Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:52 PM GMT

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

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 2.90 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.
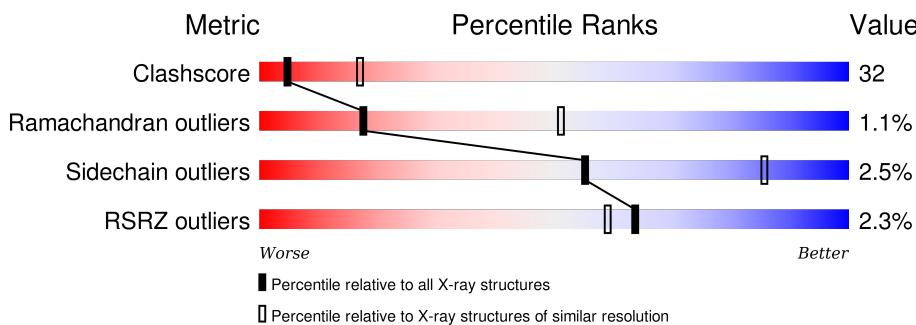
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	N	11	18% 18% 64%
2	Z	584	2% 45% 43% 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
1	N	11	Total 212	C 101	N 31	O 69	P 11	0	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Z	2	Total 2	Mg 2	0	0
3	N	2	Total 2	Mg 2	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: DNA (5'-D(*AP*TP*AP*CP*CP*TP*CP*TP*TP*GP*C)-3')

Chain N:

• Molecule 2: PROTEIN (PARVOVIRUS COAT PROTEIN)

Chain Z:
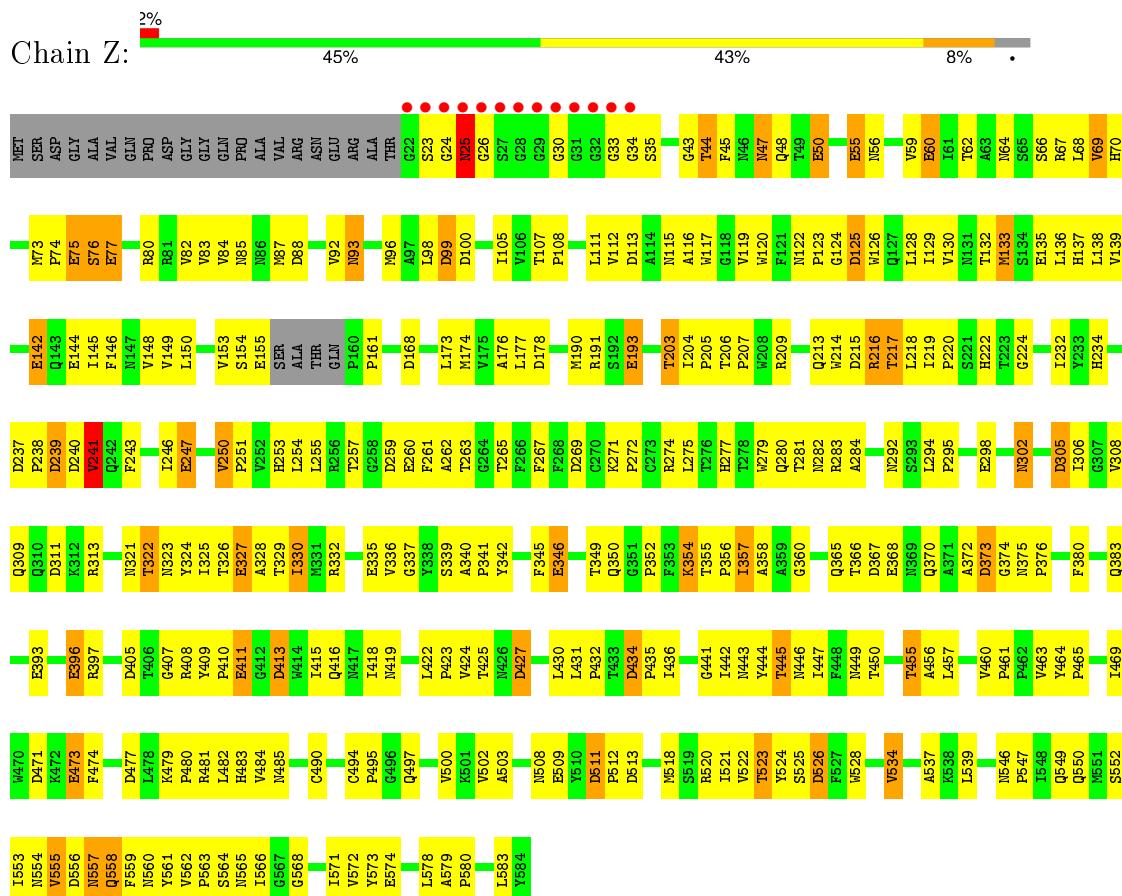
4 Data and refinement statistics (i)

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 0.268 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 115.2	EDS
Estimated twinning fraction	0.018 for l,k,-h 0.023 for h,-k,-l 0.017 for l,-k,h	Xtriage
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	2 of 1081203 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.21	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	11.28	1.38	1.25
1	N	11	DC	C1'-N1	8.80	1.60	1.49
2	Z	509	GLU	CD-OE2	8.78	1.35	1.25
2	Z	55	GLU	CD-OE1	7.89	1.34	1.25
2	Z	144	GLU	CD-OE2	7.82	1.34	1.25
2	Z	393	GLU	CD-OE2	7.79	1.34	1.25
2	Z	142	GLU	CD-OE1	7.43	1.33	1.25
2	Z	155	GLU	CD-OE2	7.05	1.33	1.25
1	N	11	DC	P-O5'	6.95	1.66	1.59
2	Z	77	GLU	CD-OE2	6.95	1.33	1.25
2	Z	260	GLU	CD-OE2	6.94	1.33	1.25
2	Z	368	GLU	CD-OE2	6.84	1.33	1.25
2	Z	50	GLU	CD-OE2	6.80	1.33	1.25
2	Z	193	GLU	CD-OE2	6.72	1.33	1.25
1	N	1	DA	P-O5'	6.66	1.66	1.59
2	Z	411	GLU	CD-OE2	6.54	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	60	GLU	CD-OE2	6.48	1.32	1.25
1	N	9	DT	C1'-N1	6.44	1.57	1.49
1	N	10	DG	C3'-O3'	6.34	1.52	1.44
2	Z	396	GLU	CD-OE2	6.31	1.32	1.25
2	Z	135	GLU	CD-OE2	6.11	1.32	1.25
2	Z	30	GLY	C-N	6.02	1.43	1.33
2	Z	298	GLU	CD-OE2	5.97	1.32	1.25
2	Z	26	GLY	C-O	5.93	1.33	1.23
2	Z	247	GLU	CD-OE2	5.91	1.32	1.25
2	Z	327	GLU	CD-OE1	5.83	1.32	1.25
2	Z	574	GLU	CD-OE2	5.82	1.32	1.25
2	Z	346	GLU	CD-OE1	5.79	1.32	1.25
2	Z	33	GLY	C-O	5.79	1.32	1.23
2	Z	35	SER	C-N	5.78	1.43	1.33
2	Z	33	GLY	C-N	5.77	1.43	1.33
2	Z	335	GLU	CD-OE2	5.72	1.31	1.25
2	Z	473	GLU	CD-OE2	5.61	1.31	1.25
2	Z	23	SER	C-N	5.51	1.43	1.33
1	N	11	DC	C2-N3	5.43	1.40	1.35
2	Z	34	GLY	CA-C	5.42	1.60	1.51
2	Z	34	GLY	N-CA	5.42	1.54	1.46
2	Z	24	GLY	C-N	5.42	1.46	1.34
2	Z	23	SER	CA-CB	5.32	1.60	1.52
1	N	11	DC	N1-C6	5.21	1.40	1.37
2	Z	33	GLY	CA-C	5.13	1.60	1.51
1	N	10	DG	C6-N1	5.07	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(°)	Ideal(°)
2	Z	240	ASP	CB-CG-OD2	11.83	128.94	118.30
2	Z	240	ASP	CB-CG-OD1	-10.15	109.17	118.30
2	Z	133	MET	CA-CB-CG	-9.11	97.81	113.30
2	Z	434	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	N	3	DA	P-O5'-C5'	-8.46	107.37	120.90
2	Z	250	VAL	C-N-CD	-8.42	102.07	120.60
2	Z	203	THR	CA-CB-CG2	-8.39	100.66	112.40
1	N	9	DT	O4'-C1'-N1	8.27	113.79	108.00
2	Z	405	ASP	CB-CG-OD1	8.26	125.73	118.30
1	N	3	DA	O4'-C1'-N9	7.95	113.57	108.00
2	Z	168	ASP	CB-CG-OD1	7.95	125.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	471	ASP	CB-CG-OD1	7.59	125.13	118.30
2	Z	25	ASN	CA-CB-CG	7.21	129.25	113.40
2	Z	513	ASP	CB-CG-OD2	-7.20	111.82	118.30
2	Z	259	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	N	8	DT	P-O3'-C3'	7.15	128.28	119.70
1	N	10	DG	O4'-C1'-N9	7.00	112.90	108.00
2	Z	269	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	N	1	DA	P-O3'-C3'	6.98	128.07	119.70
2	Z	471	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	N	10	DG	P-O3'-C3'	6.92	128.01	119.70
1	N	7	DC	O4'-C1'-N1	6.88	112.82	108.00
2	Z	113	ASP	CB-CG-OD2	-6.79	112.19	118.30
2	Z	481	ARG	NE-CZ-NH1	6.75	123.68	120.30
2	Z	427	ASP	CB-CG-OD2	-6.73	112.24	118.30
2	Z	332	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	Z	99	ASP	CB-CG-OD2	-6.69	112.28	118.30
2	Z	311	ASP	CB-CG-OD1	-6.57	112.39	118.30
2	Z	24	GLY	C-N-CA	6.50	137.94	121.70
2	Z	321	ASN	CB-CA-C	-6.49	97.41	110.40
2	Z	373	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	N	3	DA	C2-N3-C4	-6.43	107.39	110.60
2	Z	520	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	Z	269	ASP	CB-CG-OD1	6.25	123.92	118.30
2	Z	367	ASP	CB-CG-OD2	-6.23	112.70	118.30
2	Z	44	THR	CA-CB-CG2	-6.16	103.78	112.40
2	Z	477	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	Z	305	ASP	CB-CG-OD1	-6.07	112.83	118.30
2	Z	367	ASP	CB-CG-OD1	6.06	123.76	118.30
2	Z	125	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	N	3	DA	C5-C6-N1	-6.00	114.70	117.70
2	Z	178	ASP	CB-CG-OD2	-5.96	112.94	118.30
2	Z	168	ASP	CB-CG-OD2	-5.95	112.95	118.30
2	Z	209	ARG	NE-CZ-NH2	-5.87	117.36	120.30
2	Z	100	ASP	CB-CG-OD2	-5.77	113.10	118.30
2	Z	311	ASP	CB-CG-OD2	5.76	123.49	118.30
2	Z	500	VAL	CA-CB-CG2	-5.75	102.28	110.90
2	Z	88	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	Z	239	ASP	CB-CG-OD2	-5.69	113.18	118.30
2	Z	113	ASP	CB-CG-OD1	5.66	123.39	118.30
2	Z	178	ASP	CB-CG-OD1	5.65	123.39	118.30
2	Z	555	VAL	CA-CB-CG2	-5.62	102.46	110.90
2	Z	413	ASP	CB-CG-OD2	-5.61	113.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	523	THR	CA-CB-CG2	-5.51	104.68	112.40
2	Z	243	PHE	N-CA-CB	-5.49	100.72	110.60
1	N	11	DC	P-O5'-C5'	5.48	129.67	120.90
2	Z	373	ASP	CB-CG-OD1	5.48	123.23	118.30
2	Z	215	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	N	3	DA	C8-N9-C4	-5.42	103.63	105.80
2	Z	526	ASP	CB-CG-OD2	-5.40	113.44	118.30
2	Z	99	ASP	CB-CG-OD1	5.40	123.16	118.30
2	Z	100	ASP	CB-CG-OD1	5.39	123.15	118.30
2	Z	25	ASN	CB-CA-C	5.37	121.14	110.40
2	Z	534	VAL	CB-CA-C	-5.36	101.21	111.40
1	N	3	DA	N7-C8-N9	5.35	116.47	113.80
1	N	3	DA	N9-C1'-C2'	5.34	122.75	112.60
2	Z	80	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	Z	217	THR	CA-CB-CG2	-5.30	104.98	112.40
2	Z	445	THR	C-N-CA	-5.29	108.47	121.70
2	Z	513	ASP	CB-CG-OD1	5.26	123.03	118.30
1	N	3	DA	C5-N7-C8	-5.23	101.28	103.90
2	Z	241	VAL	CB-CA-C	-5.23	101.47	111.40
2	Z	357	ILE	CA-CB-CG1	-5.20	101.13	111.00
2	Z	511	ASP	CB-CG-OD2	-5.13	113.68	118.30
2	Z	534	VAL	CA-CB-CG1	-5.11	103.23	110.90
2	Z	69	VAL	CA-CB-CG2	-5.05	103.33	110.90
2	Z	255	LEU	CB-CA-C	-5.04	100.62	110.20
2	Z	455	THR	CA-CB-CG2	-5.04	105.35	112.40
1	N	4	DC	N1-C2-O2	5.03	121.92	118.90
2	Z	445	THR	CA-CB-CG2	-5.02	105.37	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	11	0
2	Z	4390	0	4172	275	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	1.07
1:N:3:DA:H61	2:Z:267:PHE:H	1.03	1.02
1:N:3:DA:N6	2:Z:267:PHE:H	1.60	0.99
2:Z:75:GLU:HG3	2:Z:76:SER:N	1.77	0.97
2:Z:554:ASN:H	2:Z:557:ASN:HD21	0.98	0.95
2:Z:366:THR:HA	2:Z:370:GLN:HB2	1.52	0.92
2:Z:557:ASN:HD22	2:Z:558:GLN:H	1.19	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	0.89
2:Z:173:LEU:HD12	2:Z:174:MET:N	1.88	0.89
2:Z:354:LYS:HD2	2:Z:355:THR:N	1.90	0.86
2:Z:204:ILE:HB	2:Z:205:PRO:HD2	1.59	0.84
2:Z:479:LYS:HB3	2:Z:480:PRO:HD2	1.58	0.84
2:Z:360:GLY:HA2	2:Z:374:GLY:HA3	1.59	0.83
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	0.82
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
2:Z:562:VAL:HG13	2:Z:563:PRO:HD2	1.65	0.77
1:N:10:DG:H3'	1:N:11:DC:H5''	1.65	0.77
2:Z:562:VAL:CG1	2:Z:563:PRO:HD2	2.14	0.77
2:Z:232:ILE:HD11	2:Z:234:HIS:CE1	2.21	0.76
2:Z:73:MET:HB2	2:Z:74:PRO:HD2	1.65	0.76
2:Z:422:LEU:HB2	2:Z:423:PRO:HA	1.68	0.75
2:Z:431:LEU:HB3	2:Z:432:PRO:HD2	1.68	0.75
2:Z:77:GLU:HG3	2:Z:518:MET:CE	2.17	0.74
2:Z:173:LEU:HD12	2:Z:174:MET:H	1.49	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:3:DA:H61	2:Z:267:PHE:N	1.83	0.73
2:Z:557:ASN:ND2	2:Z:558:GLN:N	2.32	0.73
2:Z:366:THR:HA	2:Z:370:GLN:CB	2.19	0.72
2:Z:322:THR:HB	2:Z:324:TYR:H	1.55	0.72
2:Z:422:LEU:N	2:Z:422:LEU:HD23	2.05	0.71
2:Z:219:ILE:CG2	2:Z:220:PRO:HD2	2.21	0.71
2:Z:366:THR:O	2:Z:370:GLN:HG2	1.89	0.70
2:Z:271:LYS:HB3	2:Z:272:PRO:HD2	1.72	0.70
2:Z:494:CYS:HB3	2:Z:495:PRO:HD2	1.73	0.69
2:Z:430:LEU:C	2:Z:431:LEU:HD23	2.12	0.69
2:Z:457:LEU:HD23	2:Z:457:LEU:N	2.06	0.69
2:Z:68:LEU:HD12	2:Z:69:VAL:N	2.08	0.69
2:Z:326:THR:O	2:Z:329:THR:N	2.26	0.69
2:Z:422:LEU:H	2:Z:422:LEU:HD23	1.58	0.69
2:Z:111:LEU:HD12	2:Z:112:VAL:N	2.08	0.69
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:250:VAL:HG12	2:Z:251:PRO:N	2.08	0.67
2:Z:340:ALA:HB1	2:Z:341:PRO:HD2	1.75	0.67
2:Z:206:THR:HB	2:Z:207:PRO:HD2	1.77	0.67
2:Z:203:THR:OG1	2:Z:204:ILE:N	2.27	0.67
2:Z:92:VAL:O	2:Z:93:ASN:HB2	1.95	0.67
1:N:3:DA:N6	2:Z:267:PHE:N	2.40	0.66
2:Z:150:LEU:N	2:Z:150:LEU:HD12	2.11	0.66
2:Z:583:LEU:O	2:Z:583:LEU:HD23	1.95	0.66
2:Z:204:ILE:CB	2:Z:205:PRO:HD2	2.22	0.65
2:Z:425:THR:HG22	2:Z:427:ASP:N	2.09	0.65
2:Z:354:LYS:HD2	2:Z:354:LYS:C	2.16	0.65
2:Z:557:ASN:ND2	2:Z:557:ASN:H	1.94	0.65
2:Z:326:THR:H	2:Z:329:THR:HB	1.61	0.65
2:Z:149:VAL:C	2:Z:150:LEU:HD12	2.16	0.65
2:Z:59:VAL:HG12	2:Z:60:GLU:N	2.12	0.65
1:N:10:DG:H2'	1:N:11:DC:O4'	1.96	0.64
2:Z:422:LEU:HA	2:Z:423:PRO:O	1.96	0.64
2:Z:422:LEU:HB2	2:Z:423:PRO:CA	2.26	0.64
2:Z:43:GLY:HA3	2:Z:146:PHE:CD2	2.32	0.64
1:N:3:DA:H5'	1:N:9:DT:H5"	1.79	0.63
2:Z:366:THR:HA	2:Z:370:GLN:CG	2.29	0.63
2:Z:357:ILE:HG22	2:Z:358:ALA:N	2.13	0.62
2:Z:96:MET:HG2	2:Z:220:PRO:HA	1.82	0.62
2:Z:150:LEU:HG	2:Z:525:SER:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:583:LEU:C	2:Z:583:LEU:HD23	2.20	0.61
2:Z:525:SER:OG	2:Z:526:ASP:N	2.31	0.61
2:Z:579:ALA:HB1	2:Z:580:PRO:HD2	1.82	0.61
2:Z:111:LEU:HD12	2:Z:112:VAL:H	1.66	0.61
2:Z:204:ILE:O	2:Z:204:ILE:HG13	2.01	0.61
2:Z:206:THR:HB	2:Z:207:PRO:CD	2.31	0.60
2:Z:396:GLU:HG3	2:Z:397:ARG:N	2.14	0.60
2:Z:365:GLN:O	2:Z:370:GLN:HG3	2.02	0.60
2:Z:66:SER:C	2:Z:67:ARG:HG2	2.21	0.59
2:Z:302:ASN:N	2:Z:302:ASN:OD1	2.35	0.59
2:Z:557:ASN:ND2	2:Z:557:ASN:N	2.47	0.59
2:Z:554:ASN:O	2:Z:557:ASN:ND2	2.35	0.58
2:Z:217:THR:HG22	2:Z:218:LEU:N	2.17	0.58
2:Z:219:ILE:HG23	2:Z:220:PRO:HD2	1.83	0.58
2:Z:336:VAL:O	2:Z:408:ARG:NH2	2.36	0.58
2:Z:410:PRO:HA	2:Z:413:ASP:OD2	2.04	0.57
2:Z:219:ILE:HG22	2:Z:220:PRO:HD2	1.86	0.57
2:Z:204:ILE:CB	2:Z:205:PRO:CD	2.79	0.57
2:Z:122:ASN:HB2	2:Z:123:PRO:CD	2.33	0.57
2:Z:431:LEU:HB3	2:Z:432:PRO:CD	2.35	0.56
2:Z:441:GLY:O	2:Z:442:ILE:HD13	2.05	0.56
2:Z:494:CYS:HB3	2:Z:495:PRO:CD	2.35	0.56
2:Z:193:GLU:HB3	2:Z:206:THR:CG2	2.29	0.56
2:Z:482:LEU:N	2:Z:482:LEU:HD23	2.20	0.56
2:Z:483:HIS:HB3	2:Z:485:ASN:OD1	2.05	0.56
2:Z:349:THR:HG22	2:Z:350:GLN:HG3	1.87	0.56
2:Z:237:ASP:OD1	2:Z:238:PRO:HD2	2.07	0.55
2:Z:139:VAL:HB	2:Z:534:VAL:HG12	1.88	0.55
2:Z:345:PHE:N	2:Z:345:PHE:CD1	2.73	0.55
2:Z:563:PRO:HA	2:Z:568:GLY:O	2.05	0.55
2:Z:294:LEU:HB3	2:Z:295:PRO:HD2	1.88	0.55
2:Z:218:LEU:HD12	2:Z:219:ILE:N	2.22	0.55
2:Z:473:GLU:OE1	2:Z:473:GLU:HA	2.06	0.55
2:Z:250:VAL:CG1	2:Z:251:PRO:N	2.69	0.54
2:Z:360:GLY:HA2	2:Z:374:GLY:CA	2.35	0.54
2:Z:132:THR:C	2:Z:133:MET:HG3	2.26	0.54
2:Z:410:PRO:HD2	2:Z:411:GLU:OE1	2.08	0.54
2:Z:380:PHE:N	2:Z:380:PHE:CD1	2.75	0.54
2:Z:339:SER:O	2:Z:449:ASN:HA	2.08	0.54
2:Z:75:GLU:CG	2:Z:76:SER:N	2.60	0.54
2:Z:73:MET:HB2	2:Z:74:PRO:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:442:ILE:HG22	2:Z:443:ASN:N	2.22	0.54
2:Z:357:ILE:CG2	2:Z:358:ALA:N	2.71	0.54
2:Z:485:ASN:N	2:Z:485:ASN:OD1	2.25	0.54
2:Z:177:LEU:HD22	2:Z:263:THR:HG22	1.87	0.54
2:Z:546:ASN:HB2	2:Z:547:PRO:HD2	1.90	0.54
2:Z:119:VAL:O	2:Z:119:VAL:HG12	2.08	0.54
2:Z:572:VAL:CG1	2:Z:573:TYR:N	2.71	0.54
2:Z:271:LYS:HB3	2:Z:272:PRO:CD	2.38	0.53
2:Z:119:VAL:HB	2:Z:120:TRP:CD1	2.43	0.53
2:Z:502:VAL:HG12	2:Z:503:ALA:N	2.24	0.53
2:Z:407:GLY:O	2:Z:408:ARG:HD3	2.09	0.53
2:Z:47:ASN:HD22	2:Z:47:ASN:C	2.11	0.53
2:Z:422:LEU:N	2:Z:422:LEU:CD2	2.72	0.52
2:Z:463:VAL:HG12	2:Z:463:VAL:O	2.07	0.52
2:Z:578:LEU:CD1	2:Z:578:LEU:N	2.72	0.52
2:Z:555:VAL:HG23	2:Z:556:ASP:N	2.24	0.52
1:N:3:DA:H5'	1:N:9:DT:C5'	2.39	0.52
2:Z:443:ASN:H	2:Z:446:ASN:HD22	1.56	0.52
2:Z:274:ARG:O	2:Z:275:LEU:HD23	2.10	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:N	2.24	0.52
2:Z:422:LEU:CA	2:Z:423:PRO:C	2.78	0.52
2:Z:432:PRO:O	2:Z:443:ASN:ND2	2.37	0.52
2:Z:552:SER:OG	2:Z:553:ILE:N	2.42	0.52
2:Z:572:VAL:HG12	2:Z:573:TYR:O	2.09	0.52
2:Z:565:ASN:O	2:Z:566:ILE:HD13	2.10	0.51
2:Z:139:VAL:HB	2:Z:534:VAL:O	2.11	0.51
1:N:10:DG:H3'	1:N:11:DC:C5'	2.38	0.51
2:Z:523:THR:HG22	2:Z:524:TYR:N	2.26	0.51
2:Z:431:LEU:HD23	2:Z:431:LEU:N	2.22	0.51
2:Z:511:ASP:OD1	2:Z:512:PRO:HD2	2.11	0.51
2:Z:142:GLU:HB3	2:Z:265:THR:HA	1.92	0.51
2:Z:117:TRP:HA	2:Z:469:ILE:HD11	1.93	0.50
2:Z:66:SER:O	2:Z:67:ARG:HG2	2.12	0.50
2:Z:562:VAL:HG12	2:Z:563:PRO:HD2	1.93	0.50
2:Z:281:THR:O	2:Z:283:ARG:N	2.45	0.50
2:Z:436:ILE:HG12	2:Z:443:ASN:HA	1.94	0.49
2:Z:203:THR:CB	2:Z:383:GLN:HE22	2.25	0.49
2:Z:217:THR:CG2	2:Z:218:LEU:N	2.75	0.49
2:Z:564:SER:C	2:Z:566:ILE:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:557:ASN:HD22	2:Z:557:ASN:C	2.02	0.49
2:Z:479:LYS:CB	2:Z:480:PRO:HD2	2.29	0.49
2:Z:326:THR:O	2:Z:328:ALA:N	2.46	0.49
2:Z:203:THR:CB	2:Z:383:GLN:NE2	2.76	0.48
2:Z:218:LEU:HD12	2:Z:218:LEU:C	2.33	0.48
2:Z:55:GLU:O	2:Z:56:ASN:HB2	2.12	0.48
2:Z:68:LEU:HD12	2:Z:69:VAL:H	1.76	0.48
2:Z:203:THR:C	2:Z:204:ILE:HG23	2.33	0.48
2:Z:125:ASP:O	2:Z:126:TRP:C	2.52	0.48
2:Z:444:TYR:O	2:Z:447:ILE:HG12	2.14	0.48
2:Z:360:GLY:CA	2:Z:374:GLY:HA3	2.38	0.48
2:Z:59:VAL:CG1	2:Z:60:GLU:N	2.76	0.48
2:Z:455:THR:HG22	2:Z:456:ALA:N	2.28	0.48
2:Z:561:TYR:C	2:Z:562:VAL:HG23	2.34	0.48
1:N:7:DC:H2'	1:N:8:DT:C6	2.49	0.47
2:Z:122:ASN:CB	2:Z:123:PRO:CD	2.91	0.47
2:Z:562:VAL:CG1	2:Z:563:PRO:CD	2.89	0.47
2:Z:69:VAL:HG12	2:Z:70:HIS:N	2.29	0.47
2:Z:557:ASN:N	2:Z:557:ASN:HD22	2.12	0.47
2:Z:85:ASN:OD1	2:Z:87:MET:HB2	2.14	0.47
2:Z:432:PRO:C	2:Z:443:ASN:HD22	2.17	0.47
2:Z:68:LEU:C	2:Z:68:LEU:HD12	2.34	0.47
2:Z:579:ALA:HB1	2:Z:580:PRO:CD	2.44	0.47
2:Z:473:GLU:HG3	2:Z:474:PHE:N	2.29	0.47
2:Z:528:TRP:CD1	2:Z:528:TRP:N	2.81	0.47
2:Z:153:VAL:HG12	2:Z:154:SER:N	2.27	0.47
2:Z:173:LEU:C	2:Z:173:LEU:HD12	2.31	0.47
2:Z:117:TRP:CE2	2:Z:469:ILE:HG12	2.49	0.47
2:Z:82:VAL:HG12	2:Z:83:VAL:N	2.28	0.47
2:Z:149:VAL:HG12	2:Z:150:LEU:N	2.29	0.47
2:Z:578:LEU:N	2:Z:578:LEU:HD12	2.29	0.47
2:Z:241:VAL:HG12	2:Z:241:VAL:O	2.09	0.46
2:Z:176:ALA:HB1	2:Z:250:VAL:HG11	1.96	0.46
2:Z:346:GLU:HG3	2:Z:355:THR:OG1	2.16	0.46
2:Z:326:THR:C	2:Z:328:ALA:N	2.68	0.46
2:Z:508:ASN:OD1	2:Z:508:ASN:N	2.46	0.46
2:Z:146:PHE:N	2:Z:146:PHE:CD1	2.84	0.46
2:Z:281:THR:O	2:Z:282:ASN:C	2.52	0.46
2:Z:342:TYR:O	2:Z:342:TYR:CG	2.69	0.46
2:Z:557:ASN:O	2:Z:559:PHE:N	2.48	0.45
2:Z:145:ILE:HG22	2:Z:146:PHE:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:549:GLN:O	2:Z:550:GLN:HG2	2.16	0.45
2:Z:465:PRO:HG3	2:Z:571:ILE:CG2	2.45	0.45
2:Z:330:ILE:HG23	2:Z:330:ILE:O	2.15	0.45
2:Z:261:PHE:CG	2:Z:262:ALA:N	2.85	0.45
2:Z:356:PRO:O	2:Z:357:ILE:HD13	2.16	0.45
2:Z:281:THR:C	2:Z:283:ARG:N	2.69	0.45
2:Z:431:LEU:CB	2:Z:432:PRO:CD	2.95	0.45
2:Z:253:HIS:C	2:Z:254:LEU:HD23	2.37	0.45
2:Z:557:ASN:O	2:Z:558:GLN:C	2.55	0.45
2:Z:99:ASP:CG	2:Z:216:ARG:HH21	2.19	0.45
2:Z:148:VAL:HG12	2:Z:149:VAL:N	2.30	0.45
2:Z:340:ALA:HB1	2:Z:341:PRO:CD	2.45	0.45
2:Z:465:PRO:HG3	2:Z:571:ILE:HG22	1.98	0.45
2:Z:564:SER:C	2:Z:566:ILE:N	2.71	0.44
2:Z:237:ASP:OD1	2:Z:239:ASP:OD2	2.35	0.44
2:Z:415:ILE:HG22	2:Z:416:GLN:N	2.32	0.44
2:Z:219:ILE:CG2	2:Z:220:PRO:CD	2.95	0.44
2:Z:443:ASN:OD1	2:Z:443:ASN:N	2.48	0.44
2:Z:443:ASN:H	2:Z:446:ASN:ND2	2.15	0.44
2:Z:105:ILE:HA	2:Z:105:ILE:HD13	1.77	0.44
2:Z:455:THR:CG2	2:Z:456:ALA:N	2.79	0.44
2:Z:354:LYS:HD2	2:Z:355:THR:C	2.38	0.44
2:Z:77:GLU:HG3	2:Z:518:MET:HE2	1.96	0.43
2:Z:357:ILE:HA	2:Z:357:ILE:HD13	1.31	0.43
2:Z:430:LEU:O	2:Z:431:LEU:HD23	2.18	0.43
2:Z:565:ASN:OD1	2:Z:566:ILE:HG12	2.18	0.43
2:Z:325:ILE:O	2:Z:325:ILE:HG22	2.18	0.43
2:Z:204:ILE:HB	2:Z:205:PRO:CD	2.36	0.43
2:Z:322:THR:HB	2:Z:323:ASN:H	1.60	0.43
2:Z:579:ALA:CB	2:Z:580:PRO:CD	2.95	0.43
2:Z:539:LEU:HA	2:Z:539:LEU:HD23	1.72	0.43
2:Z:424:VAL:HG22	2:Z:425:THR:N	2.34	0.43
2:Z:216:ARG:HG3	2:Z:216:ARG:O	2.13	0.43
2:Z:280:GLN:HB3	2:Z:284:ALA:HB3	2.01	0.43
2:Z:554:ASN:OD1	2:Z:554:ASN:C	2.57	0.43
2:Z:566:ILE:HD13	2:Z:566:ILE:HA	1.54	0.43
2:Z:45:PHE:CE2	2:Z:66:SER:HB2	2.53	0.43
2:Z:83:VAL:CG1	2:Z:84:VAL:N	2.80	0.43
2:Z:464:TYR:HA	2:Z:465:PRO:HA	1.80	0.43
2:Z:308:VAL:HG12	2:Z:309:GLN:N	2.33	0.43
2:Z:247:GLU:CD	2:Z:247:GLU:H	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:204:ILE:HA	2:Z:205:PRO:HD3	1.68	0.42
2:Z:122:ASN:OD1	2:Z:122:ASN:C	2.56	0.42
2:Z:564:SER:O	2:Z:566:ILE:N	2.52	0.42
2:Z:375:ASN:HA	2:Z:376:PRO:HD3	1.83	0.42
2:Z:444:TYR:O	2:Z:445:THR:C	2.54	0.42
2:Z:130:VAL:HG12	2:Z:130:VAL:O	2.18	0.42
2:Z:222:HIS:ND1	2:Z:224:GLY:N	2.68	0.42
2:Z:484:VAL:HG22	2:Z:484:VAL:H	1.59	0.42
2:Z:346:GLU:O	2:Z:352:PRO:HA	2.19	0.42
2:Z:473:GLU:CA	2:Z:473:GLU:OE1	2.68	0.42
2:Z:464:TYR:CD1	2:Z:465:PRO:HA	2.54	0.42
2:Z:213:GLN:CD	2:Z:214:TRP:N	2.73	0.42
2:Z:98:LEU:HD23	2:Z:98:LEU:HA	1.71	0.42
2:Z:555:VAL:HG22	2:Z:555:VAL:H	1.35	0.42
2:Z:579:ALA:HA	2:Z:580:PRO:HD3	1.62	0.42
2:Z:139:VAL:HB	2:Z:534:VAL:CG1	2.49	0.42
2:Z:206:THR:HA	2:Z:207:PRO:HD3	1.81	0.42
2:Z:107:THR:HB	2:Z:108:PRO:HD2	2.02	0.42
2:Z:277:HIS:O	2:Z:580:PRO:HA	2.19	0.41
2:Z:123:PRO:O	2:Z:124:GLY:C	2.54	0.41
2:Z:549:GLN:CG	2:Z:550:GLN:N	2.83	0.41
2:Z:177:LEU:HD12	2:Z:497:GLN:O	2.20	0.41
2:Z:309:GLN:O	2:Z:313:ARG:HG3	2.20	0.41
2:Z:372:ALA:HB1	2:Z:373:ASP:H	1.53	0.41
2:Z:246:ILE:HD13	2:Z:246:ILE:HA	1.77	0.41
2:Z:137:HIS:CE1	2:Z:272:PRO:HB3	2.55	0.41
2:Z:115:ASN:OD1	2:Z:469:ILE:N	2.41	0.41
2:Z:521:ILE:HG22	2:Z:522:VAL:N	2.34	0.41
2:Z:434:ASP:HA	2:Z:435:PRO:HD3	1.49	0.41
2:Z:337:GLY:C	2:Z:408:ARG:NH2	2.73	0.41
2:Z:116:ALA:O	2:Z:117:TRP:C	2.58	0.41
2:Z:138:LEU:HD12	2:Z:138:LEU:HA	1.80	0.41
2:Z:216:ARG:NH2	2:Z:218:LEU:HD22	2.36	0.41
2:Z:279:TRP:CE3	2:Z:280:GLN:HA	2.55	0.41
2:Z:75:GLU:HG3	2:Z:76:SER:HB3	2.02	0.41
2:Z:44:THR:CG2	2:Z:45:PHE:N	2.79	0.41
2:Z:337:GLY:HA3	2:Z:408:ARG:HH21	1.86	0.41
2:Z:153:VAL:CG1	2:Z:154:SER:N	2.79	0.41
2:Z:460:VAL:HG23	2:Z:460:VAL:O	2.15	0.41
2:Z:136:LEU:HD12	2:Z:537:ALA:HB2	2.01	0.41
2:Z:128:LEU:O	2:Z:129:ILE:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:418:ILE:HG23	2:Z:419:ASN:N	2.36	0.41
2:Z:48:GLN:H	2:Z:64:ASN:HB2	1.86	0.40
2:Z:430:LEU:HD12	2:Z:430:LEU:HA	1.75	0.40
2:Z:560:ASN:N	2:Z:560:ASN:ND2	2.67	0.40
2:Z:305:ASP:OD1	2:Z:306:ILE:N	2.54	0.40
2:Z:292:ASN:HB2	2:Z:306:ILE:O	2.22	0.40
2:Z:408:ARG:HD3	2:Z:408:ARG:HA	1.52	0.40
2:Z:247:GLU:N	2:Z:247:GLU:OE1	2.40	0.40
2:Z:50:GLU:HB2	2:Z:62:THR:HB	2.03	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%)	17	51

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%)	55 85

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

Some 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

Continued from previous page...

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 carbohydrates 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)

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, 95th 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(Å²)	Q<0.9
1	N	11/11 (100%)	-0.10	0	100	100	24, 36, 69, 73	0
2	Z	559/584 (95%)	-0.29	13 (2%)	64	59	1, 17, 45, 85	13 (2%)
All	All	570/595 (95%)	-0.29	13 (2%)	64	59	1, 17, 46, 85	13 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	30	GLY	8.3
2	Z	32	GLY	8.1
2	Z	23	SER	7.8
2	Z	27	SER	6.7
2	Z	22	GLY	6.6
2	Z	28	GLY	6.5
2	Z	25	ASN	6.3
2	Z	24	GLY	6.2
2	Z	29	GLY	6.1
2	Z	26	GLY	5.9
2	Z	33	GLY	5.5
2	Z	31	GLY	5.2
2	Z	34	GLY	4.3

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)

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, 95th 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^2)	Q<0.9
3	MG	N	13	1/1	0.94	0.13	-1.22	7,7,7,7	0
3	MG	N	12	1/1	0.99	0.14	-1.74	1,1,1,1	0
3	MG	Z	586	1/1	0.99	0.13	-	6,6,6,6	0
3	MG	Z	585	1/1	0.99	0.09	-	1,1,1,1	0

6.5 Other polymers (i)

There are no such residues in this entry.