



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 11:39 AM EDT

PDB ID : 1IJS
Title : CPV (STRAIN D) mutant A300D, complex (VIRAL COAT/DNA), VP2,
PH=7.5, T=4 DEGREES C
Authors : Llamas-Saiz, A.L.; Agbandje-McKenna, M.; Parker, J.S.L.; Wahid, A.T.M.;
Parrish, C.R.; Rossmann, M.G.
Deposited on : 1996-09-12
Resolution : 3.25 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

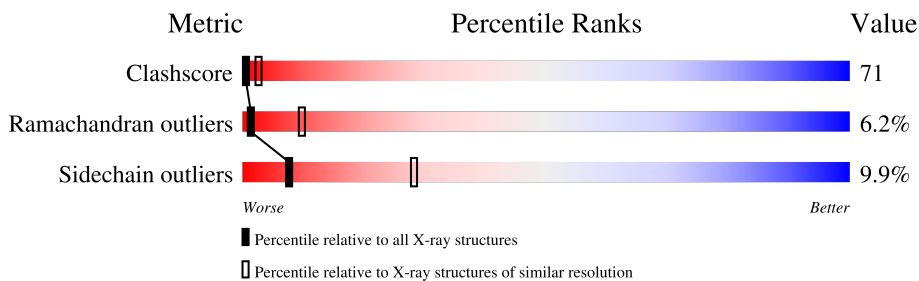
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	N	9	33% (green) 67% (yellow)
2	A	2	100% (yellow)
3	P	584	29% (green) 51% (yellow) 11% (orange) 6% (red) 3% (grey)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4571 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(*CP*CP*AP*CP*CP*CP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	N	9	178	84	33	52	9	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	A	2	40	19	8	11	2	0	0	0

- Molecule 3 is a protein called PROTEIN (PARVOVIRUS COAT PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	P	548	4353	2765	742	830	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	300	ASP	ALA	engineered mutation	UNP P30129
P	386	GLN	LYS	conflict	UNP P30129

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.

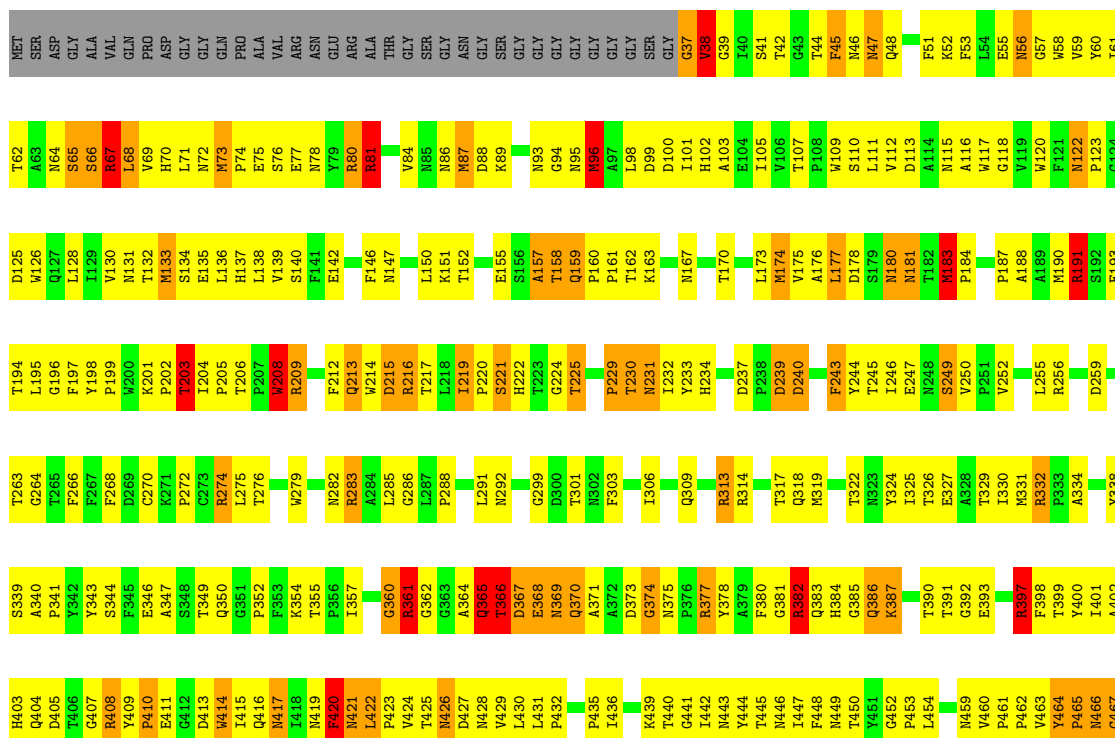
- Molecule 1: DNA (5'-D(*CP*CP*AP*CP*CP*CP*AP*A)-3')



- Molecule 2: DNA (5'-D(*AP*C)-3')



- Molecule 3: PROTEIN (PARVOVIRUS COAT PROTEIN)



Q468	I469	W470	D471	K472	E473	F474	R481	L482	P487	F488	V489	C490	N493	C494	P495	G496	F499	V500	K501	V502	A503	P504	N505	N508	Q509	Y510	N517	M518	S519	R520	I521	V522	T523	Y524	S525	D526	F527	W528	W529	K530	G531	K532	L533	V534	F535	K536	A537	K538	L539	R540	A541	S542	H543
T544	W545	I548	Q549	Q550	M551	S552	I553	N554	N557	Q558	F559	N560	Y561	V562	P563	S564	M565	I566	G567	M569	K570	I571	V572	Y573	E574	K575	S576	Q577	L578	A579	P580	R581	Y584																				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	267.60Å 268.50Å 274.30Å 61.90° 62.60° 60.20°	Depositor
Resolution (Å)	(Not available) – 3.25 15.01 – 3.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.25) 32.5 (15.01-3.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.97 (at 3.25Å)	Xtriage
Refinement program	NONE	Depositor
R, R_{free}	(Not available) , (Not available) 0.529 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for -h+k,-h,-h+l 0.014 for -k,h-k,-k+l 0.028 for h,h-k,h-l 0.035 for -h+k,k,k-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.06	EDS
Total number of atoms	4571	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	1.29	1/198 (0.5%)	1.10	0/299
2	A	1.07	0/44	1.07	0/65
3	P	1.11	10/4483 (0.2%)	1.25	37/6133 (0.6%)
All	All	1.12	11/4725 (0.2%)	1.25	37/6497 (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
3	P	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	81	ARG	CD-NE	12.24	1.67	1.46
3	P	490	CYS	N-CA	-10.05	1.26	1.46
3	P	490	CYS	CA-C	9.46	1.77	1.52
3	P	239	ASP	C-N	-8.09	1.15	1.34
1	N	1	DC	C2'-C1'	-7.39	1.44	1.52
3	P	37	GLY	CA-C	6.17	1.61	1.51
3	P	252	VAL	N-CA	-6.01	1.34	1.46
3	P	203	THR	N-CA	5.79	1.57	1.46
3	P	496	GLY	C-N	-5.78	1.20	1.34
3	P	208	TRP	NE1-CE2	-5.20	1.30	1.37
3	P	47	ASN	C-N	-5.10	1.22	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	81	ARG	CG-CD-NE	12.11	137.24	111.80
3	P	490	CYS	N-CA-CB	11.21	130.77	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	81	ARG	NE-CZ-NH2	8.14	124.37	120.30
3	P	81	ARG	CA-CB-CG	7.98	130.96	113.40
3	P	314	ARG	NE-CZ-NH2	7.73	124.17	120.30
3	P	361	ARG	NE-CZ-NH2	7.66	124.13	120.30
3	P	216	ARG	NE-CZ-NH2	7.58	124.09	120.30
3	P	209	ARG	NE-CZ-NH2	7.57	124.08	120.30
3	P	274	ARG	NE-CZ-NH2	7.49	124.04	120.30
3	P	382	ARG	NE-CZ-NH2	7.47	124.04	120.30
3	P	67	ARG	NE-CZ-NH2	7.45	124.03	120.30
3	P	581	ARG	NE-CZ-NH2	7.44	124.02	120.30
3	P	191	ARG	NE-CZ-NH2	7.44	124.02	120.30
3	P	80	ARG	NE-CZ-NH2	7.41	124.00	120.30
3	P	332	ARG	NE-CZ-NH2	7.37	123.99	120.30
3	P	540	ARG	NE-CZ-NH2	7.37	123.98	120.30
3	P	313	ARG	NE-CZ-NH2	7.36	123.98	120.30
3	P	256	ARG	NE-CZ-NH2	7.36	123.98	120.30
3	P	481	ARG	NE-CZ-NH2	7.35	123.97	120.30
3	P	520	ARG	NE-CZ-NH2	7.33	123.96	120.30
3	P	283	ARG	NE-CZ-NH2	7.31	123.95	120.30
3	P	408	ARG	NE-CZ-NH2	7.28	123.94	120.30
3	P	397	ARG	NE-CZ-NH2	7.16	123.88	120.30
3	P	377	ARG	NE-CZ-NH2	7.14	123.87	120.30
3	P	190	MET	CG-SD-CE	6.25	110.20	100.20
3	P	551	MET	CG-SD-CE	6.19	110.10	100.20
3	P	518	MET	CG-SD-CE	6.17	110.07	100.20
3	P	331	MET	CG-SD-CE	6.17	110.07	100.20
3	P	174	MET	CG-SD-CE	6.16	110.06	100.20
3	P	569	MET	CG-SD-CE	6.14	110.02	100.20
3	P	319	MET	CG-SD-CE	6.14	110.02	100.20
3	P	96	MET	CG-SD-CE	6.13	110.01	100.20
3	P	183	MET	CG-SD-CE	6.13	110.00	100.20
3	P	73	MET	CG-SD-CE	6.10	109.96	100.20
3	P	87	MET	CG-SD-CE	6.10	109.96	100.20
3	P	133	MET	CG-SD-CE	6.08	109.92	100.20
3	P	38	VAL	CB-CA-C	-5.02	101.87	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	81	ARG	Sidechain

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	178	0	99	7	0
2	A	40	0	23	12	0
3	P	4353	0	4142	605	0
All	All	4571	0	4264	624	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 71.

All (624) 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)
3:P:96:MET:CE	3:P:221:SER:H	1.02	1.57
3:P:424:VAL:HG21	3:P:429:VAL:CG2	1.35	1.51
3:P:490:CYS:C	3:P:490:CYS:CA	1.77	1.49
2:A:1:DA:C3'	2:A:2:DC:H5''	1.48	1.44
3:P:276:THR:CG2	3:P:581:ARG:HB2	1.48	1.44
2:A:1:DA:C2'	2:A:2:DC:H5''	1.44	1.44
3:P:424:VAL:CG2	3:P:429:VAL:CG2	2.00	1.40
3:P:70:HIS:CD2	3:P:526:ASP:OD2	1.74	1.38
3:P:150:LEU:CD2	3:P:525:SER:HB3	1.54	1.38
3:P:96:MET:CE	3:P:221:SER:N	1.83	1.37
3:P:159:GLN:HB2	3:P:160:PRO:CD	1.53	1.32
3:P:130:VAL:CG1	3:P:578:LEU:HD21	1.60	1.30
3:P:158:THR:O	3:P:160:PRO:HD2	1.25	1.28
3:P:113:ASP:O	3:P:195:LEU:CD1	1.84	1.26
3:P:150:LEU:HD23	3:P:525:SER:CB	1.63	1.26
3:P:70:HIS:HD2	3:P:526:ASP:OD2	0.95	1.25
3:P:113:ASP:O	3:P:195:LEU:HD12	1.33	1.25
3:P:75:GLU:CG	3:P:76:SER:H	1.43	1.24
3:P:111:LEU:HD23	3:P:112:VAL:N	1.52	1.24
3:P:505:ASN:OD1	3:P:521:ILE:HD12	1.38	1.23
3:P:160:PRO:CB	3:P:161:PRO:O	1.87	1.21
3:P:75:GLU:HG3	3:P:76:SER:N	1.53	1.19
3:P:424:VAL:CG2	3:P:429:VAL:HG23	1.63	1.16
3:P:263:THR:HG22	3:P:264:GLY:H	1.11	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:361:ARG:O	3:P:373:ASP:OD2	1.66	1.14
3:P:96:MET:HE2	3:P:221:SER:N	1.48	1.12
3:P:193:GLU:HB3	3:P:206:THR:HG21	1.21	1.12
3:P:109:TRP:NE1	3:P:247:GLU:OE2	1.82	1.12
3:P:160:PRO:HB2	3:P:161:PRO:O	0.95	1.11
3:P:424:VAL:HG22	3:P:429:VAL:HG23	1.26	1.11
2:A:1:DA:C2'	2:A:2:DC:C5'	2.30	1.09
3:P:365:GLN:OE1	3:P:365:GLN:HA	1.46	1.09
3:P:424:VAL:HG21	3:P:429:VAL:HG21	1.32	1.09
3:P:361:ARG:HG2	3:P:362:GLY:H	1.04	1.08
3:P:75:GLU:HG2	3:P:76:SER:H	1.08	1.08
3:P:134:SER:O	3:P:275:LEU:HB2	1.53	1.08
3:P:194:THR:HG22	3:P:195:LEU:H	1.12	1.07
3:P:361:ARG:CG	3:P:362:GLY:H	1.66	1.07
3:P:174:MET:HE3	3:P:503:ALA:HA	1.33	1.07
3:P:276:THR:CG2	3:P:581:ARG:CB	2.31	1.06
3:P:276:THR:HG21	3:P:581:ARG:CB	1.83	1.06
3:P:367:ASP:OD2	3:P:409:TYR:CE2	2.09	1.05
3:P:517:ASN:O	3:P:518:MET:O	1.74	1.05
2:A:1:DA:H2''	2:A:2:DC:O4'	1.55	1.04
3:P:130:VAL:HG12	3:P:578:LEU:HD21	1.32	1.04
3:P:381:GLY:HA2	3:P:386:GLN:NE2	1.70	1.04
3:P:193:GLU:HB3	3:P:206:THR:CG2	1.87	1.04
3:P:75:GLU:CG	3:P:76:SER:N	2.01	1.04
2:A:1:DA:C3'	2:A:2:DC:C5'	2.35	1.04
3:P:75:GLU:O	3:P:520:ARG:NH2	1.91	1.03
3:P:424:VAL:HG21	3:P:429:VAL:HG22	1.35	1.03
2:A:1:DA:H2''	2:A:2:DC:C4'	1.89	1.03
3:P:157:ALA:HA	3:P:161:PRO:HB3	1.35	1.02
3:P:52:LYS:HB3	3:P:60:TYR:HB3	1.38	1.01
3:P:159:GLN:CB	3:P:160:PRO:HD3	1.88	1.01
3:P:96:MET:HE2	3:P:221:SER:H	0.97	1.01
3:P:465:PRO:HG3	3:P:571:ILE:CG2	1.89	1.01
2:A:1:DA:H2''	2:A:2:DC:C5'	1.90	1.01
2:A:1:DA:H2''	2:A:2:DC:H5''	1.38	1.01
3:P:96:MET:HE3	3:P:221:SER:H	1.23	1.00
3:P:101:ILE:HG21	3:P:216:ARG:HD2	1.44	1.00
3:P:74:PRO:O	3:P:520:ARG:NH2	1.94	1.00
2:A:1:DA:H3'	2:A:2:DC:H5''	1.39	1.00
3:P:213:GLN:OE1	3:P:237:ASP:HB2	1.63	0.99
3:P:431:LEU:HB3	3:P:432:PRO:HD2	1.45	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:96:MET:HE1	3:P:221:SER:H	1.24	0.98
3:P:118:GLY:HA3	3:P:197:PHE:CE2	1.99	0.96
3:P:367:ASP:OD2	3:P:409:TYR:HE2	1.41	0.95
3:P:53:PHE:CD1	3:P:59:VAL:HG22	2.02	0.95
3:P:429:VAL:HG12	3:P:431:LEU:CD1	1.97	0.95
3:P:370:GLN:HE21	3:P:399:THR:HG21	1.30	0.94
3:P:96:MET:HE1	3:P:221:SER:N	1.79	0.94
3:P:158:THR:O	3:P:160:PRO:CD	2.15	0.94
3:P:381:GLY:HA2	3:P:386:GLN:HE21	1.26	0.93
3:P:38:VAL:HG22	3:P:38:VAL:O	1.64	0.93
3:P:465:PRO:HG3	3:P:571:ILE:HG21	1.48	0.93
3:P:365:GLN:OE1	3:P:365:GLN:CA	2.16	0.93
3:P:197:PHE:HE2	3:P:465:PRO:HB2	1.33	0.92
3:P:276:THR:HG21	3:P:581:ARG:HB2	0.93	0.92
3:P:466:ASN:O	3:P:467:GLY:O	1.88	0.92
3:P:443:ASN:HB2	3:P:446:ASN:OD1	1.68	0.92
3:P:99:ASP:OD2	3:P:216:ARG:NH1	2.02	0.91
3:P:159:GLN:HB2	3:P:160:PRO:HD3	0.92	0.91
3:P:193:GLU:CB	3:P:206:THR:HG21	2.01	0.90
3:P:322:THR:CG2	3:P:420:PHE:CD2	2.55	0.90
3:P:219:ILE:HG13	3:P:230:THR:HB	1.54	0.90
3:P:96:MET:HE1	3:P:220:PRO:CB	2.01	0.90
3:P:131:ASN:HD21	3:P:551:MET:HB3	1.37	0.89
3:P:73:MET:CE	3:P:520:ARG:HG3	2.02	0.89
3:P:99:ASP:CG	3:P:216:ARG:NH1	2.26	0.89
3:P:77:GLU:HG2	3:P:520:ARG:NH1	1.88	0.89
3:P:361:ARG:CG	3:P:362:GLY:N	2.30	0.89
3:P:469:ILE:CG2	3:P:470:TRP:HE3	1.86	0.89
3:P:38:VAL:O	3:P:38:VAL:CG2	2.20	0.89
3:P:361:ARG:HG2	3:P:362:GLY:N	1.86	0.88
3:P:73:MET:HE1	3:P:520:ARG:HG3	1.54	0.88
3:P:274:ARG:HD3	3:P:581:ARG:HH12	1.39	0.88
3:P:194:THR:HG22	3:P:195:LEU:N	1.89	0.88
3:P:73:MET:HE3	3:P:520:ARG:NE	1.88	0.88
3:P:416:GLN:HB3	3:P:429:VAL:HG22	1.55	0.88
3:P:130:VAL:CG1	3:P:578:LEU:CD2	2.50	0.87
3:P:279:TRP:HE3	3:P:279:TRP:O	1.58	0.87
3:P:424:VAL:CG2	3:P:429:VAL:HG21	1.89	0.87
3:P:263:THR:CG2	3:P:264:GLY:H	1.88	0.86
3:P:157:ALA:HA	3:P:161:PRO:CB	2.05	0.86
1:N:3:DA:H5'	1:N:9:DA:H5''	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:469:ILE:CG2	3:P:470:TRP:CE3	2.59	0.86
3:P:505:ASN:OD1	3:P:521:ILE:CD1	2.23	0.85
3:P:111:LEU:CD2	3:P:112:VAL:N	2.37	0.85
3:P:415:ILE:HD11	3:P:444:TYR:CE2	2.12	0.85
3:P:118:GLY:HA3	3:P:197:PHE:CD2	2.12	0.84
3:P:194:THR:CG2	3:P:195:LEU:H	1.83	0.84
3:P:378:TYR:O	3:P:397:ARG:CB	2.26	0.84
3:P:409:TYR:CE1	3:P:411:GLU:HB2	2.12	0.84
3:P:429:VAL:HG12	3:P:431:LEU:HD11	1.59	0.84
3:P:111:LEU:HD23	3:P:112:VAL:CA	2.09	0.83
3:P:159:GLN:CB	3:P:160:PRO:CD	2.42	0.83
3:P:160:PRO:HB2	3:P:161:PRO:C	1.98	0.83
3:P:565:ASN:ND2	3:P:566:ILE:HG13	1.93	0.83
1:N:2:DC:H4'	1:N:3:DA:OP1	1.79	0.83
3:P:137:HIS:HB2	3:P:536:LYS:O	1.78	0.83
3:P:578:LEU:HD23	3:P:578:LEU:H	1.41	0.83
3:P:197:PHE:CE2	3:P:465:PRO:HB2	2.13	0.82
1:N:2:DC:H2'	1:N:2:DC:O2	1.79	0.82
3:P:343:TYR:CE2	3:P:371:ALA:HB1	2.13	0.82
2:A:1:DA:H3'	2:A:2:DC:C5'	2.06	0.81
3:P:322:THR:HG21	3:P:420:PHE:CE2	2.16	0.81
3:P:263:THR:HG22	3:P:264:GLY:N	1.93	0.81
3:P:150:LEU:CD2	3:P:525:SER:CB	2.38	0.80
3:P:415:ILE:CD1	3:P:444:TYR:CE2	2.64	0.80
3:P:193:GLU:CD	3:P:209:ARG:HH22	1.85	0.80
3:P:340:ALA:HB3	3:P:357:ILE:HD11	1.61	0.80
3:P:158:THR:O	3:P:158:THR:CG2	2.30	0.80
3:P:215:ASP:HB3	3:P:234:HIS:HB2	1.62	0.80
3:P:99:ASP:OD1	3:P:216:ARG:NH1	2.14	0.80
3:P:130:VAL:HG13	3:P:578:LEU:HD21	1.59	0.80
3:P:364:ALA:O	3:P:366:THR:N	2.14	0.80
3:P:464:TYR:HA	3:P:465:PRO:O	1.82	0.80
3:P:313:ARG:O	3:P:325:ILE:HD12	1.81	0.80
3:P:86:ASN:ND2	3:P:100:ASP:HB2	1.97	0.80
3:P:465:PRO:HG3	3:P:571:ILE:HG22	1.62	0.80
3:P:415:ILE:HD11	3:P:444:TYR:CD2	2.17	0.80
3:P:122:ASN:HB2	3:P:123:PRO:HD2	1.61	0.79
3:P:51:PHE:CZ	3:P:128:LEU:HD23	2.18	0.79
3:P:193:GLU:OE1	3:P:209:ARG:NH2	2.16	0.79
3:P:494:CYS:HB3	3:P:495:PRO:HD2	1.62	0.79
3:P:276:THR:HG22	3:P:581:ARG:CB	2.12	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:93:ASN:HD22	3:P:221:SER:HB2	1.47	0.79
3:P:380:PHE:CD1	3:P:466:ASN:OD1	2.36	0.79
3:P:93:ASN:HD21	3:P:229:PRO:HG3	1.46	0.78
3:P:77:GLU:CG	3:P:520:ARG:NH1	2.46	0.78
3:P:378:TYR:O	3:P:397:ARG:HB3	1.83	0.78
3:P:134:SER:O	3:P:275:LEU:CB	2.31	0.78
3:P:274:ARG:NE	3:P:581:ARG:NH1	2.31	0.78
3:P:469:ILE:HG21	3:P:470:TRP:CE3	2.18	0.78
3:P:52:LYS:HB3	3:P:60:TYR:CB	2.14	0.78
3:P:174:MET:HE3	3:P:504:PRO:CD	2.14	0.78
3:P:99:ASP:CG	3:P:216:ARG:HH12	1.85	0.77
3:P:432:PRO:O	3:P:443:ASN:ND2	2.16	0.77
3:P:471:ASP:O	3:P:472:LYS:O	2.01	0.77
3:P:469:ILE:HG22	3:P:470:TRP:HE3	1.50	0.77
3:P:137:HIS:CE1	3:P:272:PRO:HB3	2.19	0.77
3:P:93:ASN:ND2	3:P:229:PRO:HG3	2.00	0.77
3:P:322:THR:HG21	3:P:420:PHE:CD2	2.20	0.77
3:P:61:ILE:HD11	3:P:133:MET:HE3	1.67	0.76
3:P:373:ASP:OD2	3:P:407:GLY:HA3	1.85	0.76
3:P:413:ASP:O	3:P:414:TRP:HB3	1.86	0.76
3:P:279:TRP:O	3:P:279:TRP:CE3	2.39	0.76
3:P:415:ILE:CD1	3:P:444:TYR:CD2	2.69	0.76
3:P:46:ASN:HB3	3:P:530:LYS:HE3	1.66	0.75
3:P:217:THR:OG1	3:P:234:HIS:HE1	1.68	0.75
3:P:361:ARG:CD	3:P:405:ASP:OD1	2.34	0.75
3:P:564:SER:O	3:P:567:GLY:N	2.17	0.75
3:P:152:THR:HG23	3:P:521:ILE:HG22	1.68	0.75
3:P:96:MET:CE	3:P:220:PRO:CA	2.65	0.75
3:P:174:MET:CE	3:P:504:PRO:HD2	2.15	0.75
3:P:343:TYR:HE2	3:P:371:ALA:CB	1.99	0.75
3:P:448:PHE:CE2	3:P:450:THR:CG2	2.70	0.75
3:P:68:LEU:HB2	3:P:528:TRP:CE3	2.22	0.75
3:P:66:SER:HA	3:P:530:LYS:HA	1.68	0.74
3:P:96:MET:HE1	3:P:220:PRO:CA	2.17	0.74
3:P:146:PHE:HD2	3:P:147:ASN:HD22	1.32	0.74
3:P:150:LEU:HD23	3:P:525:SER:HB3	0.78	0.74
3:P:431:LEU:HB3	3:P:432:PRO:CD	2.16	0.74
3:P:69:VAL:HG13	3:P:205:PRO:HD3	1.68	0.74
3:P:139:VAL:HG12	3:P:140:SER:N	2.02	0.74
3:P:276:THR:O	3:P:577:GLN:NE2	2.21	0.74
3:P:131:ASN:OD1	3:P:550:GLN:HB3	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:429:VAL:HG12	3:P:431:LEU:HD12	1.69	0.74
3:P:430:LEU:HD21	3:P:436:ILE:HD11	1.70	0.74
3:P:283:ARG:HE	3:P:327:GLU:HB3	1.53	0.74
3:P:84:VAL:HG21	3:P:102:HIS:CE1	2.22	0.74
3:P:113:ASP:O	3:P:195:LEU:HD13	1.86	0.74
3:P:533:LEU:CD2	3:P:535:PHE:CZ	2.71	0.74
3:P:138:LEU:HD13	3:P:535:PHE:CE1	2.23	0.74
3:P:111:LEU:HD23	3:P:112:VAL:H	1.52	0.73
3:P:93:ASN:ND2	3:P:221:SER:HB2	2.03	0.73
3:P:429:VAL:CG1	3:P:431:LEU:HD11	2.18	0.73
3:P:444:TYR:O	3:P:448:PHE:HB2	1.89	0.73
3:P:578:LEU:HD23	3:P:578:LEU:N	2.04	0.73
3:P:68:LEU:HD23	3:P:202:PRO:HB3	1.70	0.73
3:P:424:VAL:HG22	3:P:429:VAL:CG2	1.95	0.72
3:P:533:LEU:HD21	3:P:535:PHE:HZ	1.53	0.72
3:P:47:ASN:ND2	3:P:65:SER:HA	2.05	0.72
3:P:424:VAL:HG11	3:P:429:VAL:HG21	1.71	0.72
3:P:490:CYS:C	3:P:490:CYS:CB	2.58	0.72
3:P:533:LEU:HD21	3:P:535:PHE:CZ	2.25	0.72
3:P:217:THR:O	3:P:231:ASN:HA	1.89	0.72
3:P:368:GLU:O	3:P:369:ASN:HB2	1.88	0.71
3:P:424:VAL:CG1	3:P:429:VAL:HG21	2.19	0.71
3:P:464:TYR:CD1	3:P:464:TYR:C	2.64	0.71
3:P:361:ARG:HG2	3:P:405:ASP:OD1	1.91	0.71
3:P:365:GLN:HG2	3:P:401:ILE:HD13	1.72	0.71
3:P:53:PHE:CD1	3:P:59:VAL:CG2	2.74	0.71
3:P:61:ILE:HD11	3:P:133:MET:CE	2.20	0.70
3:P:274:ARG:CD	3:P:581:ARG:HH12	2.03	0.70
3:P:361:ARG:O	3:P:407:GLY:HA3	1.91	0.70
3:P:152:THR:HG23	3:P:521:ILE:CG2	2.21	0.70
3:P:77:GLU:HG2	3:P:520:ARG:HH12	1.53	0.70
3:P:93:ASN:O	3:P:222:HIS:O	2.10	0.69
3:P:422:LEU:HA	3:P:423:PRO:C	2.12	0.69
3:P:465:PRO:CG	3:P:571:ILE:HG22	2.23	0.69
3:P:158:THR:O	3:P:158:THR:HG22	1.92	0.69
3:P:274:ARG:NE	3:P:581:ARG:HH11	1.90	0.69
3:P:448:PHE:CE2	3:P:450:THR:HG23	2.28	0.69
3:P:430:LEU:HD11	3:P:436:ILE:HD11	1.75	0.69
3:P:53:PHE:HD1	3:P:59:VAL:HG22	1.58	0.69
3:P:64:ASN:HA	3:P:531:GLY:O	1.93	0.69
3:P:482:LEU:N	3:P:482:LEU:HD23	2.08	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:576:SER:O	3:P:578:LEU:CD2	2.41	0.69
3:P:378:TYR:CE2	3:P:463:VAL:HG11	2.27	0.68
3:P:111:LEU:HD23	3:P:112:VAL:C	2.12	0.68
3:P:109:TRP:CE3	3:P:501:LYS:HB2	2.29	0.68
3:P:157:ALA:CA	3:P:161:PRO:HB3	2.18	0.68
3:P:501:LYS:HG2	3:P:502:VAL:N	2.09	0.68
3:P:70:HIS:HD2	3:P:526:ASP:CG	1.93	0.67
3:P:414:TRP:HE1	3:P:416:GLN:NE2	1.92	0.67
3:P:403:HIS:HD2	3:P:578:LEU:HA	1.58	0.67
3:P:340:ALA:HB1	3:P:341:PRO:HD2	1.75	0.67
3:P:95:ASN:HB3	3:P:98:LEU:HD12	1.77	0.67
3:P:431:LEU:HD12	3:P:431:LEU:N	2.11	0.66
3:P:65:SER:OG	3:P:67:ARG:NH2	2.23	0.66
3:P:390:THR:HG22	3:P:391:THR:N	2.10	0.66
3:P:93:ASN:HD21	3:P:229:PRO:HD3	1.61	0.66
3:P:93:ASN:HD21	3:P:229:PRO:CG	2.09	0.66
3:P:174:MET:CE	3:P:504:PRO:CD	2.73	0.66
3:P:216:ARG:HG2	3:P:232:ILE:O	1.96	0.66
3:P:422:LEU:HB2	3:P:423:PRO:HA	1.78	0.66
3:P:55:GLU:O	3:P:56:ASN:HB2	1.96	0.65
3:P:126:TRP:O	3:P:130:VAL:HG23	1.96	0.65
3:P:361:ARG:CG	3:P:405:ASP:OD1	2.44	0.65
1:N:3:DA:H5'	1:N:9:DA:C5'	2.26	0.65
3:P:274:ARG:CZ	3:P:581:ARG:NH1	2.59	0.65
1:N:2:DC:O2	1:N:2:DC:C2'	2.43	0.65
3:P:96:MET:HE2	3:P:220:PRO:C	2.17	0.65
3:P:115:ASN:OD1	3:P:469:ILE:HB	1.97	0.65
3:P:370:GLN:NE2	3:P:399:THR:HG21	2.10	0.65
3:P:155:GLU:OE2	3:P:163:LYS:HE2	1.97	0.64
3:P:322:THR:CG2	3:P:420:PHE:HD2	2.07	0.64
3:P:96:MET:CE	3:P:220:PRO:C	2.62	0.64
3:P:51:PHE:CE1	3:P:128:LEU:HD23	2.33	0.64
3:P:469:ILE:HG22	3:P:470:TRP:CE3	2.27	0.64
3:P:564:SER:O	3:P:566:ILE:N	2.30	0.64
3:P:417:ASN:HB2	3:P:428:ASN:HD22	1.63	0.64
3:P:109:TRP:CZ3	3:P:501:LYS:HB3	2.32	0.63
3:P:343:TYR:CE2	3:P:371:ALA:CB	2.77	0.63
3:P:158:THR:C	3:P:159:GLN:HG2	2.18	0.63
3:P:452:GLY:C	3:P:454:LEU:H	2.00	0.63
3:P:274:ARG:CZ	3:P:581:ARG:HH11	2.11	0.63
3:P:66:SER:HB3	3:P:530:LYS:HG3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:469:ILE:HG21	3:P:470:TRP:HE3	1.56	0.63
3:P:183:MET:HG2	3:P:208:TRP:HH2	1.63	0.63
3:P:203:THR:OG1	3:P:204:ILE:N	2.32	0.63
3:P:370:GLN:HA	3:P:375:ASN:OD1	1.98	0.63
3:P:414:TRP:HE1	3:P:416:GLN:HE21	1.47	0.63
3:P:245:THR:O	3:P:249:SER:OG	2.16	0.62
3:P:174:MET:HE3	3:P:503:ALA:CA	2.20	0.62
3:P:107:THR:OG1	3:P:208:TRP:HB3	1.99	0.62
3:P:313:ARG:O	3:P:325:ILE:CD1	2.45	0.62
3:P:270:CYS:HB3	3:P:490:CYS:HA	1.82	0.62
3:P:508:ASN:ND2	3:P:509:GLN:HG3	2.15	0.62
3:P:174:MET:HE3	3:P:504:PRO:HD3	1.81	0.62
3:P:341:PRO:HB2	3:P:344:SER:HB2	1.82	0.62
3:P:533:LEU:HG	3:P:535:PHE:CE2	2.34	0.62
3:P:75:GLU:HG3	3:P:76:SER:HB2	1.82	0.62
3:P:116:ALA:O	3:P:120:TRP:HD1	1.83	0.62
3:P:183:MET:CG	3:P:184:PRO:HD2	2.30	0.62
3:P:326:THR:H	3:P:329:THR:HB	1.64	0.62
3:P:158:THR:C	3:P:160:PRO:HD2	2.16	0.62
3:P:500:VAL:HG11	3:P:527:PHE:CZ	2.35	0.62
3:P:390:THR:HG22	3:P:391:THR:H	1.65	0.61
3:P:443:ASN:HB3	3:P:445:THR:H	1.65	0.61
3:P:37:GLY:O	3:P:39:GLY:N	2.26	0.61
3:P:232:ILE:HG22	3:P:233:TYR:N	2.16	0.61
3:P:426:ASN:C	3:P:428:ASN:H	2.04	0.61
3:P:70:HIS:CG	3:P:526:ASP:OD2	2.50	0.60
3:P:88:ASP:OD1	3:P:89:LYS:HG2	2.00	0.60
3:P:138:LEU:CD1	3:P:535:PHE:CE1	2.83	0.60
3:P:216:ARG:CG	3:P:232:ILE:O	2.50	0.60
3:P:459:ASN:HA	3:P:482:LEU:HD12	1.83	0.60
3:P:385:GLY:O	3:P:386:GLN:O	2.19	0.60
3:P:482:LEU:HD23	3:P:482:LEU:H	1.66	0.60
3:P:533:LEU:CD2	3:P:535:PHE:HZ	2.11	0.60
3:P:219:ILE:HG13	3:P:230:THR:CB	2.28	0.60
3:P:317:THR:HG23	3:P:329:THR:HG22	1.84	0.60
3:P:93:ASN:HD21	3:P:229:PRO:CD	2.15	0.60
3:P:292:ASN:HB2	3:P:306:ILE:O	2.02	0.60
3:P:96:MET:CE	3:P:220:PRO:HA	2.31	0.59
3:P:197:PHE:HE2	3:P:465:PRO:CB	2.12	0.59
3:P:276:THR:HG22	3:P:581:ARG:HB3	1.83	0.59
3:P:578:LEU:O	3:P:578:LEU:HG	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:96:MET:HE1	3:P:220:PRO:HB2	1.81	0.59
3:P:174:MET:HE3	3:P:504:PRO:HD2	1.77	0.59
3:P:361:ARG:HG3	3:P:362:GLY:N	2.14	0.59
3:P:368:GLU:HB2	3:P:370:GLN:H	1.68	0.59
3:P:80:ARG:O	3:P:105:ILE:HG23	2.02	0.59
3:P:56:ASN:O	3:P:58:TRP:CD1	2.56	0.59
3:P:152:THR:CG2	3:P:521:ILE:CG2	2.80	0.59
3:P:322:THR:HG22	3:P:420:PHE:HD2	1.68	0.59
2:A:1:DA:C2'	2:A:2:DC:O4'	2.42	0.58
3:P:160:PRO:HG2	3:P:162:THR:OG1	2.04	0.58
3:P:557:ASN:O	3:P:560:ASN:HB2	2.02	0.58
3:P:364:ALA:O	3:P:367:ASP:N	2.36	0.58
3:P:465:PRO:CG	3:P:571:ILE:CG2	2.73	0.58
3:P:111:LEU:O	3:P:205:PRO:CB	2.52	0.58
3:P:448:PHE:CE2	3:P:450:THR:HG21	2.37	0.58
3:P:343:TYR:HE2	3:P:371:ALA:HB1	1.56	0.58
3:P:160:PRO:CB	3:P:161:PRO:C	2.65	0.58
3:P:198:TYR:OH	3:P:570:LYS:HA	2.03	0.58
3:P:562:VAL:HG13	3:P:563:PRO:HD2	1.85	0.58
3:P:274:ARG:CD	3:P:581:ARG:NH1	2.66	0.58
3:P:471:ASP:C	3:P:472:LYS:O	2.42	0.58
3:P:551:MET:HE3	3:P:574:GLU:OE1	2.04	0.58
3:P:75:GLU:HG3	3:P:76:SER:CB	2.33	0.57
3:P:77:GLU:CG	3:P:520:ARG:HH11	2.17	0.57
3:P:324:TYR:O	3:P:329:THR:HG21	2.05	0.57
3:P:339:SER:HB2	3:P:450:THR:OG1	2.04	0.57
3:P:409:TYR:C	3:P:411:GLU:H	2.08	0.57
3:P:73:MET:CE	3:P:520:ARG:CG	2.80	0.57
3:P:285:LEU:HD22	3:P:584:TYR:HB3	1.86	0.57
3:P:447:ILE:O	3:P:447:ILE:HG22	2.05	0.57
3:P:93:ASN:ND2	3:P:221:SER:CB	2.66	0.57
3:P:415:ILE:HD12	3:P:444:TYR:CD2	2.38	0.57
3:P:490:CYS:C	3:P:490:CYS:N	2.48	0.57
3:P:84:VAL:O	3:P:101:ILE:HG13	2.03	0.57
3:P:111:LEU:O	3:P:205:PRO:HB3	2.04	0.57
3:P:188:ALA:HB1	3:P:193:GLU:O	2.05	0.57
3:P:115:ASN:ND2	3:P:470:TRP:O	2.30	0.57
3:P:122:ASN:ND2	3:P:125:ASP:CG	2.59	0.57
3:P:354:LYS:HD2	3:P:355:THR:N	2.19	0.57
3:P:140:SER:H	3:P:534:VAL:HB	1.70	0.57
3:P:279:TRP:CE3	3:P:279:TRP:C	2.78	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:47:ASN:HD22	3:P:66:SER:H	1.53	0.56
3:P:136:LEU:HD12	3:P:537:ALA:HB2	1.86	0.56
3:P:142:GLU:HB2	3:P:264:GLY:O	2.03	0.56
3:P:122:ASN:HB2	3:P:123:PRO:CD	2.34	0.56
3:P:142:GLU:CB	3:P:264:GLY:O	2.53	0.56
3:P:77:GLU:OE2	3:P:520:ARG:NH1	2.39	0.56
3:P:180:ASN:O	3:P:181:ASN:C	2.44	0.56
3:P:219:ILE:CG1	3:P:230:THR:HB	2.29	0.56
3:P:109:TRP:CE3	3:P:501:LYS:CB	2.89	0.56
3:P:117:TRP:CZ2	3:P:462:PRO:HB3	2.41	0.56
3:P:68:LEU:HB2	3:P:528:TRP:CZ3	2.41	0.56
3:P:93:ASN:O	3:P:221:SER:O	2.23	0.56
3:P:110:SER:HB2	3:P:500:VAL:O	2.05	0.56
3:P:548:ILE:HG23	3:P:580:PRO:CD	2.36	0.55
3:P:132:THR:O	3:P:540:ARG:HG2	2.06	0.55
3:P:361:ARG:HD3	3:P:405:ASP:OD1	2.05	0.55
3:P:365:GLN:HG2	3:P:401:ILE:CD1	2.35	0.55
3:P:426:ASN:O	3:P:428:ASN:N	2.39	0.55
3:P:122:ASN:HD21	3:P:125:ASP:CG	2.10	0.55
3:P:73:MET:HE3	3:P:520:ARG:CD	2.37	0.55
3:P:75:GLU:C	3:P:520:ARG:HH22	2.09	0.55
3:P:73:MET:HE3	3:P:520:ARG:HE	1.71	0.55
3:P:75:GLU:HG3	3:P:76:SER:CA	2.32	0.55
3:P:461:PRO:HB3	3:P:577:GLN:OE1	2.07	0.55
3:P:578:LEU:CD2	3:P:578:LEU:N	2.69	0.55
3:P:419:ASN:O	3:P:421:ASN:N	2.37	0.55
3:P:548:ILE:HG23	3:P:580:PRO:HD2	1.88	0.55
3:P:326:THR:HG22	3:P:327:GLU:N	2.22	0.55
3:P:409:TYR:O	3:P:411:GLU:N	2.40	0.55
3:P:422:LEU:CA	3:P:423:PRO:C	2.75	0.55
3:P:111:LEU:CD2	3:P:112:VAL:C	2.75	0.55
3:P:373:ASP:OD2	3:P:407:GLY:CA	2.54	0.54
3:P:538:LYS:HG3	3:P:539:LEU:N	2.23	0.54
3:P:130:VAL:HG13	3:P:578:LEU:CD2	2.27	0.54
3:P:381:GLY:CA	3:P:386:GLN:NE2	2.59	0.54
3:P:194:THR:HB	3:P:384:HIS:CE1	2.42	0.54
3:P:255:LEU:HD13	3:P:259:ASP:HB3	1.88	0.54
3:P:472:LYS:HG2	3:P:473:GLU:H	1.72	0.54
3:P:377:ARG:CZ	3:P:397:ARG:HG3	2.38	0.54
3:P:501:LYS:CG	3:P:502:VAL:N	2.71	0.54
3:P:47:ASN:HA	3:P:64:ASN:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:482:LEU:N	3:P:482:LEU:CD2	2.71	0.54
3:P:57:GLY:O	3:P:539:LEU:HG	2.08	0.54
3:P:339:SER:O	3:P:449:ASN:HA	2.07	0.54
3:P:177:LEU:O	3:P:250:VAL:HG13	2.08	0.53
3:P:517:ASN:C	3:P:518:MET:O	2.47	0.53
3:P:70:HIS:CD2	3:P:526:ASP:CG	2.74	0.53
1:N:4:DC:H3'	1:N:5:DC:H5'	1.89	0.53
3:P:557:ASN:HB3	3:P:561:TYR:HE2	1.74	0.53
3:P:420:PHE:O	3:P:421:ASN:C	2.47	0.53
3:P:110:SER:O	3:P:500:VAL:O	2.27	0.53
3:P:422:LEU:HA	3:P:424:VAL:N	2.23	0.52
3:P:459:ASN:HD22	3:P:482:LEU:HB2	1.74	0.52
3:P:136:LEU:HD11	3:P:535:PHE:HB3	1.89	0.52
3:P:494:CYS:HB3	3:P:495:PRO:CD	2.35	0.52
3:P:193:GLU:HB3	3:P:206:THR:HG22	1.86	0.52
3:P:247:GLU:CD	3:P:247:GLU:H	2.13	0.52
3:P:432:PRO:HA	3:P:443:ASN:ND2	2.24	0.52
3:P:232:ILE:CG2	3:P:233:TYR:N	2.73	0.52
3:P:243:PHE:CD1	3:P:243:PHE:C	2.82	0.52
3:P:343:TYR:HE2	3:P:371:ALA:HB2	1.73	0.52
3:P:576:SER:O	3:P:578:LEU:HD22	2.08	0.52
3:P:468:GLN:OE1	3:P:471:ASP:HB2	2.10	0.52
3:P:103:ALA:HB3	3:P:212:PHE:O	2.10	0.52
3:P:197:PHE:CE2	3:P:465:PRO:CB	2.89	0.52
3:P:443:ASN:CB	3:P:445:THR:OG1	2.58	0.51
3:P:136:LEU:HA	3:P:537:ALA:HB2	1.91	0.51
3:P:158:THR:H	3:P:161:PRO:HB3	1.76	0.51
3:P:57:GLY:HA2	3:P:539:LEU:HD12	1.93	0.51
3:P:426:ASN:C	3:P:428:ASN:N	2.64	0.51
3:P:452:GLY:C	3:P:454:LEU:N	2.64	0.51
3:P:86:ASN:CG	3:P:86:ASN:O	2.49	0.51
3:P:183:MET:HG2	3:P:184:PRO:HD2	1.92	0.51
3:P:390:THR:CG2	3:P:391:THR:H	2.23	0.51
3:P:111:LEU:CD2	3:P:112:VAL:H	2.14	0.50
3:P:413:ASP:O	3:P:414:TRP:CB	2.59	0.50
3:P:541:ALA:HB3	3:P:543:HIS:CE1	2.47	0.50
3:P:554:ASN:HB2	3:P:557:ASN:HD22	1.76	0.50
3:P:45:PHE:HE1	3:P:47:ASN:HB2	1.76	0.50
3:P:101:ILE:O	3:P:101:ILE:HG23	2.10	0.50
3:P:390:THR:CG2	3:P:391:THR:N	2.74	0.50
3:P:137:HIS:CB	3:P:536:LYS:O	2.57	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:113:ASP:OD2	3:P:188:ALA:N	2.43	0.50
3:P:139:VAL:CG1	3:P:140:SER:N	2.69	0.50
3:P:338:TYR:CE1	3:P:357:ILE:HD13	2.47	0.50
3:P:410:PRO:HA	3:P:413:ASP:OD1	2.11	0.50
3:P:417:ASN:CB	3:P:428:ASN:HD22	2.25	0.49
3:P:216:ARG:HG2	3:P:217:THR:H	1.77	0.49
3:P:73:MET:HB2	3:P:523:THR:O	2.12	0.49
3:P:158:THR:O	3:P:158:THR:HG23	2.10	0.49
3:P:382:ARG:HG2	3:P:382:ARG:HH11	1.77	0.49
3:P:116:ALA:O	3:P:120:TRP:CD1	2.64	0.49
3:P:414:TRP:NE1	3:P:416:GLN:NE2	2.53	0.49
3:P:96:MET:HE2	3:P:220:PRO:HA	1.95	0.49
3:P:96:MET:HE1	3:P:220:PRO:C	2.27	0.49
3:P:125:ASP:O	3:P:128:LEU:HB3	2.12	0.49
3:P:75:GLU:HG2	3:P:76:SER:N	1.92	0.48
3:P:96:MET:CE	3:P:220:PRO:CB	2.84	0.48
3:P:77:GLU:CD	3:P:520:ARG:NH1	2.67	0.48
3:P:403:HIS:NE2	3:P:549:GLN:NE2	2.61	0.48
3:P:463:VAL:O	3:P:465:PRO:O	2.31	0.48
3:P:109:TRP:CG	3:P:246:ILE:HD12	2.48	0.48
3:P:282:ASN:O	3:P:332:ARG:NE	2.46	0.48
3:P:435:PRO:HB3	3:P:439:LYS:O	2.12	0.48
3:P:65:SER:O	3:P:529:TRP:CZ3	2.67	0.48
3:P:137:HIS:ND1	3:P:272:PRO:HB3	2.28	0.48
3:P:198:TYR:CE1	3:P:571:ILE:HG13	2.48	0.48
3:P:219:ILE:HG22	3:P:220:PRO:HD2	1.95	0.48
3:P:576:SER:OG	3:P:577:GLN:N	2.46	0.48
3:P:67:ARG:N	3:P:529:TRP:O	2.46	0.48
3:P:510:TYR:HE1	3:P:518:MET:HG2	1.79	0.48
3:P:313:ARG:C	3:P:325:ILE:HD12	2.33	0.48
3:P:442:ILE:HG22	3:P:443:ASN:N	2.29	0.48
3:P:472:LYS:HG2	3:P:473:GLU:N	2.29	0.48
3:P:96:MET:HE2	3:P:220:PRO:CA	2.40	0.47
3:P:111:LEU:CG	3:P:112:VAL:N	2.77	0.47
3:P:431:LEU:CD1	3:P:431:LEU:N	2.75	0.47
3:P:432:PRO:HA	3:P:443:ASN:HD22	1.79	0.47
3:P:565:ASN:HD21	3:P:566:ILE:HG13	1.76	0.47
3:P:53:PHE:CE1	3:P:59:VAL:CG2	2.98	0.47
3:P:184:PRO:HD3	3:P:244:TYR:CE2	2.49	0.47
3:P:53:PHE:CE1	3:P:59:VAL:HG21	2.50	0.47
3:P:360:GLY:HA3	3:P:404:GLN:HG3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:408:ARG:O	3:P:410:PRO:HD3	2.15	0.47
3:P:430:LEU:HD21	3:P:436:ILE:CD1	2.42	0.47
3:P:391:THR:HG22	3:P:392:GLY:N	2.30	0.47
3:P:469:ILE:HG22	3:P:470:TRP:N	2.29	0.47
3:P:221:SER:CB	3:P:229:PRO:HG3	2.45	0.46
3:P:381:GLY:HA2	3:P:386:GLN:HE22	1.72	0.46
3:P:140:SER:HA	3:P:266:PHE:O	2.15	0.46
3:P:158:THR:N	3:P:161:PRO:HB3	2.31	0.46
3:P:103:ALA:CB	3:P:214:TRP:HB3	2.44	0.46
3:P:291:LEU:CD2	3:P:306:ILE:HG12	2.46	0.46
3:P:255:LEU:CD1	3:P:259:ASP:HB3	2.45	0.46
3:P:283:ARG:HD2	3:P:327:GLU:O	2.14	0.46
3:P:95:ASN:CB	3:P:98:LEU:HD12	2.45	0.46
3:P:283:ARG:NE	3:P:327:GLU:HB3	2.26	0.46
3:P:400:TYR:OH	3:P:575:LYS:HA	2.15	0.46
3:P:299:GLY:C	3:P:301:THR:H	2.19	0.46
3:P:422:LEU:HB2	3:P:423:PRO:CA	2.45	0.46
3:P:378:TYR:O	3:P:397:ARG:HB2	2.14	0.46
3:P:380:PHE:CE1	3:P:398:PHE:CE1	3.04	0.46
3:P:557:ASN:O	3:P:560:ASN:N	2.48	0.46
3:P:151:LYS:HE2	3:P:167:ASN:OD1	2.16	0.46
3:P:286:GLY:O	3:P:288:PRO:HD3	2.16	0.46
3:P:576:SER:O	3:P:578:LEU:HD23	2.16	0.46
3:P:37:GLY:C	3:P:39:GLY:H	2.16	0.46
3:P:365:GLN:OE1	3:P:365:GLN:C	2.55	0.46
3:P:111:LEU:HD23	3:P:111:LEU:C	2.27	0.45
3:P:540:ARG:HG3	3:P:540:ARG:O	2.16	0.45
3:P:572:VAL:HG12	3:P:573:TYR:O	2.16	0.45
3:P:62:THR:HG21	3:P:532:LYS:HE3	1.98	0.45
3:P:73:MET:HE3	3:P:520:ARG:CG	2.45	0.45
3:P:473:GLU:OE2	3:P:489:VAL:HG11	2.16	0.45
3:P:466:ASN:O	3:P:467:GLY:C	2.53	0.45
3:P:551:MET:CE	3:P:574:GLU:OE1	2.64	0.45
3:P:67:ARG:NH1	3:P:196:GLY:O	2.50	0.45
3:P:103:ALA:HB3	3:P:214:TRP:HB3	1.98	0.45
3:P:443:ASN:HB3	3:P:445:THR:OG1	2.17	0.45
3:P:216:ARG:HG2	3:P:217:THR:N	2.32	0.45
3:P:383:GLN:O	3:P:383:GLN:HG2	2.16	0.45
3:P:459:ASN:CG	3:P:460:VAL:N	2.70	0.45
3:P:109:TRP:CD1	3:P:246:ILE:HD12	2.51	0.45
3:P:174:MET:CE	3:P:504:PRO:HD3	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:224:GLY:O	3:P:225:THR:C	2.55	0.45
3:P:387:LYS:HA	3:P:570:LYS:HB3	1.98	0.45
3:P:150:LEU:HD21	3:P:525:SER:CB	2.38	0.45
3:P:45:PHE:CD1	3:P:46:ASN:N	2.86	0.44
3:P:191:ARG:O	3:P:193:GLU:HG3	2.17	0.44
3:P:199:PRO:C	3:P:201:LYS:H	2.20	0.44
3:P:471:ASP:O	3:P:472:LYS:C	2.55	0.44
3:P:533:LEU:CD2	3:P:535:PHE:CE2	2.99	0.44
3:P:93:ASN:ND2	3:P:229:PRO:CG	2.74	0.44
3:P:135:GLU:O	3:P:537:ALA:HB1	2.17	0.44
3:P:138:LEU:HD11	3:P:533:LEU:HD11	1.98	0.44
3:P:160:PRO:CG	3:P:161:PRO:C	2.86	0.44
3:P:391:THR:CG2	3:P:392:GLY:N	2.81	0.44
3:P:505:ASN:O	3:P:520:ARG:HB2	2.18	0.44
3:P:160:PRO:HG2	3:P:161:PRO:C	2.37	0.44
3:P:552:SER:OG	3:P:553:ILE:N	2.51	0.44
3:P:117:TRP:HZ2	3:P:487:PRO:HG2	1.81	0.44
3:P:221:SER:HB3	3:P:229:PRO:HG3	1.99	0.44
3:P:325:ILE:HG23	3:P:330:ILE:HG12	1.99	0.44
3:P:158:THR:O	3:P:159:GLN:CB	2.65	0.44
3:P:317:THR:HG22	3:P:318:GLN:N	2.33	0.44
3:P:382:ARG:H	3:P:386:GLN:HB3	1.82	0.44
3:P:474:PHE:CD1	3:P:474:PHE:N	2.85	0.44
3:P:422:LEU:HB2	3:P:424:VAL:N	2.32	0.43
3:P:140:SER:HB2	3:P:534:VAL:CG2	2.47	0.43
3:P:175:VAL:HG23	3:P:255:LEU:HD23	2.00	0.43
3:P:448:PHE:CZ	3:P:450:THR:CG2	3.01	0.43
3:P:470:TRP:HA	3:P:488:PHE:O	2.19	0.43
3:P:80:ARG:O	3:P:105:ILE:HA	2.19	0.43
3:P:422:LEU:HB2	3:P:424:VAL:H	1.82	0.43
3:P:217:THR:OG1	3:P:234:HIS:CE1	2.59	0.43
3:P:545:TRP:CD1	3:P:545:TRP:C	2.91	0.43
3:P:572:VAL:HG12	3:P:573:TYR:N	2.34	0.43
3:P:130:VAL:HG11	3:P:578:LEU:HD21	1.79	0.43
3:P:134:SER:OG	3:P:135:GLU:N	2.51	0.43
3:P:383:GLN:HB3	3:P:384:HIS:CD2	2.53	0.43
3:P:71:LEU:HD21	3:P:502:VAL:HG23	2.01	0.43
3:P:181:ASN:HD22	3:P:493:ASN:HD21	1.67	0.43
3:P:183:MET:HG2	3:P:208:TRP:CH2	2.50	0.43
3:P:68:LEU:HB2	3:P:528:TRP:CD2	2.54	0.43
3:P:346:GLU:O	3:P:352:PRO:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:122:ASN:ND2	3:P:125:ASP:H	2.16	0.42
3:P:130:VAL:HG13	3:P:576:SER:O	2.19	0.42
3:P:334:ALA:HB1	3:P:454:LEU:O	2.19	0.42
3:P:564:SER:C	3:P:566:ILE:N	2.71	0.42
3:P:71:LEU:HD12	3:P:72:ASN:N	2.35	0.42
3:P:110:SER:O	3:P:500:VAL:N	2.50	0.42
3:P:111:LEU:CG	3:P:112:VAL:H	2.32	0.42
3:P:138:LEU:HD13	3:P:535:PHE:HE1	1.78	0.42
3:P:158:THR:HG23	3:P:159:GLN:HG2	2.01	0.42
3:P:403:HIS:CD2	3:P:577:GLN:O	2.72	0.42
3:P:93:ASN:O	3:P:222:HIS:C	2.57	0.42
3:P:139:VAL:O	3:P:268:PHE:HB2	2.20	0.42
3:P:196:GLY:HA2	3:P:383:GLN:HG2	2.00	0.42
3:P:263:THR:CG2	3:P:264:GLY:N	2.60	0.42
3:P:45:PHE:CD1	3:P:45:PHE:C	2.92	0.42
3:P:45:PHE:HD1	3:P:46:ASN:N	2.17	0.42
3:P:219:ILE:CD1	3:P:230:THR:HB	2.50	0.42
3:P:425:THR:O	3:P:428:ASN:HB2	2.19	0.42
2:A:1:DA:H2'	2:A:2:DC:H5''	1.74	0.42
3:P:86:ASN:O	3:P:86:ASN:OD1	2.37	0.42
3:P:177:LEU:O	3:P:250:VAL:CG1	2.67	0.42
3:P:361:ARG:NE	3:P:405:ASP:OD1	2.52	0.42
3:P:368:GLU:HB2	3:P:369:ASN:H	1.11	0.42
3:P:378:TYR:O	3:P:397:ARG:CA	2.67	0.42
3:P:415:ILE:HG13	3:P:444:TYR:CE2	2.55	0.42
3:P:557:ASN:O	3:P:558:GLN:C	2.57	0.42
3:P:84:VAL:O	3:P:101:ILE:HA	2.19	0.42
3:P:93:ASN:C	3:P:221:SER:O	2.58	0.42
3:P:178:ASP:OD2	3:P:181:ASN:HA	2.20	0.42
3:P:462:PRO:O	3:P:576:SER:HB3	2.20	0.42
1:N:9:DA:H2'	1:N:9:DA:N3	2.35	0.41
3:P:340:ALA:HB1	3:P:341:PRO:CD	2.48	0.41
3:P:373:ASP:O	3:P:374:GLY:C	2.57	0.41
3:P:162:THR:HG22	3:P:163:LYS:N	2.35	0.41
3:P:347:ALA:HB2	3:P:352:PRO:HA	2.01	0.41
3:P:366:THR:O	3:P:366:THR:CG2	2.68	0.41
3:P:139:VAL:O	3:P:268:PHE:HD2	2.03	0.41
3:P:548:ILE:HG23	3:P:580:PRO:HD3	2.03	0.41
3:P:44:THR:HG22	3:P:45:PHE:N	2.35	0.41
3:P:131:ASN:ND2	3:P:551:MET:HB3	2.19	0.41
3:P:440:THR:O	3:P:442:ILE:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:101:ILE:O	3:P:101:ILE:CG2	2.68	0.41
3:P:213:GLN:HG3	3:P:240:ASP:HB2	2.02	0.41
3:P:465:PRO:HB2	3:P:466:ASN:H	1.64	0.41
3:P:197:PHE:HB3	3:P:571:ILE:HD12	2.02	0.41
3:P:47:ASN:HD22	3:P:66:SER:N	2.17	0.41
3:P:59:VAL:CG1	3:P:60:TYR:N	2.84	0.41
3:P:59:VAL:HG12	3:P:60:TYR:N	2.35	0.41
3:P:93:ASN:ND2	3:P:229:PRO:HD3	2.34	0.41
3:P:160:PRO:CG	3:P:161:PRO:O	2.62	0.41
3:P:309:GLN:O	3:P:313:ARG:HG3	2.21	0.41
3:P:68:LEU:CD2	3:P:202:PRO:HB3	2.47	0.41
3:P:68:LEU:HD13	3:P:528:TRP:CE2	2.56	0.41
3:P:408:ARG:C	3:P:410:PRO:HD3	2.41	0.41
3:P:452:GLY:O	3:P:454:LEU:N	2.54	0.41
3:P:409:TYR:C	3:P:411:GLU:N	2.73	0.40
3:P:62:THR:CG2	3:P:532:LYS:HE3	2.51	0.40
3:P:301:THR:O	3:P:303:PHE:CE2	2.75	0.40
3:P:326:THR:O	3:P:330:ILE:HG13	2.20	0.40
3:P:237:ASP:C	3:P:239:ASP:H	2.23	0.40
3:P:176:ALA:HB3	3:P:499:PHE:HB2	2.03	0.40
3:P:214:TRP:NE1	3:P:350:GLN:O	2.53	0.40
3:P:380:PHE:HE1	3:P:398:PHE:CE1	2.39	0.40
3:P:187:PRO:HB2	3:P:468:GLN:NE2	2.36	0.40
3:P:430:LEU:CD2	3:P:436:ILE:HD11	2.46	0.40
3:P:464:TYR:CD1	3:P:465:PRO:N	2.89	0.40
3:P:562:VAL:CG1	3:P:563:PRO:HD2	2.49	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
3	P	546/584 (94%)	442 (81%)	70 (13%)	34 (6%)	1 10

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	38	VAL
3	P	159	GLN
3	P	369	ASN
3	P	370	GLN
3	P	386	GLN
3	P	402	ALA
3	P	465	PRO
3	P	466	ASN
3	P	467	GLY
3	P	472	LYS
3	P	518	MET
3	P	558	GLN
3	P	565	ASN
3	P	56	ASN
3	P	157	ALA
3	P	229	PRO
3	P	360	GLY
3	P	365	GLN
3	P	366	THR
3	P	374	GLY
3	P	427	ASP
3	P	522	VAL
3	P	181	ASN
3	P	221	SER
3	P	421	ASN
3	P	441	GLY
3	P	230	THR
3	P	225	THR
3	P	414	TRP
3	P	420	PHE
3	P	426	ASN
3	P	410	PRO
3	P	453	PRO
3	P	94	GLY

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
3	P	477/496 (96%)	430 (90%)	47 (10%)	8 28

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

Mol	Chain	Res	Type
3	P	41	SER
3	P	42	THR
3	P	45	PHE
3	P	48	GLN
3	P	65	SER
3	P	66	SER
3	P	67	ARG
3	P	68	LEU
3	P	78	ASN
3	P	81	ARG
3	P	87	MET
3	P	96	MET
3	P	122	ASN
3	P	158	THR
3	P	170	THR
3	P	173	LEU
3	P	177	LEU
3	P	180	ASN
3	P	183	MET
3	P	191	ARG
3	P	203	THR
3	P	208	TRP
3	P	213	GLN
3	P	215	ASP
3	P	219	ILE
3	P	231	ASN
3	P	240	ASP
3	P	243	PHE
3	P	249	SER
3	P	349	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	361	ARG
3	P	365	GLN
3	P	366	THR
3	P	367	ASP
3	P	368	GLU
3	P	382	ARG
3	P	387	LYS
3	P	393	GLU
3	P	397	ARG
3	P	417	ASN
3	P	420	PHE
3	P	422	LEU
3	P	464	TYR
3	P	482	LEU
3	P	490	CYS
3	P	518	MET
3	P	578	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
3	P	47	ASN
3	P	48	GLN
3	P	64	ASN
3	P	70	HIS
3	P	85	ASN
3	P	93	ASN
3	P	122	ASN
3	P	137	HIS
3	P	147	ASN
3	P	180	ASN
3	P	181	ASN
3	P	234	HIS
3	P	282	ASN
3	P	292	ASN
3	P	370	GLN
3	P	384	HIS
3	P	386	GLN
3	P	403	HIS
3	P	428	ASN
3	P	443	ASN
3	P	508	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	543	HIS
3	P	549	GLN
3	P	554	ASN
3	P	557	ASN
3	P	565	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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	239:ASP	C	240:ASP	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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