Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2023 – 08:54 PM EDT

PDB ID	:	4DPV
Title	:	PARVOVIRUS/DNA COMPLEX
Authors	:	Chapman, M.S.; Rossmann, M.G.
Deposited on	:	1996-02-01
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

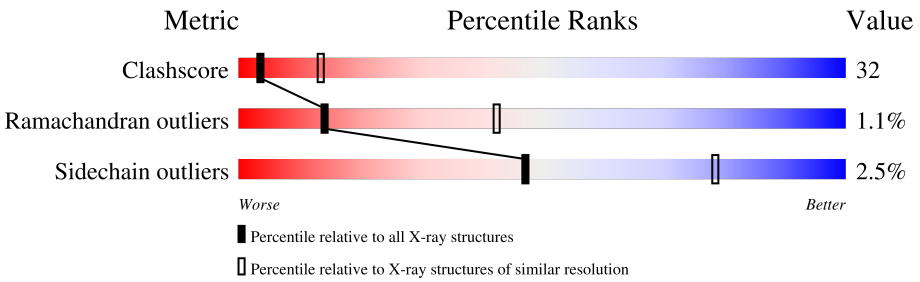
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	N	11	18% 18% 64%
2	Z	584	45% 42% 8% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4606 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 DNA chain called DNA (5'-D(*AP*TP*AP*CP*CP*TP*CP*TP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	N	11	212	101	31	69	11	0	0	0

- Molecule 2 is a protein called PROTEIN (PARVOVIRUS COAT PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Z	559	4390	2780	753	841	16	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	N	2	2	2	0	0
3	Z	2	2	2	0	0

3 Residue-property plots (i)

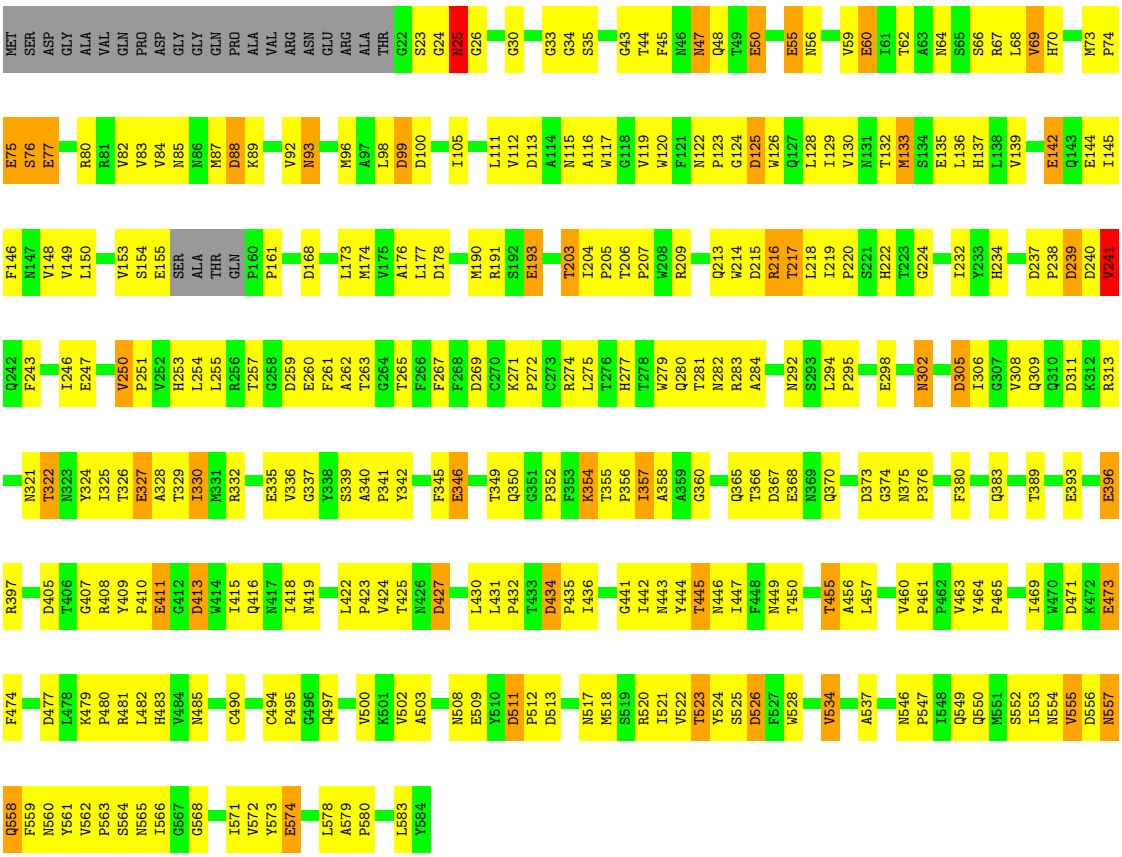
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: DNA (5'-D(*AP*TP*AP*CP*CP*TP*CP*TP*TP*GP*C)-3')

Chain N: 18% 18% 64%

- Molecule 2: PROTEIN (PARVOVIRUS COAT PROTEIN)

Chain Z: 45% 42% 8% •



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	263.21Å 349.01Å 267.32Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 124.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 65.2 (124.81-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 2.52Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , 0.283 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.018 for l,k,-h 0.023 for h,-k,-l 0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	4606	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	N	2.37	8/233 (3.4%)	2.16	17/354 (4.8%)
2	Z	1.32	35/4518 (0.8%)	1.55	65/6172 (1.1%)
All	All	1.39	43/4751 (0.9%)	1.59	82/6526 (1.3%)

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
2	Z	0	2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	75	GLU	CD-OE2	11.24	1.38	1.25
1	N	11	DC	C1'-N1	8.77	1.60	1.49
2	Z	509	GLU	CD-OE2	8.73	1.35	1.25
2	Z	55	GLU	CD-OE1	7.88	1.34	1.25
2	Z	144	GLU	CD-OE2	7.84	1.34	1.25
2	Z	393	GLU	CD-OE2	7.71	1.34	1.25
2	Z	142	GLU	CD-OE1	7.40	1.33	1.25
2	Z	155	GLU	CD-OE2	7.07	1.33	1.25
2	Z	260	GLU	CD-OE2	6.96	1.33	1.25
2	Z	77	GLU	CD-OE2	6.91	1.33	1.25
1	N	11	DC	P-O5'	6.87	1.66	1.59
2	Z	368	GLU	CD-OE2	6.86	1.33	1.25
2	Z	50	GLU	CD-OE2	6.83	1.33	1.25
2	Z	193	GLU	CD-OE2	6.74	1.33	1.25
1	N	1	DA	P-O5'	6.70	1.66	1.59
2	Z	411	GLU	CD-OE2	6.57	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	60	GLU	CD-OE2	6.52	1.32	1.25
1	N	9	DT	C1'-N1	6.44	1.57	1.49
1	N	10	DG	C3'-O3'	6.42	1.52	1.44
2	Z	396	GLU	CD-OE2	6.29	1.32	1.25
2	Z	135	GLU	CD-OE2	6.04	1.32	1.25
2	Z	30	GLY	C-N	5.98	1.43	1.33
2	Z	26	GLY	C-O	5.98	1.33	1.23
2	Z	298	GLU	CD-OE2	5.96	1.32	1.25
2	Z	327	GLU	CD-OE1	5.91	1.32	1.25
2	Z	247	GLU	CD-OE2	5.86	1.32	1.25
2	Z	35	SER	C-N	5.82	1.43	1.33
2	Z	574	GLU	CD-OE2	5.82	1.32	1.25
2	Z	33	GLY	C-O	5.78	1.32	1.23
2	Z	33	GLY	C-N	5.75	1.43	1.33
2	Z	335	GLU	CD-OE2	5.73	1.31	1.25
2	Z	346	GLU	CD-OE1	5.72	1.31	1.25
2	Z	473	GLU	CD-OE2	5.69	1.31	1.25
2	Z	23	SER	C-N	5.51	1.43	1.33
1	N	11	DC	C2-N3	5.48	1.40	1.35
2	Z	34	GLY	CA-C	5.47	1.60	1.51
2	Z	24	GLY	C-N	5.43	1.46	1.34
2	Z	34	GLY	N-CA	5.38	1.54	1.46
2	Z	23	SER	CA-CB	5.29	1.60	1.52
1	N	11	DC	N1-C6	5.20	1.40	1.37
2	Z	33	GLY	CA-C	5.17	1.60	1.51
1	N	10	DG	C6-N1	5.09	1.43	1.39
2	Z	24	GLY	C-O	5.05	1.31	1.23

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	240	ASP	CB-CG-OD2	11.86	128.97	118.30
2	Z	240	ASP	CB-CG-OD1	-10.15	109.16	118.30
2	Z	133	MET	CA-CB-CG	-9.11	97.81	113.30
2	Z	434	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	N	3	DA	P-O5'-C5'	-8.46	107.37	120.90
2	Z	250	VAL	C-N-CD	-8.43	102.05	120.60
2	Z	203	THR	CA-CB-CG2	-8.39	100.65	112.40
1	N	9	DT	O4'-C1'-N1	8.32	113.83	108.00
2	Z	405	ASP	CB-CG-OD1	8.29	125.76	118.30
1	N	3	DA	O4'-C1'-N9	7.97	113.58	108.00
2	Z	168	ASP	CB-CG-OD1	7.92	125.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	471	ASP	CB-CG-OD1	7.57	125.11	118.30
2	Z	25	ASN	CA-CB-CG	7.21	129.25	113.40
2	Z	259	ASP	CB-CG-OD2	-7.20	111.83	118.30
2	Z	513	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	N	8	DT	P-O3'-C3'	7.16	128.29	119.70
1	N	1	DA	P-O3'-C3'	6.99	128.09	119.70
2	Z	269	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	N	10	DG	O4'-C1'-N9	6.94	112.86	108.00
2	Z	471	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	N	10	DG	P-O3'-C3'	6.89	127.97	119.70
1	N	7	DC	O4'-C1'-N1	6.88	112.82	108.00
2	Z	113	ASP	CB-CG-OD2	-6.77	112.21	118.30
2	Z	332	ARG	NE-CZ-NH1	6.73	123.66	120.30
2	Z	99	ASP	CB-CG-OD2	-6.73	112.25	118.30
2	Z	427	ASP	CB-CG-OD2	-6.72	112.25	118.30
2	Z	481	ARG	NE-CZ-NH1	6.71	123.65	120.30
2	Z	311	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	N	3	DA	C2-N3-C4	-6.50	107.35	110.60
2	Z	24	GLY	C-N-CA	6.49	137.93	121.70
2	Z	321	ASN	CB-CA-C	-6.48	97.44	110.40
2	Z	373	ASP	CB-CG-OD2	-6.46	112.49	118.30
2	Z	367	ASP	CB-CG-OD2	-6.25	112.68	118.30
2	Z	520	ARG	NE-CZ-NH1	6.21	123.41	120.30
2	Z	269	ASP	CB-CG-OD1	6.20	123.88	118.30
2	Z	44	THR	CA-CB-CG2	-6.15	103.79	112.40
1	N	3	DA	C5-C6-N1	-6.10	114.65	117.70
2	Z	477	ASP	CB-CG-OD2	-6.09	112.82	118.30
2	Z	305	ASP	CB-CG-OD1	-6.06	112.85	118.30
2	Z	367	ASP	CB-CG-OD1	6.05	123.75	118.30
2	Z	178	ASP	CB-CG-OD2	-5.98	112.92	118.30
2	Z	125	ASP	CB-CG-OD2	-5.97	112.93	118.30
2	Z	168	ASP	CB-CG-OD2	-5.88	113.00	118.30
2	Z	209	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	Z	88	ASP	CB-CG-OD2	-5.77	113.11	118.30
2	Z	311	ASP	CB-CG-OD2	5.76	123.48	118.30
2	Z	500	VAL	CA-CB-CG2	-5.75	102.28	110.90
2	Z	100	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	Z	239	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	Z	113	ASP	CB-CG-OD1	5.65	123.39	118.30
2	Z	178	ASP	CB-CG-OD1	5.63	123.37	118.30
2	Z	555	VAL	CA-CB-CG2	-5.59	102.51	110.90
2	Z	413	ASP	CB-CG-OD2	-5.57	113.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	373	ASP	CB-CG-OD1	5.53	123.27	118.30
2	Z	523	THR	CA-CB-CG2	-5.52	104.67	112.40
2	Z	243	PHE	N-CA-CB	-5.49	100.71	110.60
1	N	11	DC	P-O5'-C5'	5.47	129.65	120.90
2	Z	215	ASP	CB-CG-OD2	-5.46	113.38	118.30
2	Z	99	ASP	CB-CG-OD1	5.43	123.19	118.30
2	Z	526	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	Z	25	ASN	CB-CA-C	5.38	121.17	110.40
2	Z	100	ASP	CB-CG-OD1	5.37	123.13	118.30
2	Z	534	VAL	CB-CA-C	-5.37	101.20	111.40
2	Z	80	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	N	3	DA	N9-C1'-C2'	5.33	122.73	112.60
1	N	3	DA	C8-N9-C4	-5.33	103.67	105.80
1	N	3	DA	N7-C8-N9	5.30	116.45	113.80
2	Z	217	THR	CA-CB-CG2	-5.30	104.97	112.40
2	Z	445	THR	C-N-CA	-5.29	108.47	121.70
2	Z	513	ASP	CB-CG-OD1	5.27	123.04	118.30
1	N	3	DA	C5-N7-C8	-5.24	101.28	103.90
2	Z	241	VAL	CB-CA-C	-5.24	101.45	111.40
2	Z	357	ILE	CA-CB-CG1	-5.19	101.14	111.00
2	Z	511	ASP	CB-CG-OD2	-5.14	113.68	118.30
2	Z	534	VAL	CA-CB-CG1	-5.09	103.26	110.90
1	N	4	DC	N1-C2-O2	5.06	121.94	118.90
2	Z	455	THR	CA-CB-CG2	-5.05	105.33	112.40
2	Z	69	VAL	CA-CB-CG2	-5.04	103.34	110.90
2	Z	255	LEU	CB-CA-C	-5.04	100.63	110.20
2	Z	445	THR	CA-CB-CG2	-5.03	105.36	112.40
1	N	6	DT	P-O5'-C5'	-5.02	112.87	120.90
2	Z	322	THR	CB-CA-C	-5.01	98.08	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Z	241	VAL	Mainchain
2	Z	25	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	212	0	121	12	0
2	Z	4390	0	4172	274	0
3	N	2	0	0	0	0
3	Z	2	0	0	0	0
All	All	4606	0	4293	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 32.

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)
2:Z:557:ASN:HD22	2:Z:558:GLN:N	1.49	1.09
2:Z:75:GLU:HG3	2:Z:76:SER:N	1.77	1.00
1:N:3:DA:N6	2:Z:267:PHE:H	1.60	0.99
1:N:3:DA:H61	2:Z:267:PHE:H	1.03	0.98
2:Z:554:ASN:H	2:Z:557:ASN:HD21	0.97	0.93
2:Z:366:THR:HA	2:Z:370:GLN:HB2	1.52	0.91
2:Z:193:GLU:HB3	2:Z:206:THR:HG21	1.51	0.90
2:Z:425:THR:HG22	2:Z:427:ASP:H	1.36	0.88
2:Z:173:LEU:HD12	2:Z:174:MET:N	1.88	0.88
2:Z:354:LYS:HD2	2:Z:355:THR:N	1.90	0.87
2:Z:557:ASN:HD22	2:Z:558:GLN:H	1.19	0.86
2:Z:479:LYS:HB3	2:Z:480:PRO:HD2	1.58	0.85
2:Z:204:ILE:HB	2:Z:205:PRO:HD2	1.59	0.84
2:Z:360:GLY:HA2	2:Z:374:GLY:HA3	1.58	0.84
2:Z:122:ASN:HB2	2:Z:123:PRO:HD2	1.60	0.83
2:Z:148:VAL:O	2:Z:257:THR:HG23	1.78	0.83
1:N:6:DT:H2"	1:N:7:DC:H5'	1.61	0.82
2:Z:554:ASN:N	2:Z:557:ASN:HD21	1.79	0.80
1:N:10:DG:H3'	1:N:11:DC:H5"	1.65	0.78
2:Z:73:MET:HB2	2:Z:74:PRO:HD2	1.65	0.78
2:Z:562:VAL:CG1	2:Z:563:PRO:HD2	2.14	0.78
1:N:3:DA:H61	2:Z:267:PHE:N	1.83	0.76
2:Z:562:VAL:HG13	2:Z:563:PRO:HD2	1.65	0.76
2:Z:232:ILE:HD11	2:Z:234:HIS:CE1	2.21	0.76
2:Z:431:LEU:HB3	2:Z:432:PRO:HD2	1.68	0.75
2:Z:422:LEU:HB2	2:Z:423:PRO:HA	1.68	0.75
2:Z:77:GLU:HG3	2:Z:518:MET:CE	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:173:LEU:HD12	2:Z:174:MET:H	1.49	0.73
2:Z:366:THR:HA	2:Z:370:GLN:CB	2.19	0.72
2:Z:366:THR:O	2:Z:370:GLN:HG2	1.89	0.72
2:Z:557:ASN:ND2	2:Z:558:GLN:N	2.32	0.72
2:Z:271:LYS:HB3	2:Z:272:PRO:HD2	1.72	0.71
2:Z:322:THR:HB	2:Z:324:TYR:H	1.55	0.71
2:Z:457:LEU:N	2:Z:457:LEU:HD23	2.06	0.71
2:Z:494:CYS:HB3	2:Z:495:PRO:HD2	1.73	0.70
2:Z:219:ILE:CG2	2:Z:220:PRO:HD2	2.21	0.70
2:Z:430:LEU:C	2:Z:431:LEU:HD23	2.12	0.70
2:Z:422:LEU:HD23	2:Z:422:LEU:N	2.05	0.70
2:Z:68:LEU:HD12	2:Z:69:VAL:N	2.08	0.69
2:Z:111:LEU:HD12	2:Z:112:VAL:N	2.08	0.69
1:N:3:DA:N6	2:Z:267:PHE:N	2.40	0.69
2:Z:250:VAL:HG12	2:Z:251:PRO:N	2.08	0.68
2:Z:326:THR:O	2:Z:329:THR:N	2.26	0.68
2:Z:340:ALA:HB1	2:Z:341:PRO:HD2	1.75	0.68
2:Z:422:LEU:HD23	2:Z:422:LEU:H	1.58	0.68
2:Z:409:TYR:CE2	2:Z:411:GLU:HB2	2.29	0.68
2:Z:422:LEU:HA	2:Z:423:PRO:C	2.15	0.67
2:Z:92:VAL:O	2:Z:93:ASN:HB2	1.95	0.66
1:N:10:DG:H2'	1:N:11:DC:O4'	1.96	0.66
2:Z:354:LYS:HD2	2:Z:354:LYS:C	2.16	0.66
2:Z:583:LEU:HD23	2:Z:583:LEU:O	1.95	0.66
2:Z:206:THR:HB	2:Z:207:PRO:HD2	1.77	0.66
2:Z:150:LEU:N	2:Z:150:LEU:HD12	2.11	0.65
2:Z:425:THR:HG22	2:Z:427:ASP:N	2.09	0.65
2:Z:203:THR:OG1	2:Z:204:ILE:N	2.27	0.65
2:Z:422:LEU:HA	2:Z:423:PRO:O	1.96	0.65
2:Z:149:VAL:C	2:Z:150:LEU:HD12	2.16	0.65
2:Z:43:GLY:HA3	2:Z:146:PHE:CD2	2.32	0.65
2:Z:326:THR:H	2:Z:329:THR:HB	1.61	0.65
2:Z:557:ASN:ND2	2:Z:557:ASN:H	1.94	0.65
2:Z:422:LEU:HB2	2:Z:423:PRO:CA	2.26	0.64
1:N:3:DA:H5'	1:N:9:DT:H5"	1.79	0.64
2:Z:485:ASN:OD1	2:Z:485:ASN:N	2.25	0.64
2:Z:204:ILE:CB	2:Z:205:PRO:HD2	2.22	0.63
2:Z:366:THR:HA	2:Z:370:GLN:CG	2.29	0.63
2:Z:150:LEU:HG	2:Z:525:SER:HB2	1.80	0.63
2:Z:583:LEU:HD23	2:Z:583:LEU:C	2.20	0.63
2:Z:357:ILE:HG22	2:Z:358:ALA:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:396:GLU:HG3	2:Z:397:ARG:N	2.14	0.62
2:Z:525:SER:OG	2:Z:526:ASP:N	2.31	0.62
2:Z:59:VAL:HG12	2:Z:60:GLU:N	2.12	0.62
2:Z:579:ALA:HB1	2:Z:580:PRO:HD2	1.82	0.61
2:Z:96:MET:HG2	2:Z:220:PRO:HA	1.82	0.61
2:Z:193:GLU:HB3	2:Z:206:THR:CG2	2.29	0.61
2:Z:219:ILE:HG23	2:Z:220:PRO:HD2	1.83	0.60
2:Z:66:SER:C	2:Z:67:ARG:HG2	2.21	0.60
2:Z:111:LEU:HD12	2:Z:112:VAL:H	1.66	0.59
2:Z:365:GLN:O	2:Z:370:GLN:HG3	2.02	0.59
2:Z:204:ILE:HG13	2:Z:204:ILE:O	2.01	0.59
2:Z:206:THR:HB	2:Z:207:PRO:CD	2.31	0.59
2:Z:302:ASN:OD1	2:Z:302:ASN:N	2.35	0.59
2:Z:557:ASN:ND2	2:Z:557:ASN:N	2.47	0.58
2:Z:554:ASN:O	2:Z:557:ASN:ND2	2.35	0.58
2:Z:410:PRO:HA	2:Z:413:ASP:OD2	2.04	0.58
2:Z:336:VAL:O	2:Z:408:ARG:NH2	2.36	0.58
2:Z:217:THR:HG22	2:Z:218:LEU:N	2.17	0.57
2:Z:494:CYS:HB3	2:Z:495:PRO:CD	2.35	0.57
2:Z:563:PRO:HA	2:Z:568:GLY:O	2.05	0.57
2:Z:75:GLU:CG	2:Z:76:SER:N	2.60	0.56
2:Z:177:LEU:HD22	2:Z:263:THR:HG22	1.88	0.56
2:Z:349:THR:HG22	2:Z:350:GLN:HG3	1.87	0.56
2:Z:483:HIS:HB3	2:Z:485:ASN:OD1	2.05	0.56
2:Z:219:ILE:HG22	2:Z:220:PRO:HD2	1.86	0.56
2:Z:250:VAL:CG1	2:Z:251:PRO:N	2.69	0.55
2:Z:473:GLU:HA	2:Z:473:GLU:OE1	2.06	0.55
2:Z:482:LEU:N	2:Z:482:LEU:HD23	2.20	0.55
2:Z:132:THR:C	2:Z:133:MET:HG3	2.26	0.55
2:Z:294:LEU:HB3	2:Z:295:PRO:HD2	1.88	0.55
2:Z:441:GLY:O	2:Z:442:ILE:HD13	2.05	0.55
2:Z:463:VAL:HG12	2:Z:463:VAL:O	2.07	0.55
2:Z:431:LEU:HB3	2:Z:432:PRO:CD	2.35	0.54
2:Z:122:ASN:HB2	2:Z:123:PRO:CD	2.33	0.54
2:Z:237:ASP:OD1	2:Z:238:PRO:HD2	2.07	0.54
2:Z:432:PRO:O	2:Z:443:ASN:ND2	2.37	0.54
2:Z:380:PHE:CD1	2:Z:380:PHE:N	2.75	0.54
2:Z:139:VAL:HB	2:Z:534:VAL:HG12	1.88	0.54
2:Z:339:SER:O	2:Z:449:ASN:HA	2.08	0.54
2:Z:410:PRO:HD2	2:Z:411:GLU:OE1	2.08	0.54
2:Z:218:LEU:HD12	2:Z:219:ILE:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:271:LYS:HB3	2:Z:272:PRO:CD	2.38	0.54
2:Z:572:VAL:CG1	2:Z:573:TYR:N	2.71	0.54
2:Z:345:PHE:N	2:Z:345:PHE:CD1	2.73	0.53
2:Z:431:LEU:HD23	2:Z:431:LEU:N	2.22	0.53
2:Z:119:VAL:HB	2:Z:120:TRP:CD1	2.43	0.53
2:Z:47:ASN:C	2:Z:47:ASN:HD22	2.11	0.53
2:Z:357:ILE:CG2	2:Z:358:ALA:N	2.71	0.53
2:Z:422:LEU:N	2:Z:422:LEU:CD2	2.72	0.53
2:Z:572:VAL:HG12	2:Z:573:TYR:N	2.24	0.53
2:Z:442:ILE:HG22	2:Z:443:ASN:N	2.22	0.53
2:Z:555:VAL:HG23	2:Z:556:ASP:N	2.24	0.53
2:Z:578:LEU:N	2:Z:578:LEU:CD1	2.72	0.53
2:Z:443:ASN:H	2:Z:446:ASN:HD22	1.56	0.52
2:Z:119:VAL:HG12	2:Z:119:VAL:O	2.08	0.52
1:N:3:DA:H5'	1:N:9:DT:C5'	2.39	0.52
2:Z:73:MET:HB2	2:Z:74:PRO:CD	2.37	0.52
2:Z:360:GLY:HA2	2:Z:374:GLY:CA	2.35	0.52
2:Z:422:LEU:CA	2:Z:423:PRO:C	2.78	0.52
2:Z:546:ASN:HB2	2:Z:547:PRO:HD2	1.90	0.52
2:Z:554:ASN:OD1	2:Z:556:ASP:N	2.42	0.52
2:Z:553:ILE:HG12	2:Z:554:ASN:N	2.25	0.52
2:Z:572:VAL:HG12	2:Z:573:TYR:O	2.09	0.52
2:Z:142:GLU:HB3	2:Z:265:THR:HA	1.92	0.52
2:Z:565:ASN:O	2:Z:566:ILE:HD13	2.10	0.52
2:Z:274:ARG:O	2:Z:275:LEU:HD23	2.10	0.51
2:Z:407:GLY:O	2:Z:408:ARG:HD3	2.09	0.51
2:Z:479:LYS:CB	2:Z:480:PRO:HD2	2.28	0.51
2:Z:511:ASP:OD1	2:Z:512:PRO:HD2	2.11	0.51
2:Z:68:LEU:HD12	2:Z:69:VAL:H	1.76	0.51
2:Z:523:THR:HG22	2:Z:524:TYR:N	2.26	0.51
2:Z:117:TRP:HA	2:Z:469:ILE:HD11	1.93	0.51
2:Z:206:THR:CB	2:Z:207:PRO:CD	2.86	0.51
2:Z:502:VAL:HG12	2:Z:503:ALA:N	2.24	0.51
2:Z:139:VAL:HB	2:Z:534:VAL:O	2.11	0.50
2:Z:552:SER:OG	2:Z:553:ILE:N	2.42	0.50
2:Z:360:GLY:CA	2:Z:374:GLY:HA3	2.37	0.50
2:Z:66:SER:O	2:Z:67:ARG:HG2	2.12	0.49
2:Z:241:VAL:O	2:Z:241:VAL:HG12	2.09	0.49
2:Z:436:ILE:HG12	2:Z:443:ASN:HA	1.94	0.49
2:Z:564:SER:C	2:Z:566:ILE:H	2.16	0.49
2:Z:203:THR:C	2:Z:204:ILE:HG23	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:281:THR:O	2:Z:283:ARG:N	2.45	0.49
2:Z:217:THR:CG2	2:Z:218:LEU:N	2.75	0.49
2:Z:203:THR:CB	2:Z:383:GLN:HE22	2.25	0.49
2:Z:455:THR:HG22	2:Z:456:ALA:N	2.28	0.49
2:Z:203:THR:CB	2:Z:383:GLN:NE2	2.76	0.48
2:Z:55:GLU:O	2:Z:56:ASN:HB2	2.13	0.48
2:Z:149:VAL:HG12	2:Z:150:LEU:N	2.29	0.48
2:Z:326:THR:O	2:Z:328:ALA:N	2.46	0.48
2:Z:432:PRO:C	2:Z:443:ASN:HD22	2.17	0.48
2:Z:561:TYR:C	2:Z:562:VAL:HG23	2.34	0.48
2:Z:82:VAL:HG12	2:Z:83:VAL:N	2.28	0.48
2:Z:68:LEU:HD12	2:Z:68:LEU:C	2.34	0.48
2:Z:528:TRP:CD1	2:Z:528:TRP:N	2.81	0.48
2:Z:85:ASN:OD1	2:Z:87:MET:HB2	2.14	0.48
2:Z:444:TYR:O	2:Z:447:ILE:HG12	2.14	0.48
2:Z:473:GLU:HG3	2:Z:474:PHE:N	2.29	0.48
2:Z:218:LEU:HD12	2:Z:218:LEU:C	2.33	0.48
2:Z:579:ALA:HB1	2:Z:580:PRO:CD	2.44	0.47
2:Z:176:ALA:HB1	2:Z:250:VAL:HG11	1.96	0.47
2:Z:69:VAL:HG12	2:Z:70:HIS:N	2.29	0.47
2:Z:578:LEU:N	2:Z:578:LEU:HD12	2.29	0.47
1:N:10:DG:H3'	1:N:11:DC:C5'	2.38	0.47
1:N:7:DC:H2'	1:N:8:DT:C6	2.49	0.47
2:Z:562:VAL:HG12	2:Z:563:PRO:HD2	1.94	0.47
2:Z:557:ASN:HD22	2:Z:557:ASN:N	2.12	0.47
2:Z:357:ILE:HD13	2:Z:357:ILE:HA	1.31	0.47
2:Z:408:ARG:HD3	2:Z:408:ARG:HA	1.52	0.47
2:Z:557:ASN:O	2:Z:559:PHE:N	2.48	0.47
2:Z:508:ASN:OD1	2:Z:508:ASN:N	2.46	0.46
2:Z:59:VAL:CG1	2:Z:60:GLU:N	2.76	0.46
2:Z:148:VAL:HG12	2:Z:149:VAL:N	2.30	0.46
2:Z:117:TRP:CE2	2:Z:469:ILE:HG12	2.49	0.46
2:Z:125:ASP:O	2:Z:126:TRP:C	2.52	0.46
2:Z:204:ILE:HB	2:Z:205:PRO:CD	2.36	0.46
2:Z:330:ILE:HG23	2:Z:330:ILE:O	2.15	0.46
2:Z:562:VAL:CG1	2:Z:563:PRO:CD	2.90	0.46
2:Z:479:LYS:HB3	2:Z:480:PRO:CD	2.39	0.46
2:Z:554:ASN:H	2:Z:557:ASN:ND2	1.83	0.46
2:Z:146:PHE:CD1	2:Z:146:PHE:N	2.84	0.46
2:Z:346:GLU:HG3	2:Z:355:THR:OG1	2.16	0.46
2:Z:455:THR:CG2	2:Z:456:ALA:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:460:VAL:O	2:Z:460:VAL:HG23	2.15	0.46
2:Z:465:PRO:HG3	2:Z:571:ILE:CG2	2.45	0.45
2:Z:153:VAL:HG12	2:Z:154:SER:N	2.27	0.45
1:N:6:DT:C2'	1:N:7:DC:H5'	2.40	0.45
2:Z:443:ASN:H	2:Z:446:ASN:ND2	2.15	0.45
2:Z:465:PRO:HG3	2:Z:571:ILE:HG22	1.98	0.45
2:Z:99:ASP:CG	2:Z:216:ARG:HH21	2.19	0.45
2:Z:356:PRO:O	2:Z:357:ILE:HD13	2.16	0.45
2:Z:443:ASN:N	2:Z:443:ASN:OD1	2.48	0.45
2:Z:549:GLN:O	2:Z:550:GLN:HG2	2.15	0.45
2:Z:122:ASN:OD1	2:Z:122:ASN:C	2.56	0.45
2:Z:415:ILE:HG22	2:Z:416:GLN:N	2.32	0.45
2:Z:77:GLU:HG3	2:Z:518:MET:HE2	1.97	0.45
2:Z:281:THR:O	2:Z:282:ASN:C	2.52	0.44
2:Z:123:PRO:O	2:Z:124:GLY:C	2.54	0.44
2:Z:281:THR:C	2:Z:283:ARG:N	2.69	0.44
2:Z:237:ASP:OD1	2:Z:239:ASP:OD2	2.35	0.44
2:Z:326:THR:C	2:Z:328:ALA:N	2.68	0.44
2:Z:145:ILE:HG22	2:Z:146:PHE:N	2.30	0.44
2:Z:219:ILE:CG2	2:Z:220:PRO:CD	2.95	0.44
2:Z:342:TYR:O	2:Z:342:TYR:CG	2.69	0.44
2:Z:566:ILE:HD13	2:Z:566:ILE:HA	1.54	0.44
2:Z:579:ALA:HA	2:Z:580:PRO:HD3	1.62	0.44
2:Z:253:HIS:C	2:Z:254:LEU:HD23	2.37	0.44
2:Z:98:LEU:HD23	2:Z:98:LEU:HA	1.72	0.44
2:Z:340:ALA:HB1	2:Z:341:PRO:CD	2.45	0.44
2:Z:153:VAL:CG1	2:Z:154:SER:N	2.79	0.44
2:Z:261:PHE:CG	2:Z:262:ALA:N	2.85	0.44
2:Z:354:LYS:HD2	2:Z:355:THR:C	2.38	0.44
2:Z:83:VAL:CG1	2:Z:84:VAL:N	2.81	0.44
2:Z:565:ASN:OD1	2:Z:566:ILE:HG12	2.18	0.44
2:Z:45:PHE:CE2	2:Z:66:SER:HB2	2.53	0.43
2:Z:434:ASP:HA	2:Z:435:PRO:HD3	1.49	0.43
2:Z:115:ASN:OD1	2:Z:469:ILE:N	2.41	0.43
2:Z:325:ILE:O	2:Z:325:ILE:HG22	2.18	0.43
2:Z:424:VAL:HG22	2:Z:425:THR:N	2.34	0.43
2:Z:564:SER:C	2:Z:566:ILE:N	2.71	0.43
2:Z:216:ARG:O	2:Z:216:ARG:HG3	2.13	0.43
2:Z:139:VAL:HB	2:Z:534:VAL:CG1	2.49	0.43
2:Z:277:HIS:O	2:Z:580:PRO:HA	2.19	0.43
2:Z:430:LEU:O	2:Z:431:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:554:ASN:OD1	2:Z:554:ASN:C	2.57	0.43
2:Z:560:ASN:N	2:Z:560:ASN:ND2	2.67	0.43
2:Z:130:VAL:O	2:Z:130:VAL:HG12	2.18	0.42
2:Z:308:VAL:HG12	2:Z:309:GLN:N	2.33	0.42
2:Z:422:LEU:CB	2:Z:423:PRO:CA	2.94	0.42
2:Z:136:LEU:HD12	2:Z:537:ALA:HB2	2.01	0.42
2:Z:280:GLN:HB3	2:Z:284:ALA:HB3	2.01	0.42
2:Z:444:TYR:O	2:Z:445:THR:C	2.54	0.42
2:Z:555:VAL:H	2:Z:555:VAL:HG22	1.35	0.42
2:Z:430:LEU:HD12	2:Z:430:LEU:HA	1.75	0.42
2:Z:521:ILE:HG22	2:Z:522:VAL:N	2.34	0.42
2:Z:464:TYR:CD1	2:Z:465:PRO:HA	2.54	0.42
2:Z:366:THR:CA	2:Z:370:GLN:HB2	2.36	0.42
2:Z:564:SER:O	2:Z:566:ILE:N	2.52	0.42
2:Z:346:GLU:O	2:Z:352:PRO:HA	2.19	0.42
2:Z:213:GLN:CD	2:Z:214:TRP:N	2.73	0.42
2:Z:279:TRP:CE3	2:Z:280:GLN:HA	2.55	0.42
2:Z:309:GLN:O	2:Z:313:ARG:HG3	2.20	0.42
2:Z:549:GLN:CG	2:Z:550:GLN:N	2.83	0.42
2:Z:222:HIS:ND1	2:Z:224:GLY:N	2.68	0.41
2:Z:464:TYR:HA	2:Z:465:PRO:HA	1.80	0.41
2:Z:502:VAL:CG1	2:Z:503:ALA:N	2.82	0.41
2:Z:137:HIS:CE1	2:Z:272:PRO:HB3	2.55	0.41
2:Z:517:ASN:HD22	2:Z:517:ASN:HA	1.64	0.41
2:Z:216:ARG:NH2	2:Z:218:LEU:HD22	2.36	0.41
2:Z:337:GLY:HA3	2:Z:408:ARG:HH21	1.86	0.41
2:Z:116:ALA:O	2:Z:117:TRP:C	2.58	0.41
2:Z:337:GLY:C	2:Z:408:ARG:NH2	2.73	0.41
2:Z:177:LEU:HD12	2:Z:497:GLN:O	2.20	0.41
2:Z:389:THR:HG23	2:Z:568:GLY:HA2	2.03	0.41
2:Z:445:THR:H	2:Z:445:THR:HG23	1.48	0.41
2:Z:473:GLU:OE1	2:Z:473:GLU:CA	2.68	0.41
2:Z:128:LEU:O	2:Z:129:ILE:C	2.57	0.41
2:Z:204:ILE:HA	2:Z:205:PRO:HD3	1.69	0.41
2:Z:418:ILE:HG23	2:Z:419:ASN:N	2.36	0.41
2:Z:557:ASN:O	2:Z:558:GLN:C	2.55	0.41
2:Z:105:ILE:HG23	2:Z:105:ILE:HD12	1.78	0.41
2:Z:203:THR:OG1	2:Z:383:GLN:NE2	2.49	0.41
2:Z:48:GLN:H	2:Z:64:ASN:HB2	1.86	0.41
2:Z:50:GLU:HB2	2:Z:62:THR:HB	2.03	0.41
2:Z:305:ASP:OD1	2:Z:306:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:70:HIS:O	2:Z:204:ILE:HG22	2.21	0.40
2:Z:75:GLU:HG3	2:Z:76:SER:HB3	2.02	0.40
2:Z:88:ASP:CG	2:Z:89:LYS:N	2.75	0.40
2:Z:246:ILE:HD13	2:Z:246:ILE:HA	1.77	0.40
2:Z:375:ASN:HA	2:Z:376:PRO:HD3	1.83	0.40
2:Z:292:ASN:HB2	2:Z:306:ILE:O	2.22	0.40
2:Z:565:ASN:OD1	2:Z:565:ASN:N	2.54	0.40
2:Z:579:ALA:CB	2:Z:580:PRO:CD	2.95	0.40
2:Z:573:TYR:C	2:Z:574:GLU:HG2	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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
2	Z	555/584 (95%)	499 (90%)	50 (9%)	6 (1%)	14 42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Z	25	ASN
2	Z	558	GLN
2	Z	93	ASN
2	Z	327	GLU
2	Z	330	ILE
2	Z	461	PRO

5.3.2 Protein sidechains (i)

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
2	Z	477/495 (96%)	465 (98%)	12 (2%)	47 78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	25	ASN
2	Z	47	ASN
2	Z	76	SER
2	Z	161	PRO
2	Z	190	MET
2	Z	191	ARG
2	Z	216	ARG
2	Z	302	ASN
2	Z	354	LYS
2	Z	450	THR
2	Z	490	CYS
2	Z	557	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	25	ASN
2	Z	93	ASN
2	Z	104	GLN
2	Z	242	GLN
2	Z	309	GLN
2	Z	323	ASN
2	Z	350	GLN
2	Z	383	GLN
2	Z	428	ASN
2	Z	446	ASN
2	Z	466	ASN
2	Z	491	GLN
2	Z	492	ASN
2	Z	517	ASN
2	Z	543	HIS
2	Z	549	GLN
2	Z	557	ASN

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Mol	Chain	Res	Type
2	Z	560	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.