



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:31 PM GMT

PDB ID : 1PEO  
Title : Ribonucleotide Reductase Protein R1E from Salmonella typhimurium  
Authors : Uppsten, M.; Farnegardh, M.; Jordan, A.; Eliasson, R.; Eklund, H.; Uhlin, U.  
Deposited on : 2003-05-22  
Resolution : 3.00 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

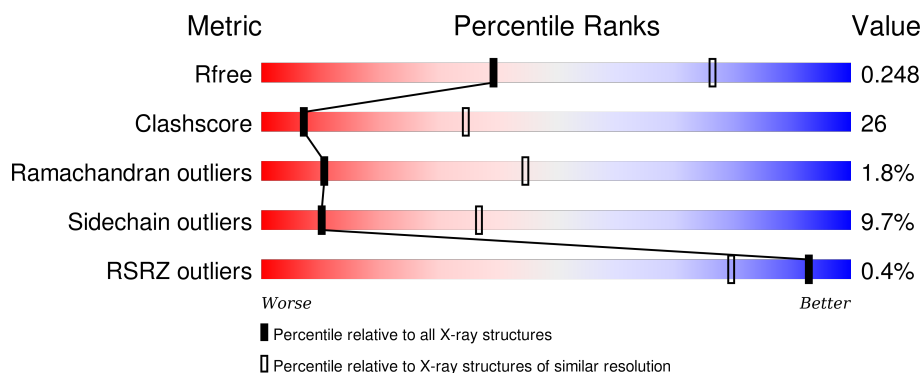
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	714	 49% 37% 8% • 5%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5465 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.

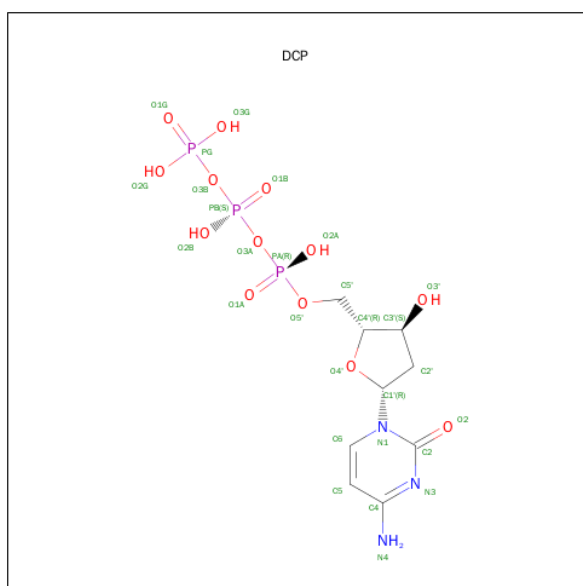
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	0	0	0
			5436	3448	961	1005	22			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula:  $C_9H_{16}N_3O_{13}P_3$ ).

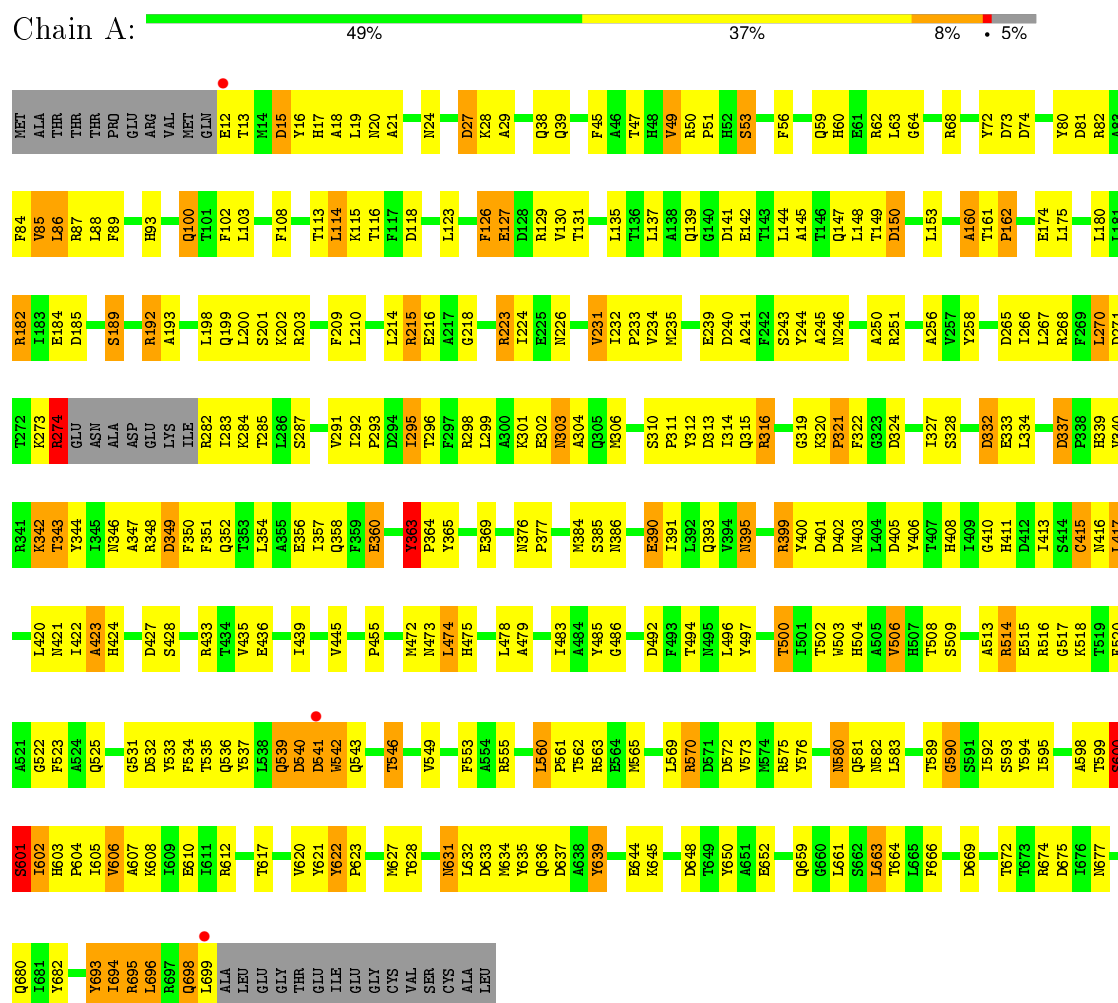


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

### 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: Ribonucleoside-diphosphate reductase 2 alpha chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.94Å 98.94Å 289.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-3.00) 99.9 (39.69-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.206 , 0.252 0.208 , 0.248	Depositor DCC
$R_{free}$ test set	1508 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29766 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

### 5.1 Standard geometry

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

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	1.33	10/5561 (0.2%)	1.27	44/7529 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	ALA	CA-CB	-5.85	1.40	1.52
1	A	595	ILE	CA-CB	-5.69	1.41	1.54
1	A	72	TYR	CE1-CZ	-5.33	1.31	1.38
1	A	483	ILE	CA-CB	-5.30	1.42	1.54
1	A	445	VAL	CB-CG2	-5.23	1.41	1.52
1	A	160	ALA	CA-CB	-5.22	1.41	1.52
1	A	423	ALA	CA-CB	-5.19	1.41	1.52
1	A	241	ALA	CA-CB	-5.11	1.41	1.52
1	A	244	TYR	CE1-CZ	-5.06	1.31	1.38
1	A	126	PHE	CD1-CE1	-5.00	1.29	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	427	ASP	CB-CG-OD2	10.13	127.42	118.30
1	A	73	ASP	CB-CG-OD2	9.61	126.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	129	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	192	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	696	LEU	CA-CB-CG	-7.51	98.04	115.30
1	A	192	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	332	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	349	ASP	CB-CG-OD2	6.88	124.50	118.30
1	A	12	GLU	N-CA-C	6.84	129.47	111.00
1	A	541	ASP	CA-C-N	-6.80	102.23	117.20
1	A	182	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	74	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	215	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	240	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	68	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	68	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	337	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	669	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	399	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	648	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	81	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	572	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	129	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	321	PRO	N-CD-CG	-5.69	94.66	103.20
1	A	363	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	A	15	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	162	PRO	N-CD-CG	-5.61	94.79	103.20
1	A	637	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	150	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	699	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	622	TYR	CB-CG-CD2	5.48	124.29	121.00
1	A	27	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	150	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	A	265	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	541	ASP	N-CA-C	-5.38	96.48	111.00
1	A	633	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	541	ASP	C-N-CA	5.20	134.69	121.70
1	A	506	VAL	CB-CA-C	-5.19	101.53	111.40
1	A	185	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	600	SER	CA-C-N	5.11	128.44	117.20
1	A	231	VAL	CB-CA-C	-5.10	101.71	111.40
1	A	363	TYR	CB-CA-C	-5.05	100.30	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	TYR	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5436	0	5325	282	0
2	A	1	0	0	0	0
3	A	28	0	12	1	0
All	All	5465	0	5337	282	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 26.

All (282) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:HH11	1:A:316:ARG:HG3	1.14	1.06
1:A:605:ILE:O	1:A:607:ALA:N	1.88	1.05
1:A:472:MET:HA	1:A:601:SER:O	1.63	0.97
1:A:608:LYS:NZ	1:A:635:TYR:O	1.98	0.95
1:A:80:TYR:CE1	1:A:135:LEU:HD22	2.00	0.95
1:A:628:THR:H	1:A:631:ASN:ND2	1.65	0.94
1:A:628:THR:N	1:A:631:ASN:HD21	1.68	0.93
1:A:59:GLN:NE2	1:A:89:PHE:CB	2.37	0.87
1:A:316:ARG:NH1	1:A:316:ARG:HG3	1.90	0.85
1:A:514:ARG:HD2	1:A:576:TYR:CG	2.13	0.83
1:A:273:LYS:NZ	1:A:283:ILE:HG22	1.96	0.80
1:A:59:GLN:HE21	1:A:89:PHE:HB2	1.46	0.80
1:A:546:THR:HG22	1:A:549:VAL:H	1.45	0.80
1:A:302:GLU:O	1:A:304:ALA:N	2.15	0.79
1:A:351:PHE:HB3	1:A:677:ASN:HD21	1.45	0.79
1:A:395:ASN:HD22	1:A:395:ASN:C	1.84	0.78
1:A:223:ARG:HH21	1:A:316:ARG:HH22	1.31	0.77
1:A:485:TYR:CZ	1:A:604:PRO:HD3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASN:HB2	1:A:598:ALA:HB1	1.69	0.75
1:A:663:LEU:C	1:A:663:LEU:HD12	2.05	0.75
1:A:80:TYR:CD1	1:A:135:LEU:HD22	2.23	0.74
1:A:223:ARG:NH2	1:A:316:ARG:HH22	1.88	0.72
1:A:605:ILE:HG13	1:A:605:ILE:O	1.89	0.72
1:A:693:TYR:CE1	1:A:695:ARG:NH1	2.58	0.71
1:A:216:GLU:OE2	1:A:311:PRO:HD2	1.91	0.70
1:A:605:ILE:O	1:A:606:VAL:C	2.29	0.70
1:A:644:GLU:HG3	1:A:682:TYR:CE2	2.26	0.70
1:A:628:THR:H	1:A:631:ASN:HD21	0.82	0.69
1:A:694:ILE:HG13	1:A:694:ILE:O	1.90	0.69
1:A:363:TYR:HB3	1:A:364:PRO:HA	1.75	0.68
1:A:210:LEU:HB2	1:A:384:MET:CE	2.22	0.68
1:A:639:TYR:CE2	1:A:666:PHE:HB3	2.29	0.67
1:A:592:ILE:HG13	1:A:593:SER:N	2.08	0.67
1:A:302:GLU:O	1:A:303:ASN:C	2.30	0.67
1:A:594:TYR:OH	1:A:612:ARG:HD3	1.93	0.67
1:A:89:PHE:CE1	1:A:131:THR:HG21	2.30	0.66
1:A:283:ILE:HG22	1:A:283:ILE:O	1.95	0.66
1:A:174:GLU:OE2	1:A:203:ARG:NH1	2.28	0.66
1:A:199:GLN:NE2	1:A:202:LYS:HE2	2.11	0.66
1:A:85:VAL:O	1:A:87:ARG:N	2.29	0.65
1:A:534:PHE:O	1:A:537:TYR:N	2.26	0.65
1:A:393:GLN:HB2	1:A:413:ILE:HD13	1.79	0.65
1:A:485:TYR:CE2	1:A:604:PRO:HD3	2.32	0.65
1:A:273:LYS:HZ2	1:A:283:ILE:HG22	1.61	0.65
1:A:59:GLN:NE2	1:A:89:PHE:CG	2.65	0.64
1:A:346:ASN:HD22	1:A:349:ASP:CG	2.00	0.64
1:A:59:GLN:NE2	1:A:89:PHE:HB3	2.13	0.64
1:A:199:GLN:HE21	1:A:202:LYS:HE2	1.63	0.64
1:A:600:SER:HB3	1:A:603:HIS:NE2	2.13	0.63
1:A:416:ASN:C	1:A:417:LEU:HD13	2.18	0.63
1:A:399:ARG:HB2	1:A:408:HIS:HB3	1.79	0.63
1:A:192:ARG:HG3	1:A:400:TYR:CE1	2.34	0.62
1:A:403:ASN:OD1	1:A:405:ASP:HB2	1.99	0.62
1:A:80:TYR:CE1	1:A:135:LEU:CD2	2.80	0.62
1:A:395:ASN:ND2	1:A:395:ASN:C	2.53	0.62
1:A:161:THR:N	1:A:162:PRO:HD2	2.13	0.62
1:A:114:LEU:HD22	1:A:115:LYS:O	2.00	0.62
1:A:672:THR:O	1:A:675:ASP:HB2	2.01	0.61
1:A:316:ARG:CG	1:A:316:ARG:HH11	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:CD1	1:A:131:THR:HG21	2.35	0.61
1:A:84:PHE:CZ	1:A:142:GLU:HB3	2.36	0.61
1:A:496:LEU:O	1:A:500:THR:HG23	1.99	0.61
1:A:223:ARG:NH2	1:A:316:ARG:NH2	2.49	0.60
1:A:631:ASN:H	1:A:631:ASN:HD22	1.49	0.60
1:A:422:ILE:HG12	1:A:497:TYR:CZ	2.36	0.60
1:A:601:SER:OG	1:A:602:ILE:N	2.33	0.60
1:A:522:GLY:O	1:A:523:PHE:C	2.40	0.60
1:A:282:ARG:NH1	1:A:284:LYS:HZ2	2.00	0.60
1:A:293:PRO:HD2	1:A:296:THR:OG1	2.01	0.60
1:A:599:THR:O	1:A:601:SER:N	2.34	0.60
1:A:84:PHE:CE1	1:A:142:GLU:HB3	2.37	0.59
1:A:605:ILE:C	1:A:607:ALA:N	2.55	0.59
1:A:282:ARG:NH1	1:A:284:LYS:NZ	2.51	0.59
1:A:218:GLY:O	1:A:226:ASN:HA	2.02	0.59
1:A:347:ALA:O	1:A:350:PHE:HB3	2.03	0.59
1:A:351:PHE:HB3	1:A:677:ASN:ND2	2.17	0.59
1:A:84:PHE:O	1:A:85:VAL:O	2.20	0.58
1:A:696:LEU:N	1:A:696:LEU:HD12	2.18	0.58
1:A:581:GLN:O	1:A:581:GLN:HG2	2.04	0.58
1:A:210:LEU:HB2	1:A:384:MET:HE2	1.85	0.57
1:A:127:GLU:N	1:A:127:GLU:OE1	2.36	0.57
1:A:56:PHE:CD1	1:A:62:ARG:HB2	2.40	0.57
1:A:589:THR:OG1	1:A:593:SER:HB3	2.03	0.57
1:A:580:ASN:ND2	1:A:580:ASN:H	2.02	0.57
1:A:631:ASN:N	1:A:631:ASN:HD22	2.01	0.57
1:A:126:PHE:O	1:A:130:VAL:HG23	2.05	0.57
1:A:232:ILE:N	1:A:233:PRO:HD2	2.20	0.56
1:A:49:VAL:O	1:A:50:ARG:C	2.44	0.56
1:A:239:GLU:OE1	1:A:285:THR:HG23	2.05	0.56
1:A:180:LEU:N	1:A:180:LEU:HD12	2.20	0.56
1:A:496:LEU:O	1:A:500:THR:CG2	2.53	0.56
1:A:180:LEU:HB2	1:A:413:ILE:HB	1.87	0.56
1:A:332:ASP:O	1:A:333:GLU:C	2.44	0.55
1:A:475:HIS:ND1	1:A:605:ILE:HG23	2.22	0.55
1:A:628:THR:O	1:A:631:ASN:ND2	2.39	0.55
1:A:580:ASN:HD22	1:A:580:ASN:H	1.54	0.55
1:A:231:VAL:HG23	1:A:232:ILE:N	2.21	0.55
1:A:59:GLN:HE21	1:A:89:PHE:CB	2.03	0.55
1:A:85:VAL:O	1:A:86:LEU:C	2.43	0.55
1:A:199:GLN:HA	1:A:199:GLN:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:O	1:A:322:PHE:C	2.45	0.55
1:A:316:ARG:CG	1:A:316:ARG:NH1	2.64	0.55
1:A:62:ARG:O	1:A:63:LEU:C	2.44	0.55
1:A:472:MET:HB3	1:A:589:THR:HG21	1.88	0.54
1:A:533:TYR:O	1:A:533:TYR:CG	2.59	0.54
1:A:415:CYS:HB2	1:A:417:LEU:HD21	1.89	0.54
1:A:20:ASN:HD21	1:A:620:VAL:HG13	1.73	0.53
1:A:390:GLU:HG2	1:A:391:ILE:HD13	1.91	0.53
1:A:343:THR:HG22	1:A:344:TYR:N	2.23	0.53
1:A:49:VAL:O	1:A:53:SER:OG	2.27	0.53
1:A:210:LEU:HB2	1:A:384:MET:HE1	1.90	0.53
1:A:59:GLN:NE2	1:A:89:PHE:HB2	2.09	0.52
1:A:232:ILE:N	1:A:233:PRO:CD	2.72	0.52
1:A:514:ARG:O	1:A:515:GLU:C	2.48	0.52
1:A:623:PRO:O	1:A:623:PRO:HG2	2.09	0.52
1:A:59:GLN:HE22	1:A:89:PHE:HB3	1.74	0.52
1:A:103:LEU:HD23	1:A:594:TYR:CG	2.45	0.52
1:A:13:THR:HG23	1:A:13:THR:O	2.09	0.52
1:A:541:ASP:HB3	1:A:542:TRP:CE3	2.44	0.52
1:A:59:GLN:HE22	1:A:89:PHE:CB	2.21	0.51
1:A:246:ASN:OD1	1:A:250:ALA:O	2.28	0.51
1:A:85:VAL:O	1:A:88:LEU:N	2.43	0.51
1:A:201:SER:OG	1:A:245:ALA:O	2.25	0.51
1:A:580:ASN:N	1:A:580:ASN:ND2	2.59	0.51
1:A:422:ILE:HG12	1:A:497:TYR:CE2	2.46	0.51
1:A:24:ASN:O	1:A:24:ASN:CG	2.50	0.51
1:A:343:THR:CG2	1:A:344:TYR:N	2.74	0.51
1:A:541:ASP:O	1:A:543:GLN:N	2.36	0.51
1:A:15:ASP:O	1:A:19:LEU:HG	2.11	0.51
1:A:562:THR:O	1:A:565:MET:N	2.44	0.51
1:A:349:ASP:O	1:A:352:GLN:HB3	2.11	0.50
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.76	0.50
1:A:17:HIS:HB3	1:A:617:THR:HG21	1.93	0.50
1:A:363:TYR:HE2	1:A:365:TYR:HH	1.57	0.50
1:A:553:PHE:CD2	1:A:560:LEU:CD1	2.94	0.50
1:A:605:ILE:O	1:A:607:ALA:CA	2.59	0.50
1:A:696:LEU:N	1:A:696:LEU:CD1	2.75	0.50
1:A:513:ALA:O	1:A:517:GLY:N	2.42	0.50
1:A:436:GLU:HG3	1:A:508:THR:HG23	1.93	0.50
1:A:161:THR:HB	1:A:162:PRO:CD	2.41	0.50
1:A:503:TRP:CZ3	1:A:504:HIS:CE1	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:SER:HB3	1:A:363:TYR:CE2	2.47	0.49
1:A:592:ILE:O	1:A:593:SER:C	2.46	0.49
1:A:312:TYR:HD2	1:A:313:ASP:OD1	1.95	0.49
1:A:312:TYR:CE2	1:A:316:ARG:NH1	2.80	0.49
1:A:354:LEU:HD11	1:A:364:PRO:HG2	1.93	0.49
1:A:327:ILE:O	1:A:328:SER:C	2.49	0.49
1:A:356:GLU:O	1:A:360:GLU:HG2	2.12	0.49
1:A:184:GLU:H	1:A:189:SER:CB	2.24	0.49
1:A:273:LYS:NZ	1:A:283:ILE:O	2.23	0.49
1:A:302:GLU:O	1:A:302:GLU:HG3	2.13	0.49
1:A:663:LEU:CD1	1:A:663:LEU:C	2.78	0.49
1:A:24:ASN:HB2	1:A:621:TYR:CE2	2.48	0.49
1:A:553:PHE:CD2	1:A:560:LEU:HD11	2.48	0.49
1:A:88:LEU:O	1:A:89:PHE:C	2.48	0.48
1:A:50:ARG:HB2	1:A:51:PRO:HD3	1.94	0.48
1:A:130:VAL:HG21	1:A:153:LEU:CD2	2.44	0.48
1:A:539:GLN:OE1	1:A:539:GLN:CA	2.62	0.48
1:A:522:GLY:O	1:A:525:GLN:N	2.41	0.48
1:A:291:VAL:CG1	1:A:369:GLU:HB2	2.44	0.48
1:A:473:ASN:HB2	1:A:598:ALA:CB	2.41	0.48
1:A:266:ILE:HG23	1:A:267:LEU:N	2.27	0.48
1:A:358:GLN:OE1	1:A:680:GLN:NE2	2.47	0.47
1:A:376:ASN:HA	1:A:377:PRO:HD3	1.77	0.47
1:A:627:MET:HG3	1:A:635:TYR:CD1	2.49	0.47
1:A:569:LEU:O	1:A:573:VAL:HG23	2.15	0.47
1:A:182:ARG:HE	1:A:395:ASN:ND2	2.12	0.47
1:A:666:PHE:CD1	1:A:666:PHE:N	2.82	0.47
1:A:509:SER:OG	1:A:580:ASN:ND2	2.32	0.47
1:A:160:ALA:HB2	1:A:417:LEU:O	2.15	0.47
1:A:27:ASP:O	1:A:29:ALA:N	2.47	0.47
1:A:663:LEU:HD12	1:A:664:THR:N	2.28	0.46
1:A:63:LEU:O	1:A:64:GLY:C	2.53	0.46
1:A:650:TYR:CG	1:A:663:LEU:HD22	2.50	0.46
1:A:539:GLN:N	1:A:539:GLN:OE1	2.48	0.46
1:A:406:TYR:CE1	1:A:455:PRO:HG2	2.51	0.46
1:A:435:VAL:O	1:A:439:ILE:HG12	2.16	0.46
1:A:546:THR:CG2	1:A:549:VAL:H	2.21	0.46
1:A:346:ASN:ND2	1:A:349:ASP:CG	2.69	0.46
1:A:500:THR:HB	1:A:561:PRO:HD3	1.97	0.46
1:A:581:GLN:HG2	1:A:582:ASN:ND2	2.31	0.46
1:A:116:THR:OG1	1:A:118:ASP:OD1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:O	1:A:417:LEU:HD13	2.16	0.46
1:A:295:ILE:O	1:A:296:THR:C	2.53	0.46
1:A:130:VAL:HG21	1:A:153:LEU:HD23	1.98	0.45
1:A:534:PHE:C	1:A:536:GLN:N	2.66	0.45
1:A:415:CYS:HB2	1:A:417:LEU:CD2	2.46	0.45
1:A:334:LEU:O	1:A:342:LYS:NZ	2.43	0.45
1:A:16:TYR:HB2	1:A:102:PHE:CE1	2.51	0.45
1:A:82:ARG:O	1:A:86:LEU:HG	2.15	0.45
1:A:631:ASN:ND2	1:A:631:ASN:N	2.62	0.45
1:A:182:ARG:NH2	1:A:324:ASP:OD2	2.50	0.45
1:A:695:ARG:C	1:A:696:LEU:HD12	2.37	0.45
1:A:644:GLU:HG3	1:A:682:TYR:HE2	1.76	0.45
1:A:313:ASP:O	1:A:314:ILE:C	2.54	0.45
1:A:38:GLN:O	1:A:39:GLN:C	2.54	0.45
1:A:322:PHE:CD1	1:A:322:PHE:C	2.89	0.45
1:A:114:LEU:HD13	1:A:123:LEU:HB2	1.98	0.45
1:A:589:THR:O	1:A:590:GLY:O	2.35	0.44
1:A:306:MET:SD	1:A:347:ALA:HA	2.57	0.44
1:A:337:ASP:O	1:A:342:LYS:NZ	2.49	0.44
1:A:337:ASP:OD1	1:A:339:HIS:HB2	2.17	0.44
1:A:199:GLN:HA	1:A:199:GLN:HE21	1.80	0.44
1:A:562:THR:O	1:A:565:MET:HB2	2.16	0.44
1:A:422:ILE:O	1:A:423:ALA:C	2.54	0.44
1:A:306:MET:HG3	1:A:347:ALA:HB2	1.99	0.44
1:A:80:TYR:CZ	1:A:135:LEU:CD2	3.01	0.44
1:A:514:ARG:HD2	1:A:576:TYR:CD1	2.52	0.44
1:A:60:HIS:HD2	1:A:82:ARG:HE	1.66	0.44
1:A:299:LEU:HD23	1:A:306:MET:HA	1.99	0.44
1:A:141:ASP:OD2	1:A:141:ASP:C	2.52	0.44
1:A:421:ASN:C	1:A:421:ASN:OD1	2.55	0.44
1:A:100:GLN:HE21	1:A:100:GLN:N	2.15	0.44
1:A:315:GLN:HA	1:A:320:LYS:O	2.18	0.44
1:A:391:ILE:HG23	1:A:659:GLN:OE1	2.17	0.44
1:A:18:ALA:O	1:A:19:LEU:C	2.56	0.44
1:A:310:SER:HA	1:A:311:PRO:HD3	1.87	0.44
1:A:147:GLN:O	1:A:148:LEU:C	2.55	0.44
1:A:410:GLY:O	1:A:411:HIS:HD2	2.01	0.43
1:A:502:THR:O	1:A:506:VAL:HG23	2.18	0.43
1:A:363:TYR:CB	1:A:364:PRO:HA	2.40	0.43
1:A:534:PHE:O	1:A:536:GLN:N	2.51	0.43
1:A:385:SER:OG	1:A:386:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:GLY:O	1:A:532:ASP:C	2.57	0.43
1:A:301:LYS:O	1:A:348:ARG:NH2	2.51	0.43
1:A:534:PHE:O	1:A:535:THR:C	2.56	0.43
1:A:144:LEU:O	1:A:145:ALA:C	2.55	0.43
1:A:258:TYR:CE1	1:A:385:SER:O	2.71	0.43
1:A:632:LEU:O	1:A:634:MET:N	2.51	0.43
1:A:193:ALA:HB1	1:A:209:PHE:CE2	2.54	0.43
1:A:89:PHE:CE1	1:A:131:THR:CG2	3.02	0.43
1:A:401:ASP:OD1	1:A:402:ASP:N	2.51	0.43
1:A:216:GLU:HG2	1:A:216:GLU:O	2.19	0.43
1:A:503:TRP:HZ3	1:A:504:HIS:CE1	2.37	0.43
1:A:492:ASP:OD2	1:A:546:THR:HB	2.19	0.42
1:A:302:GLU:O	1:A:302:GLU:CG	2.67	0.42
1:A:520:PHE:CD2	1:A:581:GLN:HA	2.54	0.42
1:A:232:ILE:HB	1:A:233:PRO:HD3	2.01	0.42
1:A:352:GLN:HE21	1:A:352:GLN:HB2	1.63	0.42
1:A:292:ILE:HA	1:A:293:PRO:HD3	1.88	0.42
1:A:622:TYR:O	1:A:622:TYR:CG	2.72	0.42
1:A:20:ASN:ND2	1:A:620:VAL:HG13	2.34	0.42
1:A:108:PHE:CZ	1:A:126:PHE:HA	2.55	0.42
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.77	0.42
1:A:239:GLU:OE2	1:A:283:ILE:HG23	2.19	0.42
1:A:130:VAL:HG11	1:A:153:LEU:HG	2.01	0.42
1:A:698:GLN:HE21	1:A:698:GLN:HB2	1.61	0.42
1:A:539:GLN:HB3	1:A:540:ASP:H	1.37	0.42
1:A:149:THR:O	1:A:153:LEU:HG	2.20	0.41
1:A:274:ARG:HH11	1:A:274:ARG:CG	2.33	0.41
1:A:403:ASN:C	1:A:403:ASN:OD1	2.56	0.41
1:A:45:PHE:HA	1:A:49:VAL:HB	2.02	0.41
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.83	0.41
1:A:266:ILE:CG2	1:A:267:LEU:N	2.84	0.41
1:A:340:VAL:O	1:A:342:LYS:HD3	2.21	0.41
1:A:534:PHE:CD1	1:A:570:ARG:HG3	2.55	0.41
1:A:93:HIS:HA	1:A:127:GLU:HG3	2.01	0.41
1:A:147:GLN:O	1:A:150:ASP:N	2.53	0.41
1:A:423:ALA:O	1:A:424:HIS:C	2.58	0.41
1:A:474:LEU:HB2	1:A:602:ILE:HG22	2.02	0.41
1:A:520:PHE:CE2	1:A:581:GLN:HA	2.55	0.41
1:A:20:ASN:HD21	1:A:621:TYR:H	1.68	0.41
1:A:18:ALA:O	1:A:21:ALA:HB3	2.20	0.41
1:A:147:GLN:CD	1:A:433:ARG:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:O	1:A:139:GLN:HG3	2.21	0.41
1:A:215:ARG:HD2	3:A:716:DCP:H4'	2.02	0.41
1:A:486:GLY:HA3	1:A:645:LYS:HG2	2.03	0.41
1:A:575:ARG:NE	1:A:576:TYR:CE2	2.89	0.41
1:A:516:ARG:HD2	1:A:516:ARG:HH11	1.75	0.41
1:A:661:LEU:HD12	1:A:661:LEU:N	2.35	0.41
1:A:270:LEU:HG	1:A:357:ILE:HD12	2.03	0.41
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.93	0.40
1:A:199:GLN:CA	1:A:199:GLN:NE2	2.78	0.40
1:A:295:ILE:O	1:A:298:ARG:N	2.54	0.40
1:A:581:GLN:CG	1:A:581:GLN:O	2.69	0.40
1:A:478:LEU:O	1:A:479:ALA:C	2.55	0.40
1:A:415:CYS:CB	1:A:417:LEU:HD21	2.52	0.40
1:A:342:LYS:N	1:A:342:LYS:HD3	2.36	0.40
1:A:315:GLN:O	1:A:319:GLY:N	2.46	0.40
1:A:234:VAL:O	1:A:235:MET:C	2.57	0.40
1:A:180:LEU:HD21	1:A:386:ASN:N	2.37	0.40
1:A:594:TYR:OH	1:A:610:GLU:OE2	2.28	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	677/714 (95%)	615 (91%)	50 (7%)	12 (2%)	11	45

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	86	LEU
1	A	303	ASN

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Mol	Chain	Res	Type
1	A	542	TRP
1	A	600	SER
1	A	606	VAL
1	A	590	GLY
1	A	601	SER
1	A	602	ILE
1	A	28	LYS
1	A	639	TYR
1	A	49	VAL

### 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	569/596 (96%)	514 (90%)	55 (10%)	10	37

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	A	53	SER
1	A	100	GLN
1	A	113	THR
1	A	114	LEU
1	A	127	GLU
1	A	175	LEU
1	A	189	SER
1	A	198	LEU
1	A	200	LEU
1	A	214	LEU
1	A	223	ARG
1	A	224	ILE
1	A	243	SER
1	A	251	ARG
1	A	268	ARG
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	271	ASP
1	A	274	ARG
1	A	295	ILE
1	A	316	ARG
1	A	342	LYS
1	A	343	THR
1	A	360	GLU
1	A	390	GLU
1	A	395	ASN
1	A	415	CYS
1	A	417	LEU
1	A	420	LEU
1	A	428	SER
1	A	474	LEU
1	A	494	THR
1	A	500	THR
1	A	514	ARG
1	A	518	LYS
1	A	539	GLN
1	A	540	ASP
1	A	546	THR
1	A	555	ARG
1	A	560	LEU
1	A	563	ARG
1	A	570	ARG
1	A	580	ASN
1	A	583	LEU
1	A	600	SER
1	A	601	SER
1	A	631	ASN
1	A	636	GLN
1	A	652	GLU
1	A	663	LEU
1	A	674	ARG
1	A	693	TYR
1	A	694	ILE
1	A	695	ARG
1	A	698	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	38	GLN
1	A	59	GLN
1	A	60	HIS
1	A	100	GLN
1	A	195	ASN
1	A	199	GLN
1	A	346	ASN
1	A	352	GLN
1	A	395	ASN
1	A	411	HIS
1	A	465	HIS
1	A	580	ASN
1	A	581	GLN
1	A	582	ASN
1	A	584	GLN
1	A	631	ASN
1	A	636	GLN
1	A	677	ASN
1	A	698	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	DCP	A	716	2	21,29,29	1.25	3 (14%)	33,45,45	2.14	11 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DCP	A	716	2	-	0/18/34/34	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	716	DCP	C4-N4	-2.77	1.27	1.35
3	A	716	DCP	C6-N1	2.34	1.39	1.35
3	A	716	DCP	C6-C5	2.42	1.43	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	716	DCP	PB-O3A-PA	-4.92	118.90	132.73
3	A	716	DCP	PB-O3B-PG	-4.64	117.11	132.67
3	A	716	DCP	O2G-PG-O3B	-3.48	89.32	105.09
3	A	716	DCP	C6-N1-C2	-2.36	117.45	121.28
3	A	716	DCP	C4'-O4'-C1'	2.16	114.94	109.47
3	A	716	DCP	O2B-PB-O1B	2.28	124.87	112.53
3	A	716	DCP	C2'-C1'-N1	2.41	120.01	114.16
3	A	716	DCP	C3'-C2'-C1'	2.68	108.85	102.40
3	A	716	DCP	O3'-C3'-C2'	2.72	119.76	110.74
3	A	716	DCP	O4'-C1'-N1	3.01	112.94	107.72
3	A	716	DCP	O2G-PG-O1G	4.14	123.89	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	716	DCP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	681/714 (95%)	-0.53	3 (0%) 93 80	19, 34, 57, 105	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	GLU	2.6
1	A	541	ASP	2.5
1	A	699	LEU	2.1

### 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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DCP	A	716	28/28	0.95	0.12	-0.85	3,21,25,30	0
2	MG	A	715	1/1	0.47	0.23	-	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.