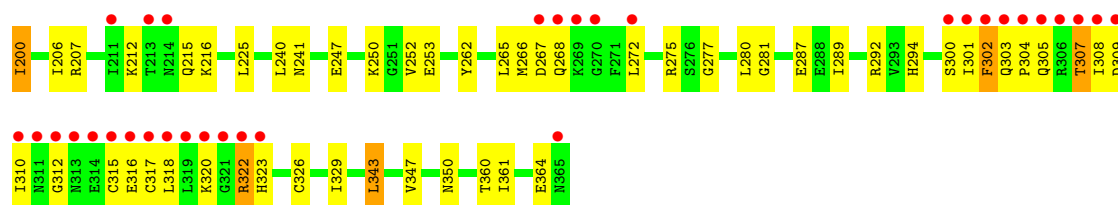
Chain B: 



#### • Molecule 1: Chorismate synthase

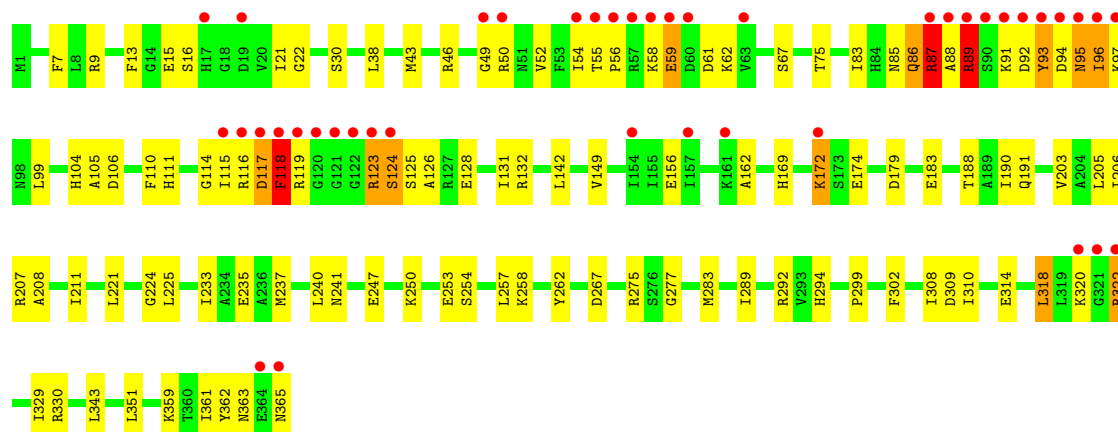
Chain C: 





● Molecule 1: Chorismate synthase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.48Å 146.48Å 132.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.13 – 2.25 21.13 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (21.13-2.25) 98.7 (21.13-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.248 0.202 , 0.248	Depositor DCC
$R_{free}$ test set	6567 reflections (10.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 53.8	EDS
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 64913 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.37	0/2857	0.64	3/3833 (0.1%)
1	B	0.33	0/2857	0.60	2/3833 (0.1%)
1	C	0.33	0/2857	0.59	2/3833 (0.1%)
1	D	0.34	0/2857	0.62	2/3833 (0.1%)
All	All	0.34	0/11428	0.61	9/15332 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	C	87	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	D	89	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	89	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	87	ARG	NE-CZ-NH2	7.29	123.95	120.30
1	B	89	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	B	87	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	D	87	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	8	LEU	N-CA-C	-5.36	96.52	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2816	0	2852	80	0
1	B	2816	0	2852	99	1
1	C	2816	0	2852	123	6
1	D	2816	0	2852	106	5
2	A	173	0	0	6	0
2	B	82	0	0	4	0
2	C	90	0	0	1	0
2	D	147	0	0	5	0
All	All	11756	0	11408	372	7

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 17.

All (372) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:197:HIS:HB3	1:C:302:PHE:HB3	1.40	0.99
1:C:307:THR:HG23	1:C:308:ILE:H	1.34	0.92
1:B:47:GLN:HE22	1:B:60:ASP:HB3	1.35	0.89
1:C:102:PRO:HG2	1:C:305:GLN:HB3	1.56	0.88
1:A:322:ARG:HH11	1:A:322:ARG:H	1.21	0.86
1:A:318:LEU:HD12	1:A:320:LYS:HE3	1.55	0.85
1:D:322:ARG:HB2	1:D:322:ARG:HH11	1.40	0.84
1:D:104:HIS:HB3	1:D:123:ARG:NH2	1.93	0.82
1:D:105:ALA:N	1:D:123:ARG:HH22	1.77	0.82
1:B:238:MET:HE3	1:B:243:VAL:O	1.80	0.81
1:A:128:GLU:HG3	1:D:225:LEU:HD13	1.62	0.81
1:D:322:ARG:HB2	1:D:322:ARG:NH1	1.95	0.81
1:D:105:ALA:H	1:D:123:ARG:HH12	1.29	0.80
1:B:281:GLY:HA3	1:C:105:ALA:HB2	1.64	0.80
1:B:105:ALA:HB3	1:B:123:ARG:HH22	1.49	0.78
1:D:105:ALA:H	1:D:123:ARG:NH1	1.82	0.77
1:D:115:ILE:O	1:D:115:ILE:HD12	1.84	0.77
1:B:250:LYS:HE2	1:B:257:LEU:HD21	1.66	0.76
1:B:67:SER:HB3	1:D:16:SER:HB3	1.66	0.76
1:C:305:GLN:HB2	1:C:317:CYS:SG	2.25	0.76
1:B:54:ILE:HB	1:B:59:GLU:HG3	1.69	0.75
1:D:21:ILE:HG13	1:D:131:ILE:HD11	1.68	0.75
1:D:123:ARG:HG2	1:D:124:SER:N	2.00	0.74
1:D:169:HIS:CD2	1:D:172:LYS:HE3	2.22	0.74
1:C:322:ARG:H	1:C:322:ARG:HD3	1.53	0.73
1:A:361:ILE:HD11	1:B:361:ILE:HD11	1.69	0.73
1:A:45:ARG:HD2	2:A:491:HOH:O	1.88	0.73
1:C:47:GLN:HE22	1:C:60:ASP:HB2	1.53	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:302:PHE:HE2	1:B:318:LEU:HD11	1.55	0.72
1:B:318:LEU:HD12	1:B:320:LYS:HE3	1.70	0.72
1:C:48:GLY:HA2	1:C:52:VAL:HG21	1.69	0.72
1:C:117:ASP:CG	1:C:118:PHE:H	1.93	0.72
1:D:50:ARG:HD3	1:D:52:VAL:O	1.91	0.71
1:B:169:HIS:HA	1:B:172:LYS:HE3	1.72	0.71
1:A:322:ARG:HB2	1:A:322:ARG:NH1	2.08	0.69
1:D:104:HIS:HB3	1:D:123:ARG:HH22	1.55	0.69
1:D:116:ARG:H	1:D:116:ARG:HD2	1.56	0.69
1:D:247:GLU:OE1	1:D:294:HIS:HE1	1.76	0.69
1:B:320:LYS:H	1:B:320:LYS:HD2	1.58	0.68
1:A:75:THR:HA	1:C:115:ILE:HD12	1.73	0.68
1:B:262:TYR:HD1	1:B:263:ASN:N	1.92	0.68
1:A:21:ILE:HG13	1:A:131:ILE:HD11	1.76	0.68
1:A:302:PHE:HE2	1:A:318:LEU:HD11	1.56	0.68
1:D:97:LYS:HA	2:D:463:HOH:O	1.93	0.68
1:C:197:HIS:CB	1:C:302:PHE:HB3	2.22	0.67
1:C:320:LYS:HD2	1:C:320:LYS:H	1.58	0.67
1:A:262:TYR:O	1:A:275:ARG:HD3	1.94	0.67
1:A:361:ILE:HD12	1:B:351:LEU:HD22	1.76	0.67
1:C:97:LYS:NZ	1:C:97:LYS:HB2	2.09	0.67
1:C:247:GLU:HB2	1:C:292:ARG:HB2	1.76	0.67
1:C:247:GLU:OE2	1:C:252:VAL:HG22	1.95	0.67
1:C:322:ARG:HB2	1:C:322:ARG:NH1	2.11	0.66
1:D:105:ALA:N	1:D:123:ARG:NH2	2.44	0.66
1:D:116:ARG:HE	1:D:310:ILE:HD12	1.60	0.66
1:B:247:GLU:OE2	1:B:252:VAL:HG22	1.96	0.66
1:D:99:LEU:HA	1:D:309:ASP:HA	1.77	0.65
1:A:97:LYS:NZ	1:A:97:LYS:HB2	2.10	0.65
1:C:197:HIS:HB2	1:C:303:GLN:HG3	1.78	0.65
1:B:169:HIS:HE1	1:B:183:GLU:OE2	1.79	0.65
1:D:85:ASN:ND2	1:D:86:GLN:HG3	2.12	0.65
1:B:101:ARG:HH11	1:B:101:ARG:HG3	1.62	0.64
1:C:322:ARG:HD3	1:C:322:ARG:N	2.11	0.64
1:C:361:ILE:HD12	1:D:351:LEU:HD22	1.80	0.64
1:C:21:ILE:HG13	1:C:131:ILE:HD11	1.80	0.64
1:D:162:ALA:HB1	1:D:179:ASP:HB2	1.79	0.64
1:B:128:GLU:HG3	1:C:225:LEU:HD13	1.81	0.63
1:B:206:ILE:HD12	1:B:206:ILE:N	2.13	0.63
2:A:501:HOH:O	1:D:258:LYS:HE3	1.99	0.62
1:C:322:ARG:H	1:C:322:ARG:HH11	1.48	0.62
1:D:206:ILE:HD12	1:D:206:ILE:N	2.14	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:212:LYS:HD3	1:C:215:GLN:HG2	1.82	0.62
1:C:100:PHE:CE2	1:C:310:ILE:HA	2.34	0.61
1:C:308:ILE:HD11	1:C:312:GLY:HA2	1.83	0.61
1:C:308:ILE:HG12	1:C:309:ASP:N	2.16	0.61
1:A:330:ARG:HB3	1:A:330:ARG:HH21	1.65	0.61
1:B:262:TYR:CD1	1:B:263:ASN:N	2.68	0.61
1:C:320:LYS:HD2	1:C:320:LYS:N	2.16	0.61
1:A:322:ARG:HH11	1:A:322:ARG:N	1.96	0.60
1:D:169:HIS:O	1:D:172:LYS:HD3	2.01	0.60
1:D:58:LYS:HG3	1:D:59:GLU:HG2	1.84	0.60
1:C:307:THR:HG23	1:C:308:ILE:N	2.11	0.60
1:D:190:ILE:HD11	1:D:329:ILE:HD11	1.84	0.60
1:A:322:ARG:HH11	1:A:322:ARG:HB2	1.68	0.59
1:D:54:ILE:CG2	1:D:58:LYS:HD2	2.33	0.59
1:D:318:LEU:HD13	1:D:320:LYS:HE3	1.83	0.59
1:D:207:ARG:HG2	1:D:208:ALA:N	2.17	0.59
1:A:123:ARG:HG3	1:A:124:SER:H	1.65	0.59
1:A:320:LYS:H	1:A:320:LYS:HD2	1.68	0.59
1:D:169:HIS:HE1	1:D:183:GLU:OE2	1.86	0.58
1:A:225:LEU:HD13	1:D:128:GLU:HG3	1.84	0.58
1:A:47:GLN:HE22	1:A:60:ASP:CG	2.06	0.58
1:B:16:SER:HB3	1:D:67:SER:HB3	1.84	0.58
1:A:16:SER:HB3	1:C:67:SER:HB3	1.84	0.58
1:D:322:ARG:CB	1:D:322:ARG:HH11	2.16	0.58
1:D:106:ASP:H	1:D:123:ARG:NH2	2.00	0.58
1:C:48:GLY:HA2	1:C:52:VAL:CG2	2.33	0.58
1:B:322:ARG:HD3	1:B:322:ARG:N	2.19	0.58
1:D:361:ILE:O	1:D:365:ASN:HB2	2.04	0.57
1:B:267:ASP:O	1:B:268:GLN:HG3	2.03	0.57
1:B:118:PHE:O	1:B:119:ARG:HD2	2.05	0.57
1:B:264:ASP:C	1:B:265:LEU:HD12	2.25	0.57
1:D:54:ILE:HG22	1:D:58:LYS:HD2	1.87	0.57
1:C:322:ARG:HB2	1:C:322:ARG:HH11	1.68	0.57
1:B:247:GLU:OE1	1:B:294:HIS:HE1	1.88	0.57
1:A:161:LYS:HE2	2:A:409:HOH:O	2.04	0.57
1:D:49:GLY:O	1:D:174:GLU:HA	2.05	0.56
1:D:105:ALA:H	1:D:123:ARG:CZ	2.18	0.56
2:B:433:HOH:O	1:D:115:ILE:HD11	2.06	0.56
1:A:156:GLU:HB2	1:A:203:VAL:HB	1.88	0.56
1:A:169:HIS:HE1	1:A:183:GLU:OE2	1.89	0.56
1:C:59:GLU:O	1:C:59:GLU:HG2	2.06	0.56
1:D:116:ARG:N	1:D:116:ARG:HD2	2.20	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:142:LEU:C	1:C:142:LEU:HD23	2.26	0.56
1:B:104:HIS:CD2	1:B:123:ARG:HH11	2.24	0.56
1:D:253:GLU:O	1:D:257:LEU:HD13	2.06	0.56
1:C:100:PHE:CZ	1:C:310:ILE:HA	2.41	0.56
1:D:116:ARG:HG2	1:D:310:ILE:HD13	1.88	0.55
1:D:247:GLU:HB2	1:D:292:ARG:HB2	1.87	0.55
1:C:304:PRO:HG3	1:C:318:LEU:CD2	2.36	0.55
1:A:264:ASP:OD1	1:A:275:ARG:HD2	2.07	0.55
1:C:162:ALA:HB1	1:C:179:ASP:HB2	1.86	0.55
1:A:101:ARG:NH1	1:A:106:ASP:OD2	2.39	0.55
1:C:206:ILE:N	1:C:206:ILE:HD12	2.21	0.55
1:C:247:GLU:OE1	1:C:294:HIS:HE1	1.88	0.55
1:D:116:ARG:CD	1:D:116:ARG:H	2.18	0.55
1:A:247:GLU:OE1	1:A:294:HIS:HE1	1.90	0.55
1:B:162:ALA:HB1	1:B:179:ASP:HB2	1.89	0.55
1:C:301:ILE:H	1:C:305:GLN:NE2	2.06	0.54
1:C:44:LYS:HE2	1:C:56:PRO:HG2	1.89	0.54
1:C:85:ASN:O	1:C:86:GLN:HB2	2.07	0.54
1:A:67:SER:HB3	1:C:16:SER:HB3	1.89	0.54
1:A:45:ARG:HH22	1:A:336:GLU:CD	2.10	0.54
1:B:97:LYS:HB3	1:B:118:PHE:CE2	2.43	0.54
1:B:115:ILE:HD12	1:D:75:THR:HA	1.90	0.54
1:A:162:ALA:HB1	1:A:179:ASP:HB2	1.88	0.54
1:B:277:GLY:O	1:B:289:ILE:HA	2.08	0.54
1:A:157:ILE:HD13	1:A:190:ILE:HD11	1.89	0.54
1:A:363:ASN:O	1:A:364:GLU:HG3	2.07	0.54
1:B:266:MET:H	1:C:307:THR:HA	1.73	0.53
1:D:169:HIS:NE2	1:D:172:LYS:HE3	2.22	0.53
1:A:51:ASN:OD1	1:A:52:VAL:HG23	2.08	0.53
1:A:99:LEU:HA	1:A:309:ASP:HA	1.90	0.53
1:C:100:PHE:HD1	1:C:106:ASP:HB3	1.73	0.53
1:A:142:LEU:C	1:A:142:LEU:HD23	2.29	0.53
1:A:21:ILE:HG23	1:A:83:ILE:HB	1.90	0.52
1:A:362:TYR:CE2	1:B:347:VAL:HG13	2.45	0.52
1:A:122:GLY:O	1:A:124:SER:N	2.43	0.52
1:C:38:LEU:HD23	1:C:42:GLU:HG2	1.90	0.52
1:C:277:GLY:O	1:C:289:ILE:HA	2.09	0.52
1:C:262:TYR:O	1:C:275:ARG:HD2	2.10	0.52
1:A:351:LEU:HD22	1:B:361:ILE:HD12	1.91	0.52
1:C:360:THR:HG23	1:C:364:GLU:OE1	2.09	0.52
1:D:330:ARG:HG3	2:D:392:HOH:O	2.09	0.52
1:A:250:LYS:HB3	1:A:254:SER:OG	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:320:LYS:N	1:D:320:LYS:HD2	2.26	0.51
1:B:20:VAL:HG22	1:B:84:HIS:ND1	2.26	0.51
1:B:258:LYS:HZ3	1:B:261:GLU:HG3	1.76	0.51
1:C:302:PHE:N	1:C:323:HIS:HD2	2.09	0.51
1:C:318:LEU:O	1:C:320:LYS:HD2	2.10	0.51
1:A:322:ARG:H	1:A:322:ARG:NH1	2.00	0.51
1:D:128:GLU:HG2	2:D:469:HOH:O	2.11	0.51
1:B:99:LEU:HA	1:B:309:ASP:HA	1.92	0.51
1:A:97:LYS:HZ2	1:A:97:LYS:HB2	1.75	0.51
1:C:77:THR:HB	1:C:78:PRO:CD	2.41	0.51
1:C:122:GLY:O	1:C:123:ARG:HG2	2.10	0.51
1:A:363:ASN:C	1:A:364:GLU:HG3	2.31	0.51
1:B:266:MET:HB2	1:C:308:ILE:HG22	1.93	0.50
1:B:261:GLU:O	1:B:275:ARG:NH1	2.39	0.50
1:A:302:PHE:HE2	1:A:318:LEU:CD1	2.25	0.50
1:B:105:ALA:HB3	1:B:123:ARG:NH2	2.22	0.50
1:B:169:HIS:O	1:B:172:LYS:HD3	2.11	0.50
1:A:330:ARG:CB	1:A:330:ARG:HH21	2.24	0.50
1:C:197:HIS:O	1:C:303:GLN:HG3	2.11	0.50
1:D:97:LYS:HB2	1:D:97:LYS:NZ	2.26	0.50
1:B:271:PHE:CZ	1:B:280:LEU:HD22	2.47	0.50
1:B:155:ILE:CG2	1:B:178:LEU:HD12	2.42	0.50
1:D:106:ASP:N	1:D:123:ARG:NH2	2.60	0.50
1:B:264:ASP:HB3	1:B:271:PHE:HD2	1.77	0.50
1:C:9:ARG:HD2	2:C:446:HOH:O	2.11	0.50
1:D:106:ASP:H	1:D:123:ARG:HH22	1.58	0.50
1:C:100:PHE:CD1	1:C:106:ASP:HB3	2.47	0.50
1:B:205:LEU:C	1:B:206:ILE:HD12	2.33	0.50
1:D:95:ASN:O	1:D:96:ILE:HB	2.11	0.50
1:A:233:ILE:O	1:A:237:MET:HG2	2.12	0.50
1:A:180:GLU:HG2	2:A:535:HOH:O	2.11	0.49
1:C:265:LEU:HD22	1:C:265:LEU:N	2.27	0.49
1:C:360:THR:O	1:C:364:GLU:HB2	2.13	0.49
1:D:105:ALA:H	1:D:123:ARG:NH2	2.09	0.49
1:C:123:ARG:HG3	1:C:124:SER:N	2.27	0.49
1:B:100:PHE:HB2	1:C:266:MET:HE3	1.94	0.49
1:D:124:SER:O	1:D:126:ALA:N	2.46	0.49
1:B:110:PHE:O	1:B:114:GLY:HA2	2.11	0.49
1:D:320:LYS:H	1:D:320:LYS:HD2	1.77	0.49
1:A:330:ARG:HB3	1:A:330:ARG:NH2	2.28	0.49
1:A:304:PRO:HB3	1:A:316:GLU:OE1	2.13	0.49
1:C:99:LEU:O	1:C:99:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:123:ARG:CG	1:D:124:SER:N	2.75	0.49
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.27	0.49
1:B:104:HIS:HD2	1:B:123:ARG:HH11	1.60	0.48
1:B:105:ALA:H	1:B:123:ARG:HH12	1.61	0.48
1:C:117:ASP:CG	1:C:118:PHE:N	2.64	0.48
1:C:58:LYS:HD3	1:C:58:LYS:H	1.78	0.48
1:A:54:ILE:HG22	1:A:55:THR:N	2.29	0.48
1:B:247:GLU:HB2	1:B:292:ARG:HB2	1.94	0.48
1:B:142:LEU:C	1:B:142:LEU:HD23	2.34	0.48
1:C:20:VAL:HG22	1:C:84:HIS:ND1	2.29	0.48
1:B:9:ARG:HD2	2:B:386:HOH:O	2.13	0.48
1:C:265:LEU:HB2	1:C:272:LEU:HD12	1.95	0.48
1:A:361:ILE:O	1:A:365:ASN:OXT	2.30	0.48
1:B:54:ILE:HG22	1:B:55:THR:N	2.29	0.47
1:B:302:PHE:CE2	1:B:318:LEU:HD11	2.42	0.47
1:A:318:LEU:O	1:A:320:LYS:HD2	2.14	0.47
1:C:123:ARG:HG3	1:C:123:ARG:HH11	1.79	0.47
1:B:116:ARG:HH11	1:B:116:ARG:HG3	1.78	0.47
1:C:21:ILE:HG23	1:C:83:ILE:HB	1.96	0.47
1:C:316:GLU:HG2	1:C:318:LEU:H	1.80	0.47
1:B:215:GLN:OE1	1:B:216:LYS:N	2.47	0.47
1:B:101:ARG:O	1:B:104:HIS:HB2	2.14	0.47
1:C:267:ASP:HB2	1:C:272:LEU:CD2	2.45	0.47
1:C:145:GLU:OE1	1:D:359:LYS:HE2	2.15	0.47
1:C:110:PHE:O	1:C:114:GLY:HA2	2.15	0.47
1:C:190:ILE:HD11	1:C:329:ILE:HD11	1.96	0.47
1:A:93:TYR:HA	1:A:320:LYS:O	2.15	0.47
1:C:38:LEU:HD23	1:C:38:LEU:C	2.36	0.47
1:C:240:LEU:HD23	1:C:241:ASN:N	2.30	0.47
1:A:302:PHE:CE2	1:A:318:LEU:HD11	2.44	0.47
1:C:100:PHE:CD2	1:C:107:PHE:HA	2.50	0.47
1:D:205:LEU:C	1:D:206:ILE:HD12	2.36	0.47
1:D:132:ARG:NH1	2:D:416:HOH:O	2.47	0.47
1:C:99:LEU:HD23	1:C:315:CYS:HB2	1.96	0.47
1:A:322:ARG:HH11	1:A:322:ARG:CB	2.28	0.46
1:B:54:ILE:HD12	1:B:59:GLU:OE2	2.15	0.46
1:D:85:ASN:HD22	1:D:86:GLN:HG3	1.77	0.46
1:D:142:LEU:C	1:D:142:LEU:HD23	2.36	0.46
1:C:309:ASP:HB3	1:C:315:CYS:SG	2.56	0.46
1:A:247:GLU:HB2	1:A:292:ARG:HB2	1.96	0.46
1:D:314:GLU:HG3	2:D:502:HOH:O	2.15	0.46
1:B:98:ASN:O	1:B:310:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:15:GLU:H	1:D:15:GLU:CD	2.18	0.46
1:A:170:ALA:HB2	1:A:178:LEU:HD23	1.98	0.46
1:C:308:ILE:CG1	1:C:312:GLY:HA2	2.45	0.46
1:D:88:ALA:O	1:D:89:ARG:HB2	2.16	0.46
1:A:75:THR:HA	1:C:115:ILE:CD1	2.45	0.46
1:C:161:LYS:O	1:C:182:GLN:HG3	2.16	0.46
1:C:38:LEU:HD22	1:C:137:ALA:HB1	1.97	0.46
1:A:347:VAL:HG13	1:B:362:TYR:CE2	2.50	0.46
1:C:322:ARG:CB	1:C:322:ARG:HH11	2.29	0.45
1:B:116:ARG:HG2	1:B:310:ILE:HD13	1.99	0.45
1:D:117:ASP:O	1:D:119:ARG:HD3	2.16	0.45
1:D:363:ASN:C	1:D:365:ASN:H	2.19	0.45
1:A:228:LYS:HD3	1:A:282:GLY:HA3	1.98	0.45
1:C:97:LYS:HB2	1:C:97:LYS:HZ2	1.79	0.45
1:C:58:LYS:N	1:C:58:LYS:HD3	2.31	0.45
1:D:61:ASP:O	1:D:62:LYS:HB2	2.15	0.45
1:C:322:ARG:HH11	1:C:322:ARG:N	2.12	0.45
1:A:47:GLN:HE22	1:A:60:ASP:CB	2.28	0.45
1:B:101:ARG:NH1	1:B:101:ARG:HG3	2.30	0.45
1:D:99:LEU:C	1:D:99:LEU:HD12	2.37	0.45
1:B:322:ARG:HD3	1:B:322:ARG:H	1.81	0.45
1:B:207:ARG:HG3	1:B:290:ILE:HD13	1.98	0.45
1:C:308:ILE:CD1	1:C:312:GLY:HA2	2.46	0.45
1:C:77:THR:HB	1:C:78:PRO:HD2	1.99	0.45
1:A:322:ARG:N	1:A:322:ARG:HD3	2.32	0.45
1:B:128:GLU:CG	1:C:225:LEU:HD13	2.45	0.45
1:A:47:GLN:HE22	1:A:60:ASP:HB3	1.81	0.45
1:D:21:ILE:HG23	1:D:83:ILE:HB	1.99	0.45
1:B:265:LEU:HD12	1:B:265:LEU:N	2.32	0.45
1:B:361:ILE:O	1:B:365:ASN:HB3	2.17	0.44
1:C:207:ARG:HA	1:C:289:ILE:O	2.17	0.44
1:C:127:ARG:HG2	1:C:127:ARG:NH1	2.31	0.44
1:A:296:LYS:HD2	1:D:262:TYR:CE1	2.52	0.44
1:C:267:ASP:CG	1:C:268:GLN:H	2.21	0.44
1:A:9:ARG:HD2	2:A:416:HOH:O	2.17	0.44
1:C:200:ILE:CD1	1:C:326:CYS:HB2	2.47	0.44
1:B:21:ILE:HG23	1:B:83:ILE:HB	1.98	0.44
1:A:128:GLU:CG	1:D:225:LEU:HD13	2.42	0.44
1:D:247:GLU:OE1	1:D:294:HIS:CE1	2.65	0.44
1:C:122:GLY:O	1:C:124:SER:N	2.45	0.44
1:D:188:THR:HA	1:D:191:GLN:NE2	2.33	0.44
1:B:327:ILE:HA	2:B:399:HOH:O	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:105:ALA:HB2	1:C:281:GLY:HA3	2.00	0.44
1:B:93:TYR:HA	1:B:320:LYS:HB2	2.00	0.44
1:A:67:SER:O	1:A:79:ILE:HA	2.17	0.44
1:C:99:LEU:HA	1:C:309:ASP:HA	1.99	0.44
1:C:67:SER:O	1:C:79:ILE:HA	2.18	0.44
1:A:116:ARG:HG3	1:A:116:ARG:HH11	1.81	0.44
1:B:156:GLU:HG2	2:B:371:HOH:O	2.17	0.44
1:C:116:ARG:NH1	1:C:310:ILE:HG21	2.33	0.44
1:C:47:GLN:NE2	1:C:60:ASP:HB2	2.27	0.43
1:C:127:ARG:HG2	1:C:127:ARG:HH11	1.82	0.43
1:D:262:TYR:O	1:D:275:ARG:HD2	2.19	0.43
1:B:97:LYS:HB3	1:B:118:PHE:CD2	2.53	0.43
1:A:361:ILE:HD11	1:B:361:ILE:CD1	2.45	0.43
1:C:216:LYS:NZ	1:C:287:GLU:OE1	2.50	0.43
1:B:61:ASP:OD2	1:B:85:ASN:HB3	2.18	0.43
1:C:304:PRO:HG3	1:C:318:LEU:HD23	1.99	0.43
1:C:99:LEU:C	1:C:99:LEU:HD12	2.38	0.43
1:B:116:ARG:NH1	1:B:116:ARG:HG3	2.33	0.43
1:D:206:ILE:CD1	1:D:206:ILE:N	2.82	0.43
1:A:2:ASN:OD1	1:C:9:ARG:NH1	2.52	0.43
1:B:92:ASP:C	1:B:94:ASP:H	2.22	0.43
1:C:183:GLU:HG2	1:C:187:LYS:HE3	2.01	0.43
1:A:320:LYS:HD2	1:A:320:LYS:N	2.32	0.43
1:D:308:ILE:HG22	1:D:314:GLU:HG2	2.01	0.43
1:A:155:ILE:CG2	1:A:178:LEU:HD12	2.49	0.43
1:D:221:LEU:O	1:D:283:MET:HA	2.19	0.43
1:B:156:GLU:HA	1:B:160:ILE:O	2.18	0.43
1:B:85:ASN:O	1:B:86:GLN:HB2	2.18	0.43
1:D:233:ILE:O	1:D:237:MET:HG2	2.19	0.43
1:C:50:ARG:O	1:C:51:ASN:HB2	2.19	0.43
1:B:242:GLY:HA2	1:B:296:LYS:HE2	2.01	0.43
1:D:169:HIS:CE1	1:D:183:GLU:OE2	2.69	0.42
1:D:54:ILE:HG21	1:D:58:LYS:HD2	2.01	0.42
1:A:106:ASP:HA	1:A:118:PHE:CZ	2.54	0.42
1:C:187:LYS:O	1:C:191:GLN:HG3	2.18	0.42
1:C:250:LYS:HE3	1:C:253:GLU:HB3	2.00	0.42
1:C:106:ASP:HA	1:C:118:PHE:CZ	2.54	0.42
2:A:519:HOH:O	1:D:111:HIS:HD2	2.02	0.42
1:D:104:HIS:CE1	1:D:299:PRO:HB2	2.55	0.42
1:A:351:LEU:HD22	1:B:361:ILE:CD1	2.49	0.42
1:B:183:GLU:HG2	1:B:187:LYS:HE3	2.01	0.42
1:C:200:ILE:H	1:C:200:ILE:HD12	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:300:SER:HA	1:C:305:GLN:HE22	1.85	0.42
1:D:43:MET:O	1:D:46:ARG:HG2	2.20	0.42
1:B:155:ILE:HG22	1:B:178:LEU:HD12	2.00	0.42
1:B:45:ARG:HH22	1:B:336:GLU:CD	2.23	0.42
1:C:97:LYS:HB2	1:C:97:LYS:HZ3	1.85	0.42
1:D:55:THR:O	1:D:58:LYS:HG2	2.19	0.42
1:D:110:PHE:O	1:D:114:GLY:N	2.50	0.42
1:D:149:VAL:HG11	1:D:211:ILE:HD12	2.01	0.42
1:B:255:SER:OG	1:C:294:HIS:HD2	2.03	0.42
1:C:156:GLU:OE1	1:C:161:LYS:HG2	2.20	0.42
1:D:156:GLU:HB2	1:D:203:VAL:HB	2.02	0.42
1:B:78:PRO:HB2	1:D:13:PHE:O	2.20	0.42
1:D:172:LYS:O	1:D:172:LYS:HG2	2.19	0.41
1:B:21:ILE:HD12	1:B:22:GLY:H	1.84	0.41
1:C:169:HIS:HA	1:C:172:LYS:HZ2	1.85	0.41
1:B:125:SER:O	1:B:127:ARG:N	2.53	0.41
1:B:262:TYR:HD1	1:B:263:ASN:H	1.59	0.41
1:C:320:LYS:CD	1:C:320:LYS:H	2.29	0.41
1:B:103:SER:C	1:C:280:LEU:HD11	2.40	0.41
1:C:343:LEU:O	1:C:347:VAL:HG23	2.20	0.41
1:C:350:ASN:HB3	1:D:362:TYR:OH	2.21	0.41
1:B:101:ARG:NH1	1:B:118:PHE:CE1	2.88	0.41
1:A:235:GLU:HB2	1:D:235:GLU:HB2	2.03	0.41
1:D:105:ALA:N	1:D:123:ARG:HH12	2.06	0.41
1:B:210:SER:HB3	1:B:215:GLN:O	2.20	0.41
1:C:53:PHE:O	1:C:54:ILE:HB	2.20	0.41
1:B:47:GLN:O	1:B:49:GLY:N	2.46	0.41
1:D:115:ILE:CD1	1:D:115:ILE:O	2.63	0.41
1:B:320:LYS:H	1:B:320:LYS:CD	2.31	0.41
1:B:115:ILE:CD1	1:D:30:SER:HB2	2.51	0.41
1:C:267:ASP:HB2	1:C:272:LEU:HD21	2.03	0.41
1:B:125:SER:O	1:B:126:ALA:HB3	2.21	0.41
1:B:70:PHE:CE2	1:B:71:GLU:HG3	2.56	0.41
1:A:91:LYS:HB2	1:A:92:ASP:H	1.64	0.41
1:A:123:ARG:CG	1:A:124:SER:H	2.30	0.41
1:A:175:ILE:HG21	1:A:190:ILE:HD12	2.03	0.41
1:D:250:LYS:HB3	1:D:254:SER:OG	2.20	0.41
1:D:267:ASP:C	1:D:267:ASP:OD2	2.58	0.40
1:A:151:GLU:OE2	1:A:207:ARG:NH1	2.45	0.40
1:C:302:PHE:HD2	1:C:302:PHE:O	2.04	0.40
1:C:215:GLN:OE1	1:C:215:GLN:HA	2.21	0.40
1:C:38:LEU:HD23	1:C:38:LEU:O	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:GLU:OE2	1:D:235:GLU:OE2	2.38	0.40
1:D:118:PHE:CD1	1:D:118:PHE:N	2.88	0.40
1:D:277:GLY:O	1:D:289:ILE:HA	2.22	0.40
1:B:250:LYS:HE2	1:B:257:LEU:CD2	2.46	0.40
1:D:21:ILE:HD12	1:D:22:GLY:H	1.86	0.40
1:D:7:PHE:O	1:D:9:ARG:HG3	2.21	0.40
1:D:322:ARG:HH11	1:D:322:ARG:H	1.69	0.40
1:A:225:LEU:HD13	1:D:128:GLU:CG	2.50	0.40

All (7) 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	Distance(Å)	Clash(Å)
1:C:182:GLN:NE2	1:D:89:ARG:NH2[7_545]	1.37	0.83
1:C:316:GLU:OE1	1:C:316:GLU:OE1[2_655]	1.70	0.50
1:C:71:GLU:OE2	1:D:87:ARG:CG[6_555]	1.71	0.49
1:C:71:GLU:OE2	1:D:87:ARG:NE[6_555]	1.92	0.28
1:C:181:GLU:O	1:D:89:ARG:NH1[7_545]	2.05	0.15
1:B:272:LEU:CD2	1:B:272:LEU:CD2[2_655]	2.07	0.13
1:C:71:GLU:OE2	1:D:87:ARG:CD[6_555]	2.14	0.06

## 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	363/365 (100%)	323 (89%)	30 (8%)	10 (3%)	8	3
1	B	363/365 (100%)	318 (88%)	34 (9%)	11 (3%)	7	2
1	C	363/365 (100%)	323 (89%)	31 (8%)	9 (2%)	9	3
1	D	363/365 (100%)	333 (92%)	17 (5%)	13 (4%)	5	1
All	All	1452/1460 (100%)	1297 (89%)	112 (8%)	43 (3%)	7	2

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	95	ASN
1	A	116	ARG
1	A	123	ARG
1	B	95	ASN
1	B	118	PHE
1	B	125	SER
1	B	262	TYR
1	B	263	ASN
1	B	271	PHE
1	C	61	ASP
1	C	117	ASP
1	C	307	THR
1	D	124	SER
1	A	52	VAL
1	B	50	ARG
1	B	51	ASN
1	B	123	ARG
1	C	124	SER
1	D	56	PRO
1	D	92	ASP
1	A	61	ASP
1	C	54	ILE
1	C	116	ARG
1	C	123	ARG
1	D	59	GLU
1	D	86	GLN
1	D	94	ASP
1	D	96	ILE
1	D	117	ASP
1	D	125	SER
1	A	87	ARG
1	A	97	LYS
1	A	120	GLY
1	D	89	ARG
1	A	92	ASP
1	C	59	GLU
1	D	93	TYR
1	D	118	PHE
1	B	90	SER
1	D	224	GLY
1	B	52	VAL
1	C	96	ILE

### 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	300/300 (100%)	292 (97%)	8 (3%)	57	67
1	B	300/300 (100%)	291 (97%)	9 (3%)	53	62
1	C	300/300 (100%)	290 (97%)	10 (3%)	50	59
1	D	300/300 (100%)	286 (95%)	14 (5%)	36	40
All	All	1200/1200 (100%)	1159 (97%)	41 (3%)	49	57

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	89	ARG
1	A	91	LYS
1	A	93	TYR
1	A	168	ASN
1	A	240	LEU
1	A	322	ARG
1	A	330	ARG
1	B	87	ARG
1	B	89	ARG
1	B	172	LYS
1	B	215	GLN
1	B	240	LEU
1	B	241	ASN
1	B	257	LEU
1	B	302	PHE
1	B	322	ARG
1	C	17	HIS
1	C	58	LYS
1	C	87	ARG
1	C	89	ARG
1	C	91	LYS
1	C	172	LYS
1	C	200	ILE
1	C	302	PHE
1	C	322	ARG

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Mol	Chain	Res	Type
1	C	343	LEU
1	D	38	LEU
1	D	87	ARG
1	D	91	LYS
1	D	93	TYR
1	D	95	ASN
1	D	118	PHE
1	D	123	ARG
1	D	172	LYS
1	D	240	LEU
1	D	241	ASN
1	D	302	PHE
1	D	318	LEU
1	D	322	ARG
1	D	343	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	85	ASN
1	A	104	HIS
1	A	168	ASN
1	A	169	HIS
1	A	182	GLN
1	A	186	GLN
1	A	215	GLN
1	A	223	GLN
1	A	241	ASN
1	A	294	HIS
1	A	313	ASN
1	B	47	GLN
1	B	51	ASN
1	B	168	ASN
1	B	169	HIS
1	B	186	GLN
1	B	191	GLN
1	B	223	GLN
1	B	241	ASN
1	B	263	ASN
1	B	294	HIS
1	B	313	ASN

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Mol	Chain	Res	Type
1	C	47	GLN
1	C	51	ASN
1	C	168	ASN
1	C	186	GLN
1	C	191	GLN
1	C	214	ASN
1	C	223	GLN
1	C	294	HIS
1	C	303	GLN
1	C	305	GLN
1	C	313	ASN
1	C	323	HIS
1	D	47	GLN
1	D	85	ASN
1	D	104	HIS
1	D	111	HIS
1	D	169	HIS
1	D	186	GLN
1	D	191	GLN
1	D	215	GLN
1	D	223	GLN
1	D	294	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 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	365/365 (100%)	0.74	43 (11%) 5 6	19, 30, 131, 176	9 (2%)
1	B	365/365 (100%)	1.36	76 (20%) 1 1	23, 41, 141, 167	9 (2%)
1	C	365/365 (100%)	1.90	86 (23%) 1 1	22, 39, 168, 183	9 (2%)
1	D	365/365 (100%)	0.45	42 (11%) 5 6	20, 34, 110, 149	9 (2%)
All	All	1460/1460 (100%)	1.11	247 (16%) 2 2	19, 36, 146, 183	36 (2%)

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	302	PHE	35.1
1	B	270	GLY	24.9
1	B	272	LEU	23.8
1	C	99	LEU	21.6
1	A	93	TYR	21.2
1	A	53	PHE	19.7
1	C	301	ILE	19.5
1	A	55	THR	17.4
1	C	306	ARG	17.2
1	B	53	PHE	16.6
1	C	96	ILE	16.3
1	A	56	PRO	15.9
1	B	51	ASN	15.7
1	C	52	VAL	14.9
1	C	98	ASN	14.8
1	A	58	LYS	14.6
1	A	92	ASP	14.2
1	C	56	PRO	13.8
1	C	315	CYS	13.6
1	B	54	ILE	13.5
1	C	313	ASN	13.5

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Mol	Chain	Res	Type	RSRZ
1	C	309	ASP	13.5
1	C	305	GLN	13.5
1	C	54	ILE	13.2
1	C	310	ILE	13.1
1	B	52	VAL	13.1
1	A	52	VAL	12.6
1	B	267	ASP	12.6
1	D	89	ARG	12.6
1	D	90	SER	12.4
1	C	93	TYR	12.1
1	B	268	GLN	11.9
1	C	95	ASN	11.9
1	C	300	SER	11.9
1	C	55	THR	11.9
1	C	307	THR	11.8
1	A	88	ALA	11.8
1	A	51	ASN	11.8
1	A	49	GLY	11.7
1	C	317	CYS	11.5
1	C	320	LYS	11.5
1	D	121	GLY	11.5
1	A	50	ARG	11.4
1	C	101	ARG	11.4
1	B	93	TYR	11.4
1	B	88	ALA	11.3
1	B	271	PHE	11.3
1	B	90	SER	11.1
1	D	88	ALA	11.0
1	A	54	ILE	11.0
1	C	321	GLY	10.9
1	A	89	ARG	10.8
1	A	91	LYS	10.8
1	B	266	MET	10.8
1	B	92	ASP	10.6
1	A	90	SER	10.4
1	A	95	ASN	10.3
1	C	88	ALA	9.8
1	B	56	PRO	9.8
1	C	314	GLU	9.7
1	B	55	THR	9.5
1	B	118	PHE	9.2
1	C	92	ASP	9.0

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Mol	Chain	Res	Type	RSRZ
1	C	94	ASP	9.0
1	C	311	ASN	8.7
1	C	90	SER	8.6
1	C	308	ILE	8.5
1	B	87	ARG	8.5
1	C	57	ARG	8.5
1	A	94	ASP	8.5
1	C	214	ASN	8.5
1	C	118	PHE	8.4
1	C	58	LYS	8.4
1	C	86	GLN	8.2
1	C	87	ARG	8.2
1	C	303	GLN	8.2
1	D	123	ARG	8.1
1	C	59	GLU	8.1
1	C	213	THR	8.0
1	B	263	ASN	8.0
1	C	102	PRO	7.8
1	B	57	ARG	7.7
1	A	96	ILE	7.7
1	C	49	GLY	7.7
1	D	120	GLY	7.7
1	C	104	HIS	7.6
1	C	319	LEU	7.6
1	C	51	ASN	7.6
1	C	103	SER	7.5
1	C	105	ALA	7.5
1	C	318	LEU	7.3
1	A	59	GLU	7.3
1	B	273	SER	7.2
1	A	121	GLY	7.2
1	A	57	ARG	7.0
1	D	91	LYS	6.8
1	A	118	PHE	6.8
1	B	58	LYS	6.8
1	C	322	ARG	6.8
1	B	50	ARG	6.8
1	B	94	ASP	6.6
1	B	91	LYS	6.5
1	C	304	PRO	6.5
1	A	120	GLY	6.5
1	C	123	ARG	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	119	ARG	6.4
1	B	89	ARG	6.3
1	C	121	GLY	6.2
1	C	91	LYS	6.2
1	D	365	ASN	6.1
1	B	265	LEU	6.1
1	C	89	ARG	6.1
1	B	119	ARG	6.0
1	C	53	PHE	5.9
1	C	312	GLY	5.9
1	D	364	GLU	5.8
1	B	264	ASP	5.8
1	B	120	GLY	5.8
1	D	94	ASP	5.7
1	A	86	GLN	5.7
1	C	365	ASN	5.5
1	D	92	ASP	5.5
1	C	48	GLY	5.5
1	D	93	TYR	5.5
1	A	365	ASN	5.5
1	D	59	GLU	5.4
1	B	214	ASN	5.2
1	B	365	ASN	5.2
1	C	100	PHE	5.1
1	B	121	GLY	5.1
1	D	58	LYS	5.1
1	B	168	ASN	4.9
1	B	122	GLY	4.9
1	C	267	ASP	4.8
1	D	49	GLY	4.8
1	A	17	HIS	4.7
1	C	85	ASN	4.7
1	D	124	SER	4.7
1	A	115	ILE	4.7
1	B	321	GLY	4.6
1	C	269	LYS	4.6
1	C	272	LEU	4.5
1	C	124	SER	4.5
1	C	119	ARG	4.5
1	A	60	ASP	4.5
1	D	119	ARG	4.3
1	D	56	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	87	ARG	4.3
1	B	172	LYS	4.3
1	B	269	LYS	4.2
1	B	59	GLU	4.2
1	C	19	ASP	4.2
1	C	316	GLU	4.2
1	B	322	ARG	4.2
1	B	97	LYS	4.1
1	C	323	HIS	4.1
1	B	306	ARG	4.0
1	B	123	ARG	4.0
1	D	17	HIS	4.0
1	B	49	GLY	4.0
1	D	122	GLY	4.0
1	B	213	THR	3.9
1	D	321	GLY	3.9
1	B	95	ASN	3.9
1	B	275	ARG	3.8
1	B	17	HIS	3.7
1	C	97	LYS	3.7
1	B	300	SER	3.7
1	D	95	ASN	3.7
1	B	116	ARG	3.5
1	B	212	LYS	3.5
1	A	123	ARG	3.5
1	C	211	ILE	3.5
1	B	313	ASN	3.5
1	C	122	GLY	3.5
1	D	57	ARG	3.5
1	A	87	ARG	3.5
1	B	301	ILE	3.5
1	B	62	LYS	3.5
1	D	118	PHE	3.4
1	B	61	ASP	3.4
1	C	17	HIS	3.4
1	D	19	ASP	3.3
1	D	55	THR	3.3
1	D	116	ARG	3.3
1	A	97	LYS	3.2
1	D	60	ASP	3.2
1	B	60	ASP	3.2
1	C	116	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	117	ASP	3.1
1	A	48	GLY	3.1
1	D	320	LYS	3.0
1	D	322	ARG	3.0
1	B	323	HIS	3.0
1	C	120	GLY	3.0
1	B	124	SER	3.0
1	A	85	ASN	2.9
1	D	115	ILE	2.9
1	C	172	LYS	2.9
1	B	191	GLN	2.9
1	B	98	ASN	2.9
1	D	97	LYS	2.8
1	A	269	LYS	2.8
1	B	312	GLY	2.7
1	D	172	LYS	2.7
1	A	116	ARG	2.7
1	B	86	GLN	2.6
1	C	270	GLY	2.6
1	B	304	PRO	2.6
1	B	99	LEU	2.6
1	B	164	ASN	2.6
1	C	268	GLN	2.5
1	D	154	ILE	2.5
1	A	122	GLY	2.5
1	B	309	ASP	2.5
1	C	60	ASP	2.4
1	C	154	ILE	2.4
1	B	302	PHE	2.4
1	A	322	ARG	2.4
1	C	109	TYR	2.4
1	A	163	LYS	2.3
1	D	63	VAL	2.3
1	A	19	ASP	2.3
1	A	117	ASP	2.3
1	C	195	LYS	2.3
1	C	164	ASN	2.3
1	A	98	ASN	2.2
1	C	110	PHE	2.2
1	B	154	ILE	2.2
1	B	307	THR	2.2
1	B	311	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	96	ILE	2.2
1	D	157	ILE	2.2
1	D	161	LYS	2.2
1	B	109	TYR	2.2
1	C	61	ASP	2.1
1	D	54	ILE	2.1
1	B	318	LEU	2.1
1	A	154	ILE	2.1
1	B	125	SER	2.1
1	C	106	ASP	2.1
1	B	197	HIS	2.1
1	D	50	ARG	2.1
1	C	197	HIS	2.1
1	C	163	LYS	2.1
1	B	33	LYS	2.0
1	B	117	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.