



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:14 AM GMT

PDB ID : 2GAF  
Title : Crystal Structure of the Vaccinia Polyadenylate Polymerase Heterodimer (apo form)  
Authors : Moure, C.M.; Bowman, B.R.; Gershon, P.D.; Quioco, F.A.  
Deposited on : 2006-03-08  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

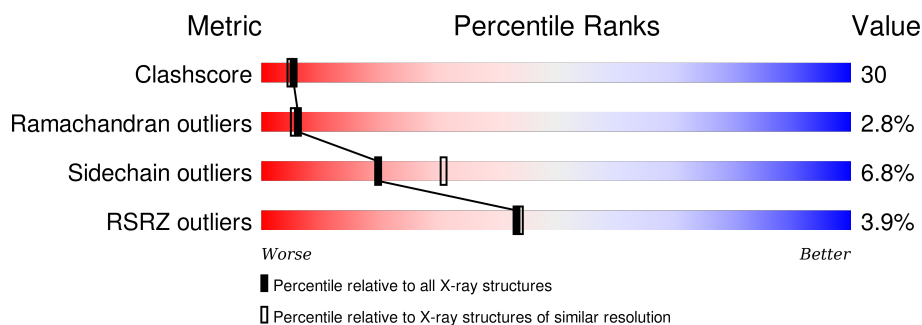
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	297	<div> <div>2%</div> <div>61% 31% . . .</div> </div>
2	D	469	<div> <div>4%</div> <div>46% 43% 6% • 5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6151 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 Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	Se	0	0	0
			2370	1547	392	419	2	10			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	11	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	92	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	140	ALA	ARG	ENGINEERED	UNP P07617
A	142	ALA	LYS	ENGINEERED	UNP P07617
A	143	ALA	ARG	ENGINEERED	UNP P07617
A	163	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	196	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	208	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	219	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	236	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	263	MSE	MET	MODIFIED RESIDUE	UNP P07617
A	266	MSE	MET	MODIFIED RESIDUE	UNP P07617

- Molecule 2 is a protein called Poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	447	Total	C	N	O	S	0	0	0
			3641	2329	607	681	24			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	36	SER	LEU	VARIANT	UNP P23371

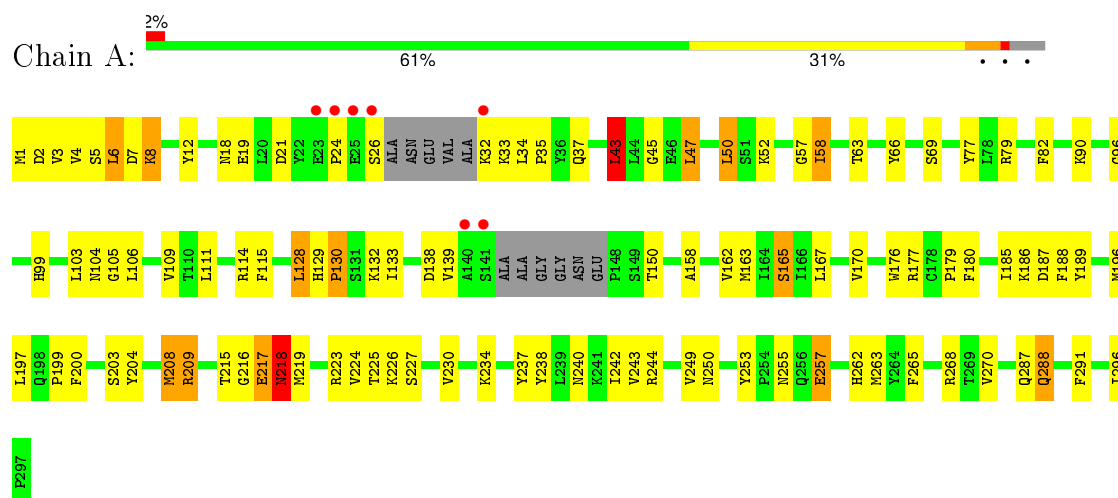
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total 59	O 59	0	0
3	D	81	Total 81	O 81	0	0

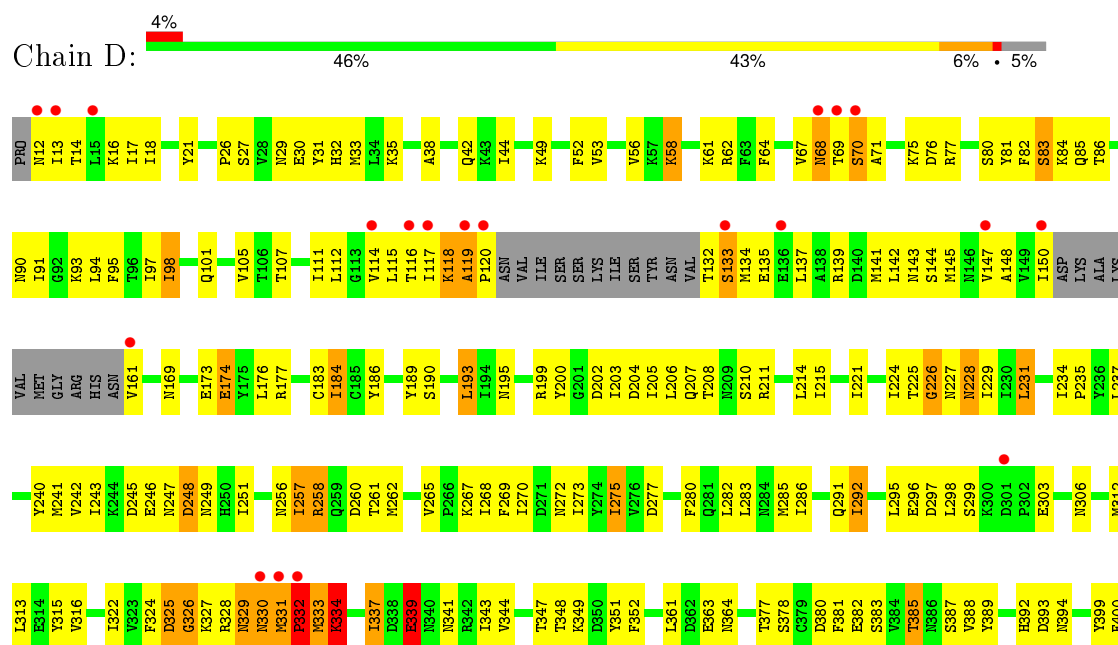
### 3 Residue-property plots

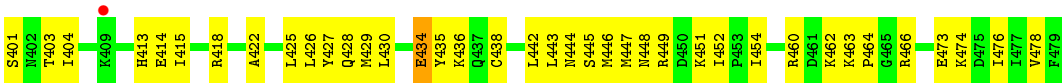
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase



- Molecule 2: Poly(A) polymerase catalytic subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.08Å 91.26Å 133.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.40 38.07 – 2.26	Depositor EDS
% Data completeness (in resolution range)	83.6 (500.00-2.40) 81.8 (38.07-2.26)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.27Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.243 , 0.288 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63502 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6151	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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	0.42	0/2423	0.68	1/3263 (0.0%)
2	D	0.43	0/3701	0.67	0/4992
All	All	0.42	0/6124	0.67	1/8255 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2370	0	2388	104	0
2	D	3641	0	3710	258	0
3	A	59	0	0	8	0
3	D	81	0	0	8	0
All	All	6151	0	6098	361	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 30.

All (361) 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)
2:D:21:TYR:CZ	2:D:85:GLN:HG2	1.91	1.05
2:D:147:VAL:HG11	2:D:452:ILE:O	1.56	1.04
1:A:215:THR:HG22	1:A:216:GLY:N	1.80	0.94
2:D:190:SER:HB2	2:D:275:ILE:HG13	1.49	0.94
1:A:34:LEU:HB2	1:A:37:GLN:OE1	1.69	0.93
2:D:378:SER:HB3	2:D:388:VAL:CG1	2.01	0.91
1:A:104:ASN:ND2	1:A:111:LEU:HD12	1.87	0.90
2:D:119:ALA:HB3	2:D:120:PRO:HD3	1.51	0.90
2:D:413:HIS:HD2	2:D:415:ILE:H	1.12	0.89
2:D:303:GLU:HA	2:D:306:ASN:HD22	1.35	0.89
2:D:443:LEU:HD23	2:D:446:MET:HE3	1.54	0.89
2:D:141:MET:HE1	2:D:313:LEU:HD11	1.56	0.88
1:A:104:ASN:HD21	1:A:111:LEU:HD12	1.38	0.88
2:D:291:GLN:HA	2:D:403:THR:HG22	1.56	0.87
2:D:147:VAL:O	2:D:147:VAL:HG12	1.73	0.86
2:D:183:CYS:SG	2:D:205:ILE:HG21	2.16	0.86
2:D:84:LYS:HG3	2:D:97:ILE:HD13	1.58	0.85
2:D:331:MET:O	2:D:332:PRO:C	2.14	0.85
1:A:215:THR:O	3:A:337:HOH:O	1.97	0.83
2:D:94:LEU:O	2:D:98:ILE:HG22	1.78	0.82
2:D:225:THR:O	2:D:227:ASN:N	2.13	0.81
1:A:7:ASP:HB2	1:A:8:LYS:NZ	1.95	0.81
2:D:269:PHE:CZ	2:D:272:ASN:HA	2.17	0.80
1:A:218:ASN:N	1:A:218:ASN:HD22	1.78	0.80
2:D:325:ASP:H	2:D:444:ASN:ND2	1.78	0.79
2:D:135:GLU:HB3	2:D:139:ARG:HH21	1.45	0.79
2:D:434:GLU:CD	2:D:434:GLU:H	1.81	0.79
2:D:378:SER:HB3	2:D:388:VAL:HG11	1.64	0.79
2:D:141:MET:CE	2:D:313:LEU:HD11	2.13	0.78
1:A:217:GLU:OE1	1:A:218:ASN:ND2	2.17	0.77
2:D:203:ILE:HG22	2:D:205:ILE:HD11	1.65	0.77
2:D:331:MET:HB3	2:D:332:PRO:CD	2.13	0.77
1:A:66:TYR:CD1	1:A:69:SER:HB3	2.20	0.76
2:D:413:HIS:HE1	2:D:452:ILE:O	1.66	0.76
2:D:184:ILE:HG21	2:D:262:MET:HE1	1.68	0.76
1:A:7:ASP:HB2	1:A:8:LYS:HZ3	1.50	0.76
2:D:392:HIS:O	2:D:394:ASN:N	2.18	0.76
2:D:331:MET:HG2	2:D:445:SER:CB	2.16	0.76
2:D:283:LEU:HD22	2:D:429:MET:CE	2.17	0.75
1:A:237:TYR:HA	3:A:304:HOH:O	1.87	0.75
1:A:215:THR:CG2	1:A:216:GLY:N	2.48	0.75
2:D:280:PHE:HA	2:D:429:MET:HE3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:PRO:O	2:D:334:LYS:N	2.19	0.74
2:D:132:THR:HG22	2:D:133:SER:H	1.51	0.74
1:A:215:THR:HG22	1:A:216:GLY:H	1.52	0.74
2:D:67:VAL:HG11	2:D:224:ILE:HG12	1.69	0.74
2:D:332:PRO:C	2:D:334:LYS:H	1.89	0.74
1:A:58:ILE:O	1:A:58:ILE:HD12	1.89	0.73
2:D:334:LYS:HG3	2:D:334:LYS:O	1.89	0.73
1:A:255:ASN:OD1	1:A:257:GLU:HB2	1.89	0.72
2:D:147:VAL:O	2:D:147:VAL:CG1	2.35	0.72
2:D:361:LEU:HD21	2:D:404:ILE:HD11	1.71	0.72
2:D:292:ILE:H	2:D:403:THR:HG21	1.55	0.72
2:D:331:MET:HG2	2:D:445:SER:OG	1.89	0.72
2:D:385:THR:HG21	2:D:389:TYR:HE1	1.53	0.71
2:D:325:ASP:H	2:D:444:ASN:HD22	1.39	0.70
2:D:385:THR:HG22	2:D:387:SER:H	1.57	0.70
1:A:106:LEU:HB2	1:A:109:VAL:HG22	1.73	0.70
2:D:378:SER:HB3	2:D:388:VAL:HG13	1.73	0.69
1:A:129:HIS:HA	3:A:300:HOH:O	1.91	0.69
1:A:165:SER:HB2	1:A:219:MSE:HE1	1.75	0.69
2:D:316:VAL:CG1	2:D:322:ILE:HD12	2.22	0.69
2:D:333:MET:CE	2:D:348:THR:HG22	2.23	0.69
1:A:165:SER:CB	1:A:219:MSE:HE1	2.23	0.69
2:D:325:ASP:N	2:D:447:MET:HE1	2.08	0.68
2:D:214:LEU:O	2:D:243:ILE:HD11	1.94	0.68
2:D:190:SER:HB2	2:D:275:ILE:CG1	2.21	0.68
2:D:385:THR:HG21	2:D:389:TYR:CE1	2.29	0.68
2:D:44:ILE:HD13	2:D:101:GLN:HE21	1.59	0.68
2:D:364:ASN:HA	3:D:518:HOH:O	1.94	0.68
2:D:147:VAL:HG22	2:D:451:LYS:HB3	1.76	0.67
2:D:268:ILE:HD12	2:D:277:ASP:HA	1.76	0.67
1:A:19:GLU:HB2	1:A:234:LYS:HB3	1.74	0.67
2:D:150:ILE:HG12	2:D:299:SER:OG	1.93	0.67
2:D:64:PHE:HB3	2:D:67:VAL:HG23	1.76	0.67
1:A:199:PRO:HD3	1:A:262:HIS:CE1	2.30	0.67
2:D:31:TYR:O	2:D:35:LYS:HB2	1.95	0.66
1:A:199:PRO:HD2	3:A:319:HOH:O	1.95	0.66
1:A:34:LEU:CD2	1:A:35:PRO:HD2	2.26	0.66
1:A:219:MSE:HG2	3:A:315:HOH:O	1.96	0.66
2:D:189:TYR:O	2:D:193:LEU:HD22	1.94	0.66
2:D:144:SER:O	2:D:147:VAL:HG23	1.95	0.66
2:D:62:ARG:HH22	2:D:118:LYS:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:N	1:A:218:ASN:ND2	2.44	0.66
1:A:33:LYS:O	1:A:33:LYS:HG3	1.96	0.65
1:A:265:PHE:HA	1:A:268:ARG:HD3	1.78	0.65
1:A:215:THR:HG21	1:A:217:GLU:OE2	1.96	0.65
1:A:263:MSE:HE1	1:A:287:GLN:NE2	2.10	0.65
2:D:331:MET:SD	2:D:442:LEU:HA	2.36	0.65
2:D:283:LEU:HD22	2:D:429:MET:HE1	1.77	0.65
2:D:176:LEU:HB3	2:D:273:ILE:HG12	1.79	0.65
2:D:64:PHE:HB3	2:D:67:VAL:CG2	2.27	0.65
2:D:119:ALA:CB	2:D:120:PRO:HD3	2.26	0.64
2:D:331:MET:HB3	2:D:332:PRO:HD3	1.78	0.64
1:A:291:PHE:HB3	1:A:296:ILE:O	1.97	0.64
2:D:332:PRO:C	2:D:334:LYS:N	2.48	0.64
2:D:418:ARG:HG2	2:D:442:LEU:HD11	1.79	0.64
2:D:147:VAL:CG1	2:D:452:ILE:O	2.39	0.64
2:D:119:ALA:HB3	2:D:120:PRO:CD	2.28	0.63
2:D:425:LEU:HD21	2:D:438:CYS:SG	2.38	0.63
2:D:58:LYS:O	2:D:61:LYS:HG2	1.99	0.63
2:D:18:ILE:HG22	2:D:26:PRO:HG3	1.78	0.63
2:D:361:LEU:HD11	2:D:404:ILE:HD12	1.81	0.63
2:D:82:PHE:C	2:D:85:GLN:HE22	2.03	0.62
2:D:331:MET:O	2:D:333:MET:N	2.32	0.62
2:D:325:ASP:H	2:D:447:MET:HE1	1.65	0.62
1:A:58:ILE:CD1	1:A:170:VAL:HG21	2.29	0.61
2:D:444:ASN:HA	2:D:447:MET:HE2	1.80	0.61
2:D:283:LEU:HD22	2:D:429:MET:HE2	1.82	0.61
2:D:12:ASN:HB3	2:D:16:LYS:HE3	1.81	0.61
1:A:188:PHE:CE2	1:A:224:VAL:HG11	2.34	0.61
2:D:205:ILE:HG22	2:D:206:LEU:N	2.16	0.61
1:A:187:ASP:OD2	1:A:225:THR:HG22	1.99	0.61
1:A:96:GLY:HA3	1:A:115:PHE:CE1	2.35	0.61
2:D:205:ILE:CG2	2:D:206:LEU:N	2.64	0.60
2:D:380:ASP:HB2	2:D:388:VAL:HG22	1.84	0.60
2:D:189:TYR:CE2	2:D:193:LEU:HD21	2.36	0.60
1:A:226:LYS:O	1:A:230:VAL:HG23	2.01	0.60
2:D:21:TYR:CE1	2:D:85:GLN:HG2	2.37	0.60
1:A:186:LYS:HA	3:A:299:HOH:O	2.02	0.60
1:A:4:VAL:HG13	1:A:6:LEU:HD11	1.84	0.59
2:D:231:LEU:HD12	2:D:241:MET:CE	2.32	0.59
2:D:184:ILE:HG21	2:D:262:MET:CE	2.32	0.59
2:D:448:ASN:HB2	3:D:493:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:333:MET:HE2	2:D:348:THR:HG22	1.85	0.59
2:D:90:ASN:HB3	2:D:93:LYS:HD3	1.83	0.59
2:D:331:MET:CB	2:D:332:PRO:CD	2.80	0.59
2:D:29:ASN:ND2	2:D:91:ILE:HD12	2.18	0.59
2:D:49:LYS:O	2:D:53:VAL:HG23	2.03	0.58
1:A:34:LEU:HD22	1:A:35:PRO:HD2	1.84	0.58
2:D:69:THR:HG22	2:D:70:SER:N	2.19	0.58
2:D:243:ILE:HG22	2:D:251:ILE:HD12	1.85	0.58
2:D:333:MET:HE1	2:D:348:THR:HG22	1.85	0.57
1:A:215:THR:CG2	1:A:216:GLY:H	2.11	0.57
2:D:137:LEU:HD11	2:D:447:MET:HG2	1.87	0.57
2:D:327:LYS:HB3	2:D:444:ASN:CG	2.25	0.57
2:D:132:THR:HG22	2:D:133:SER:N	2.18	0.57
2:D:292:ILE:O	2:D:296:GLU:HG3	2.05	0.57
2:D:462:LYS:HG2	3:D:492:HOH:O	2.04	0.57
1:A:32:LYS:N	1:A:203:SER:HG	2.03	0.57
2:D:64:PHE:HB2	2:D:224:ILE:CD1	2.35	0.57
2:D:333:MET:O	2:D:334:LYS:HB3	2.05	0.56
2:D:32:HIS:HD2	2:D:33:MET:HE1	1.70	0.56
1:A:32:LYS:HB2	1:A:37:GLN:NE2	2.20	0.56
2:D:361:LEU:HD21	2:D:404:ILE:CD1	2.35	0.56
1:A:104:ASN:ND2	1:A:111:LEU:CD1	2.65	0.56
2:D:331:MET:HG2	2:D:445:SER:HB3	1.87	0.56
2:D:83:SER:N	2:D:85:GLN:HE22	2.05	0.55
2:D:204:ASP:C	2:D:205:ILE:HD12	2.26	0.55
2:D:203:ILE:HG22	2:D:205:ILE:CD1	2.35	0.55
1:A:5:SER:HA	1:A:250:ASN:OD1	2.05	0.55
2:D:413:HIS:CD2	2:D:415:ILE:H	2.05	0.55
1:A:7:ASP:HB2	1:A:8:LYS:HZ2	1.72	0.55
2:D:85:GLN:NE2	2:D:85:GLN:H	2.05	0.55
1:A:196:MSE:HE2	1:A:209:ARG:HB2	1.88	0.55
1:A:8:LYS:H	1:A:8:LYS:HD2	1.72	0.54
1:A:250:ASN:HA	3:A:311:HOH:O	2.07	0.54
2:D:344:VAL:HG21	2:D:404:ILE:HD13	1.89	0.54
2:D:282:LEU:O	2:D:286:ILE:HG12	2.08	0.54
2:D:62:ARG:NH2	2:D:118:LYS:HB3	2.23	0.54
2:D:326:GLY:H	2:D:447:MET:CE	2.21	0.53
2:D:132:THR:CG2	2:D:133:SER:H	2.16	0.53
1:A:79:ARG:C	1:A:79:ARG:HD3	2.29	0.53
2:D:145:MET:O	2:D:147:VAL:N	2.38	0.53
1:A:6:LEU:HD12	1:A:6:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:HG11	1:A:163:MSE:HE1	1.91	0.53
2:D:280:PHE:HD1	2:D:429:MET:HE3	1.74	0.53
2:D:435:TYR:CD1	2:D:435:TYR:O	2.61	0.53
2:D:280:PHE:CD1	2:D:429:MET:HE3	2.44	0.53
2:D:237:LEU:HD23	2:D:240:TYR:CD2	2.44	0.53
2:D:117:ILE:O	2:D:117:ILE:HG23	2.08	0.53
2:D:33:MET:HG3	2:D:91:ILE:HD13	1.91	0.52
2:D:114:VAL:C	2:D:116:THR:H	2.12	0.52
2:D:361:LEU:CD1	2:D:404:ILE:HD12	2.39	0.52
2:D:326:GLY:N	2:D:447:MET:HE1	2.26	0.51
2:D:12:ASN:HB3	2:D:16:LYS:CE	2.40	0.51
1:A:34:LEU:HD23	1:A:35:PRO:HD2	1.92	0.51
2:D:280:PHE:HA	2:D:429:MET:CE	2.39	0.51
2:D:229:ILE:CG2	2:D:243:ILE:HG23	2.40	0.51
2:D:147:VAL:HG22	2:D:451:LYS:CB	2.40	0.51
2:D:221:ILE:HA	2:D:224:ILE:HG22	1.92	0.51
1:A:58:ILE:CD1	1:A:170:VAL:CG2	2.88	0.51
2:D:52:PHE:O	2:D:56:VAL:HG23	2.11	0.51
1:A:1:MSE:HG2	1:A:2:ASP:H	1.76	0.51
2:D:381:PHE:CG	2:D:430:LEU:HD13	2.46	0.51
2:D:324:PHE:HA	2:D:444:ASN:HD21	1.75	0.51
2:D:261:THR:O	2:D:265:VAL:HG23	2.10	0.51
2:D:258:ARG:HG3	2:D:382:GLU:OE2	2.10	0.51
2:D:337:ILE:HG23	2:D:344:VAL:HG22	1.92	0.50
2:D:377:THR:CG2	2:D:377:THR:O	2.59	0.50
2:D:21:TYR:OH	2:D:85:GLN:HG2	2.09	0.50
2:D:292:ILE:H	2:D:403:THR:CG2	2.21	0.50
2:D:64:PHE:HB2	2:D:224:ILE:HD11	1.94	0.50
2:D:363:GLU:HG3	2:D:399:TYR:CE2	2.47	0.50
2:D:144:SER:O	2:D:147:VAL:CG2	2.59	0.50
2:D:225:THR:O	2:D:225:THR:HG22	2.12	0.50
1:A:4:VAL:HG22	1:A:5:SER:N	2.26	0.50
1:A:47:LEU:HD13	1:A:270:VAL:HG21	1.93	0.50
2:D:385:THR:HG22	2:D:387:SER:N	2.25	0.50
1:A:8:LYS:N	1:A:8:LYS:HD2	2.27	0.50
2:D:240:TYR:CZ	2:D:242:VAL:HG13	2.47	0.50
1:A:33:LYS:O	1:A:33:LYS:CG	2.58	0.50
2:D:183:CYS:SG	2:D:205:ILE:CG2	2.94	0.49
1:A:158:ALA:O	1:A:162:VAL:HG23	2.13	0.49
2:D:237:LEU:HD23	2:D:240:TYR:CG	2.47	0.49
2:D:328:ARG:O	2:D:329:ASN:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:418:ARG:HD3	2:D:446:MET:CG	2.43	0.49
2:D:32:HIS:HD2	2:D:33:MET:CE	2.25	0.49
2:D:351:TYR:CD2	2:D:438:CYS:HB3	2.47	0.49
2:D:177:ARG:HA	2:D:272:ASN:O	2.13	0.49
2:D:148:ALA:CB	2:D:454:ILE:HD12	2.43	0.49
2:D:268:ILE:HG22	2:D:270:ILE:HG13	1.93	0.48
2:D:325:ASP:N	2:D:444:ASN:ND2	2.56	0.48
2:D:83:SER:O	2:D:86:THR:HB	2.14	0.48
1:A:253:TYR:HE2	1:A:287:GLN:HE22	1.60	0.48
2:D:331:MET:CB	2:D:332:PRO:HD3	2.44	0.48
2:D:208:THR:HA	2:D:257:ILE:O	2.14	0.48
1:A:185:ILE:HG22	1:A:186:LYS:HG2	1.95	0.48
2:D:228:ASN:O	2:D:229:ILE:HD12	2.13	0.48
2:D:325:ASP:O	2:D:327:LYS:N	2.47	0.48
2:D:381:PHE:CD2	2:D:430:LEU:HD13	2.49	0.48
2:D:77:ARG:CZ	2:D:226:GLY:CA	2.92	0.48
2:D:142:LEU:HD23	2:D:145:MET:HE3	1.96	0.47
1:A:188:PHE:CZ	1:A:224:VAL:HG11	2.48	0.47
2:D:177:ARG:HD3	3:D:486:HOH:O	2.14	0.47
2:D:107:THR:HB	2:D:111:ILE:HD13	1.95	0.47
1:A:138:ASP:OD1	1:A:209:ARG:NH2	2.38	0.47
2:D:326:GLY:N	2:D:447:MET:CE	2.78	0.47
2:D:326:GLY:H	2:D:447:MET:HE1	1.79	0.47
2:D:211:ARG:O	2:D:215:ILE:HG13	2.14	0.47
1:A:12:TYR:OH	1:A:52:LYS:NZ	2.48	0.47
2:D:327:LYS:HB3	2:D:444:ASN:ND2	2.30	0.47
1:A:52:LYS:HE2	3:D:485:HOH:O	2.15	0.47
2:D:295:LEU:O	2:D:298:LEU:HB3	2.14	0.47
2:D:245:ASP:OD1	2:D:249:ASN:HB2	2.15	0.47
1:A:217:GLU:N	1:A:217:GLU:CD	2.68	0.47
2:D:227:ASN:HB3	2:D:246:GLU:OE2	2.15	0.47
2:D:13:ILE:O	2:D:17:ILE:HG13	2.15	0.46
2:D:17:ILE:HD13	2:D:42:GLN:HG2	1.96	0.46
1:A:57:GLY:HA2	3:A:316:HOH:O	2.15	0.46
1:A:26:SER:HB3	1:A:204:TYR:CE2	2.50	0.46
2:D:69:THR:CG2	2:D:70:SER:N	2.78	0.46
2:D:231:LEU:H	2:D:231:LEU:HD23	1.80	0.46
2:D:228:ASN:C	2:D:229:ILE:HD12	2.36	0.46
2:D:418:ARG:HG2	2:D:442:LEU:CD1	2.43	0.46
1:A:128:LEU:HG	1:A:133:ILE:HD11	1.97	0.46
2:D:143:ASN:ND2	3:D:550:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:CE1	1:A:69:SER:HA	2.51	0.46
2:D:44:ILE:HA	2:D:105:VAL:HG21	1.97	0.46
2:D:268:ILE:HD11	2:D:315:TYR:OH	2.15	0.45
2:D:67:VAL:O	2:D:69:THR:N	2.49	0.45
1:A:58:ILE:HD13	1:A:170:VAL:HG21	1.98	0.45
2:D:147:VAL:HG11	2:D:452:ILE:C	2.31	0.45
2:D:62:ARG:NH2	2:D:174:GLU:HG3	2.31	0.45
2:D:339:GLU:HG3	2:D:339:GLU:H	1.34	0.45
1:A:217:GLU:H	1:A:217:GLU:CD	2.20	0.45
2:D:333:MET:O	2:D:334:LYS:CB	2.64	0.45
2:D:348:THR:HB	2:D:352:PHE:HD1	1.82	0.45
2:D:14:THR:HG21	2:D:35:LYS:HG3	1.98	0.45
2:D:202:ASP:OD2	2:D:204:ASP:OD1	2.34	0.45
1:A:3:VAL:HB	1:A:249:VAL:HG13	1.97	0.45
2:D:388:VAL:CG1	2:D:389:TYR:N	2.78	0.45
2:D:427:TYR:HD2	2:D:428:GLN:HE21	1.63	0.45
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.80	0.45
2:D:148:ALA:HB2	2:D:454:ILE:HD12	1.99	0.45
1:A:21:ASP:OD1	1:A:234:LYS:HE3	2.16	0.45
2:D:267:LYS:HE3	3:D:551:HOH:O	2.17	0.45
2:D:331:MET:HG3	2:D:332:PRO:HD3	1.99	0.45
2:D:221:ILE:O	2:D:224:ILE:HG22	2.17	0.45
2:D:399:TYR:OH	2:D:401:SER:HA	2.17	0.45
1:A:188:PHE:O	1:A:224:VAL:HG12	2.17	0.44
2:D:333:MET:HB3	2:D:347:THR:O	2.16	0.44
2:D:186:TYR:CZ	2:D:204:ASP:HB3	2.53	0.44
2:D:199:ARG:O	2:D:200:TYR:HB3	2.16	0.44
1:A:189:TYR:OH	1:A:223:ARG:NH1	2.50	0.44
2:D:240:TYR:CE2	2:D:242:VAL:HG13	2.53	0.44
2:D:229:ILE:HG21	2:D:243:ILE:HG23	1.99	0.44
1:A:43:LEU:O	1:A:47:LEU:HB2	2.17	0.44
2:D:83:SER:CA	2:D:85:GLN:HE22	2.30	0.44
2:D:329:ASN:O	2:D:329:ASN:OD1	2.35	0.44
1:A:45:GLY:HA3	1:A:196:MSE:HE1	1.98	0.44
2:D:351:TYR:CE2	2:D:438:CYS:HB3	2.53	0.44
2:D:324:PHE:HA	2:D:444:ASN:ND2	2.32	0.44
2:D:118:LYS:O	2:D:118:LYS:HG3	2.17	0.44
2:D:62:ARG:HH12	2:D:118:LYS:HB3	1.83	0.44
2:D:27:SER:OG	2:D:30:GLU:HG3	2.17	0.44
2:D:414:GLU:O	2:D:418:ARG:HB2	2.17	0.44
2:D:444:ASN:CA	2:D:447:MET:HE2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:PHE:O	2:D:401:SER:CB	2.64	0.44
2:D:341:ASN:O	2:D:343:ILE:HG13	2.18	0.43
2:D:378:SER:CB	2:D:388:VAL:HG11	2.41	0.43
2:D:443:LEU:HA	2:D:446:MET:HE3	1.99	0.43
1:A:8:LYS:O	1:A:8:LYS:HD2	2.17	0.43
2:D:44:ILE:O	2:D:49:LYS:NZ	2.51	0.43
2:D:466:ARG:HD3	2:D:478:VAL:HG12	2.01	0.43
1:A:96:GLY:HA3	1:A:115:PHE:CZ	2.53	0.43
2:D:68:ASN:O	2:D:68:ASN:OD1	2.37	0.43
1:A:150:THR:HG23	1:A:179:PRO:HB3	2.01	0.43
1:A:242:ILE:HG22	1:A:243:VAL:N	2.32	0.43
1:A:177:ARG:NH2	1:A:180:PHE:CE2	2.87	0.43
2:D:147:VAL:HG22	2:D:451:LYS:CA	2.48	0.42
1:A:52:LYS:HB2	1:A:52:LYS:HE3	1.79	0.42
2:D:141:MET:HB2	2:D:141:MET:HE3	1.77	0.42
1:A:150:THR:HG21	1:A:185:ILE:HG12	2.01	0.42
1:A:215:THR:CG2	1:A:217:GLU:OE2	2.63	0.42
1:A:253:TYR:OH	1:A:287:GLN:NE2	2.53	0.42
1:A:176:TRP:CD1	1:A:208:MSE:HG3	2.54	0.42
2:D:75:LYS:HB2	2:D:75:LYS:HE3	1.78	0.42
2:D:463:LYS:HA	2:D:464:PRO:HD2	1.87	0.42
2:D:141:MET:HE2	2:D:313:LEU:HD11	1.97	0.42
2:D:377:THR:HG22	2:D:377:THR:O	2.20	0.42
1:A:240:ASN:HA	1:A:244:ARG:HD3	2.02	0.42
2:D:247:ASN:O	2:D:248:ASP:CB	2.66	0.42
2:D:85:GLN:H	2:D:85:GLN:CD	2.23	0.42
2:D:324:PHE:HB3	2:D:447:MET:SD	2.58	0.42
2:D:76:ASP:O	2:D:80:SER:HB2	2.20	0.42
2:D:44:ILE:HD13	2:D:101:GLN:NE2	2.28	0.42
2:D:118:LYS:NZ	2:D:118:LYS:HB2	2.35	0.42
1:A:199:PRO:O	1:A:200:PHE:HB2	2.19	0.42
2:D:413:HIS:CE1	2:D:452:ILE:HB	2.54	0.42
2:D:195:ASN:C	2:D:195:ASN:OD1	2.58	0.42
2:D:422:ALA:O	2:D:426:LEU:HG	2.20	0.42
2:D:280:PHE:CA	2:D:429:MET:HE3	2.46	0.42
2:D:183:CYS:HG	2:D:205:ILE:HG21	1.84	0.41
2:D:207:GLN:O	2:D:257:ILE:N	2.46	0.41
1:A:105:GLY:HA2	2:D:95:PHE:CZ	2.54	0.41
1:A:58:ILE:HD11	1:A:170:VAL:CG2	2.50	0.41
2:D:111:ILE:HG22	2:D:112:LEU:HG	2.03	0.41
2:D:234:ILE:HG22	2:D:235:PRO:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:418:ARG:HD3	2:D:446:MET:HG2	2.02	0.41
1:A:58:ILE:HD13	1:A:170:VAL:CG2	2.50	0.41
2:D:228:ASN:HB2	2:D:473:GLU:OE2	2.20	0.41
1:A:288:GLN:HB3	1:A:288:GLN:HE21	1.72	0.41
1:A:18:ASN:HB3	1:A:238:TYR:CE2	2.56	0.41
1:A:58:ILE:HD12	1:A:132:LYS:HD3	2.03	0.41
1:A:129:HIS:ND1	1:A:130:PRO:HA	2.35	0.41
2:D:81:TYR:C	2:D:83:SER:H	2.23	0.41
2:D:325:ASP:C	2:D:327:LYS:N	2.73	0.41
2:D:325:ASP:OD1	2:D:325:ASP:N	2.54	0.41
2:D:285:MET:SD	2:D:312:MET:HE3	2.60	0.41
2:D:443:LEU:HA	2:D:446:MET:CE	2.51	0.41
2:D:12:ASN:HB3	2:D:16:LYS:NZ	2.35	0.41
2:D:240:TYR:OH	2:D:242:VAL:CG1	2.69	0.41
2:D:210:SER:HB2	2:D:256:ASN:HB2	2.02	0.41
2:D:169:ASN:O	2:D:173:GLU:HG3	2.21	0.41
1:A:99:HIS:HB3	1:A:103:LEU:HD12	2.03	0.41
2:D:111:ILE:HD12	2:D:111:ILE:N	2.36	0.41
1:A:77:TYR:C	1:A:77:TYR:CD1	2.94	0.41
2:D:474:LYS:O	2:D:476:ILE:HG13	2.21	0.41
1:A:50:LEU:HA	1:A:50:LEU:HD12	1.86	0.40
2:D:231:LEU:HA	2:D:242:VAL:O	2.21	0.40
2:D:363:GLU:HG3	2:D:399:TYR:CZ	2.56	0.40
1:A:50:LEU:HB3	1:A:82:PHE:CZ	2.56	0.40
1:A:63:THR:HA	1:A:90:LYS:O	2.21	0.40
2:D:203:ILE:HA	3:D:504:HOH:O	2.20	0.40
2:D:328:ARG:HG3	2:D:449:ARG:NH2	2.36	0.40
1:A:37:GLN:HG2	1:A:200:PHE:O	2.22	0.40
2:D:325:ASP:O	2:D:326:GLY:C	2.59	0.40
2:D:283:LEU:HD21	2:D:425:LEU:HB3	2.02	0.40
2:D:114:VAL:O	2:D:116:THR:N	2.54	0.40
1:A:114:ARG:HG3	1:A:114:ARG:NH1	2.36	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	280/297 (94%)	260 (93%)	18 (6%)	2 (1%)	26	38
2	D	441/469 (94%)	387 (88%)	36 (8%)	18 (4%)	3	3
All	All	721/766 (94%)	647 (90%)	54 (8%)	20 (3%)	6	5

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	68	ASN
2	D	71	ALA
2	D	119	ALA
2	D	226	GLY
2	D	228	ASN
2	D	331	MET
2	D	333	MET
2	D	115	LEU
2	D	325	ASP
2	D	329	ASN
2	D	332	PRO
2	D	393	ASP
1	A	218	ASN
2	D	339	GLU
1	A	24	PRO
2	D	133	SER
2	D	330	ASN
2	D	334	LYS
2	D	38	ALA
2	D	326	GLY

### 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	265/260 (102%)	247 (93%)	18 (7%)	20	31
2	D	423/443 (96%)	394 (93%)	29 (7%)	19	30
All	All	688/703 (98%)	641 (93%)	47 (7%)	20	31

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	8	LYS
1	A	43	LEU
1	A	47	LEU
1	A	50	LEU
1	A	58	ILE
1	A	128	LEU
1	A	130	PRO
1	A	165	SER
1	A	167	LEU
1	A	197	LEU
1	A	208	MSE
1	A	209	ARG
1	A	217	GLU
1	A	218	ASN
1	A	227	SER
1	A	257	GLU
1	A	288	GLN
2	D	58	LYS
2	D	70	SER
2	D	83	SER
2	D	98	ILE
2	D	118	LYS
2	D	134	MET
2	D	161	VAL
2	D	174	GLU
2	D	184	ILE
2	D	193	LEU
2	D	231	LEU
2	D	248	ASP
2	D	257	ILE
2	D	258	ARG
2	D	260	ASP
2	D	275	ILE
2	D	292	ILE

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Mol	Chain	Res	Type
2	D	297	ASP
2	D	330	ASN
2	D	332	PRO
2	D	334	LYS
2	D	337	ILE
2	D	339	GLU
2	D	349	LYS
2	D	383	SER
2	D	385	THR
2	D	434	GLU
2	D	436	LYS
2	D	460	ARG

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

Mol	Chain	Res	Type
1	A	84	ASN
1	A	104	ASN
1	A	156	ASN
1	A	183	GLN
1	A	218	ASN
1	A	287	GLN
1	A	288	GLN
2	D	29	ASN
2	D	32	HIS
2	D	59	ASN
2	D	85	GLN
2	D	101	GLN
2	D	167	ASN
2	D	250	HIS
2	D	306	ASN
2	D	341	ASN
2	D	394	ASN
2	D	413	HIS
2	D	428	GLN
2	D	444	ASN
2	D	457	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	276/297 (92%)	-0.09	7 (2%) 61 60	17, 34, 66, 89	0
2	D	447/469 (95%)	-0.03	21 (4%) 35 36	24, 40, 67, 86	0
All	All	723/766 (94%)	-0.05	28 (3%) 43 44	17, 38, 67, 89	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	LYS	6.8
1	A	26	SER	5.8
1	A	24	PRO	5.3
2	D	120	PRO	4.8
2	D	70	SER	4.6
1	A	141	SER	4.5
1	A	25	GLU	4.4
2	D	119	ALA	4.1
2	D	150	ILE	4.0
2	D	331	MET	3.8
2	D	117	ILE	3.8
2	D	13	ILE	3.6
2	D	12	ASN	3.3
2	D	332	PRO	3.2
2	D	69	THR	3.1
1	A	23	GLU	3.0
2	D	147	VAL	3.0
2	D	68	ASN	2.8
2	D	136	GLU	2.6
2	D	116	THR	2.6
2	D	15	LEU	2.6
2	D	330	ASN	2.5
2	D	161	VAL	2.4
2	D	409	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	114	VAL	2.2
2	D	133	SER	2.2
2	D	301	ASP	2.2
1	A	140	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.