



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:14 AM UTC

PDB ID : 1ALK / pdb_00001alk
Title : REACTION MECHANISM OF ALKALINE PHOSPHATASE BASED ON
CRYSTAL STRUCTURES. TWO METAL ION CATALYSIS
Authors : Kim, E.E.; Wyckoff, W.
Deposited on : 1993-03-03
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

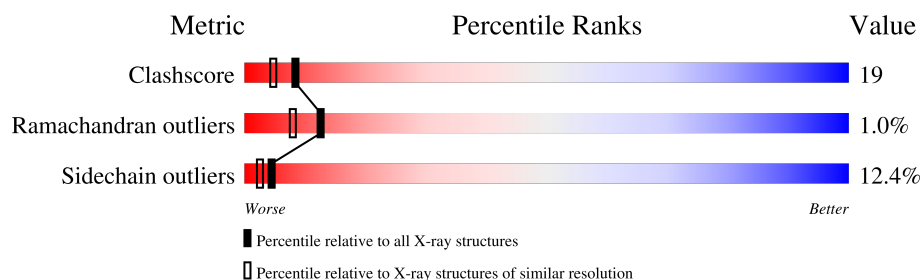
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	65% 26% 7% .
1	B	449	59% 31% 8% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6630 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALKALINE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3304	2042	582	668	12			
1	B	449	Total	C	N	O	S	0	0	0
			3304	2042	582	668	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASN	ASP	conflict	UNP P00634
A	35	ASN	ASP	conflict	UNP P00634
A	176	GLN	GLU	conflict	UNP P00634
A	228	GLU	GLN	conflict	UNP P00634
A	230	GLU	GLN	conflict	UNP P00634
B	15	ASN	ASP	conflict	UNP P00634
B	35	ASN	ASP	conflict	UNP P00634
B	176	GLN	GLU	conflict	UNP P00634
B	228	GLU	GLN	conflict	UNP P00634
B	230	GLU	GLN	conflict	UNP P00634

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

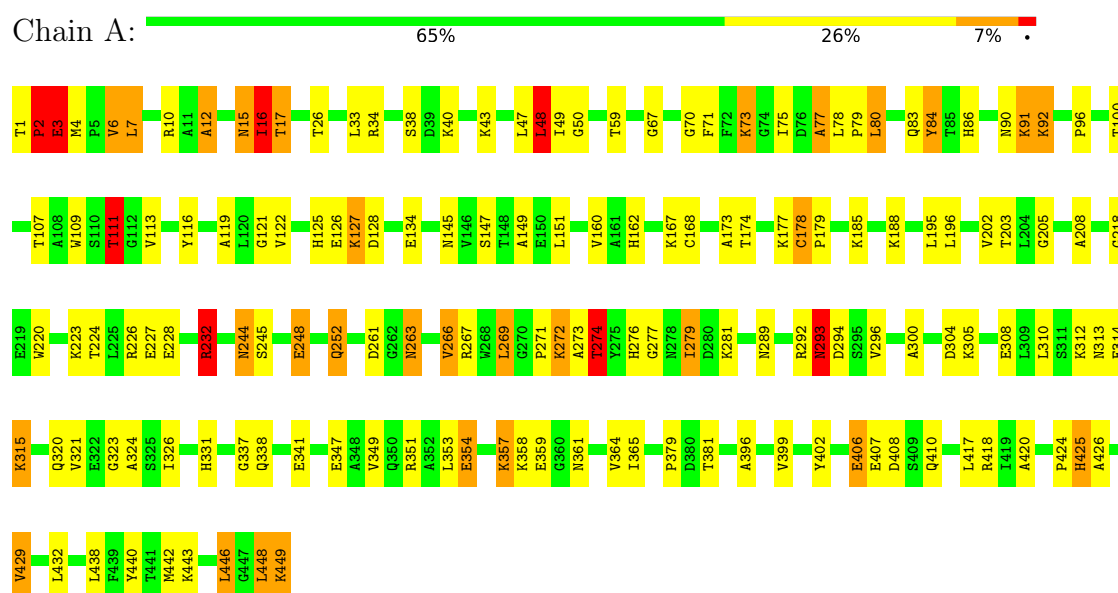
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	3	Total	O	0	0
			3	3		

3 Residue-property plots

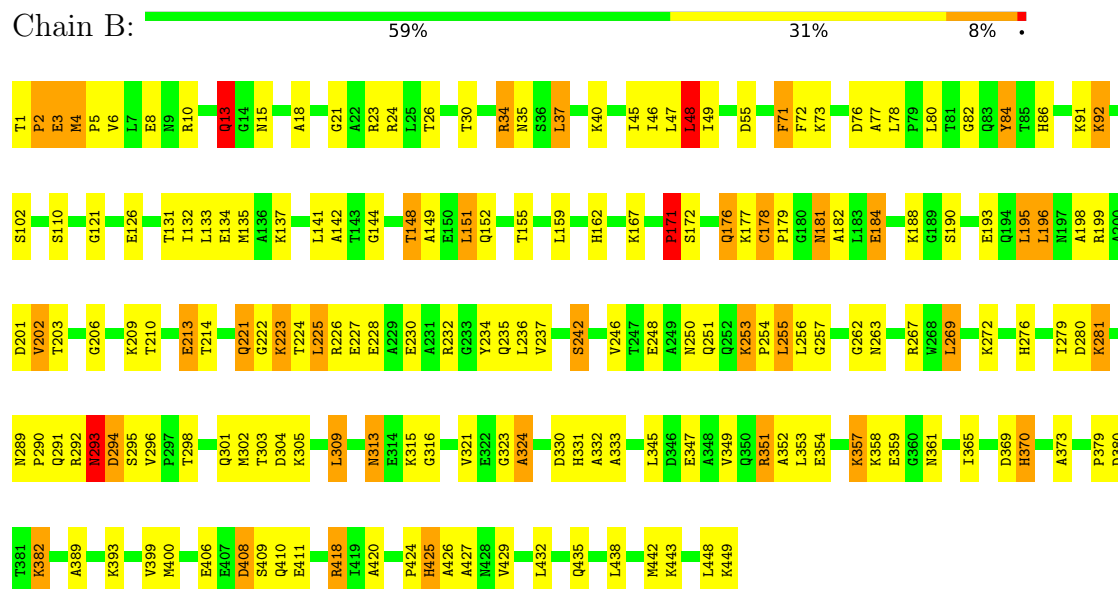
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

• Molecule 1: ALKALINE PHOSPHATASE



• Molecule 1: ALKALINE PHOSPHATASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	195.30Å 167.40Å 76.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6630	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.33	6/3359 (0.2%)	1.84	65/4560 (1.4%)
1	B	1.24	4/3359 (0.1%)	1.75	45/4560 (1.0%)
All	All	1.29	10/6718 (0.1%)	1.79	110/9120 (1.2%)

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	GLN	CD-OE1	8.05	1.38	1.23
1	B	82	GLY	N-CA	6.64	1.52	1.44
1	A	49	ILE	CA-CB	6.06	1.61	1.54
1	A	48	LEU	CB-CG	-5.53	1.42	1.53
1	B	49	ILE	CA-CB	5.37	1.61	1.54
1	B	303	THR	CA-CB	5.29	1.61	1.53
1	B	389	ALA	N-CA	5.25	1.52	1.46
1	A	17	THR	CA-CB	5.22	1.62	1.53
1	A	100	THR	CA-CB	5.13	1.61	1.53
1	A	12	ALA	N-CA	5.01	1.52	1.46

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	ARG	CD-NE-CZ	21.73	154.82	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ARG	CD-NE-CZ	16.38	147.33	124.40
1	B	418	ARG	NE-CZ-NH2	9.45	127.71	119.20
1	A	71	PHE	CA-CB-CG	9.07	122.87	113.80
1	A	354	GLU	CA-CB-CG	9.02	132.15	114.10
1	B	418	ARG	NH1-CZ-NH2	-8.90	107.73	119.30
1	A	429	VAL	N-CA-CB	-8.34	103.04	112.21
1	A	232	ARG	NE-CZ-NH1	-8.21	113.29	121.50
1	A	354	GLU	N-CA-CB	8.00	121.67	110.07
1	A	48	LEU	CA-CB-CG	7.95	144.12	116.30
1	B	3	GLU	CA-C-N	7.89	141.06	121.80
1	B	3	GLU	C-N-CA	7.89	141.06	121.80
1	B	292	ARG	CA-C-N	7.87	136.57	121.54
1	B	292	ARG	C-N-CA	7.87	136.57	121.54
1	B	71	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	111	THR	OG1-CB-CG2	7.42	124.14	109.30
1	A	6	VAL	CA-C-O	-7.32	115.90	121.68
1	A	84	TYR	CA-CB-CG	7.24	126.93	113.90
1	A	279	ILE	CB-CA-C	7.22	117.99	110.91
1	B	294	ASP	N-CA-C	-7.21	104.51	113.38
1	A	324	ALA	N-CA-C	7.11	119.11	111.36
1	B	72	PHE	CA-CB-CG	6.93	120.73	113.80
1	B	324	ALA	N-CA-C	6.91	118.89	111.36
1	A	178	CYS	O-C-N	6.86	127.08	121.05
1	A	293	ASN	N-CA-C	6.83	125.34	110.80
1	A	90	ASN	CA-CB-CG	-6.75	105.85	112.60
1	A	418	ARG	NE-CZ-NH2	6.70	125.23	119.20
1	A	86	HIS	CA-CB-CG	-6.70	107.10	113.80
1	A	75	ILE	N-CA-C	6.69	116.84	110.42
1	B	293	ASN	N-CA-C	6.64	124.94	110.80
1	A	160	VAL	N-CA-CB	-6.56	104.52	112.33
1	B	26	THR	CA-CB-OG1	-6.33	100.10	109.60
1	B	18	ALA	O-C-N	6.28	126.85	121.20
1	A	364	VAL	CA-C-O	-6.23	113.91	120.39
1	B	370	HIS	CA-CB-CG	-6.20	107.60	113.80
1	B	316	GLY	CA-C-O	-6.14	117.89	122.37
1	A	232	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	A	273	ALA	N-CA-C	-6.09	102.45	110.43
1	A	126	GLU	CB-CG-CD	6.03	122.85	112.60
1	A	111	THR	CA-CB-CG2	5.95	120.61	110.50
1	A	274	THR	N-CA-CB	-5.91	101.78	111.66
1	A	326	ILE	N-CA-C	-5.89	104.77	110.42
1	B	178	CYS	O-C-N	5.87	126.56	121.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	PRO	CA-C-N	5.84	131.79	123.14
1	A	96	PRO	C-N-CA	5.84	131.79	123.14
1	B	373	ALA	N-CA-C	5.84	118.87	111.69
1	A	125	HIS	CA-CB-CG	-5.81	107.99	113.80
1	B	48	LEU	CA-CB-CG	5.78	136.54	116.30
1	B	181	ASN	CA-CB-CG	5.73	118.33	112.60
1	B	425	HIS	CA-CB-CG	-5.73	108.07	113.80
1	A	244	ASN	CB-CA-C	5.71	122.71	110.21
1	A	263	ASN	O-C-N	5.68	129.56	122.86
1	B	330	ASP	CA-CB-CG	5.67	118.28	112.60
1	B	86	HIS	CA-CB-CG	-5.67	108.13	113.80
1	B	34	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	A	425	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	16	ILE	CA-CB-CG2	5.62	120.05	110.50
1	B	202	VAL	CA-C-N	5.57	130.63	122.77
1	B	202	VAL	C-N-CA	5.57	130.63	122.77
1	A	407	GLU	CA-C-N	5.57	132.18	121.54
1	A	407	GLU	C-N-CA	5.57	132.18	121.54
1	A	218	GLY	CA-C-N	5.56	128.50	120.38
1	A	218	GLY	C-N-CA	5.56	128.50	120.38
1	B	323	GLY	N-CA-C	-5.55	100.02	113.18
1	A	6	VAL	N-CA-C	-5.53	101.82	109.46
1	B	330	ASP	N-CA-C	-5.52	105.18	111.14
1	A	34	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	B	352	ALA	CA-C-N	5.46	127.60	120.28
1	B	352	ALA	C-N-CA	5.46	127.60	120.28
1	B	365	ILE	CA-C-O	-5.42	114.69	120.39
1	A	109	TRP	CA-C-N	-5.42	112.88	122.26
1	A	109	TRP	C-N-CA	-5.42	112.88	122.26
1	A	47	LEU	CA-C-N	-5.41	115.53	123.00
1	A	47	LEU	C-N-CA	-5.41	115.53	123.00
1	A	338	GLN	CA-C-O	5.40	126.49	120.82
1	B	13	GLN	CB-CG-CD	5.39	121.76	112.60
1	A	77	ALA	N-CA-C	5.36	119.44	113.01
1	B	408	ASP	N-CA-C	5.36	116.81	110.97
1	A	2	PRO	CA-C-N	5.36	131.77	121.54
1	A	2	PRO	C-N-CA	5.36	131.77	121.54
1	B	55	ASP	CA-CB-CG	-5.36	107.24	112.60
1	A	50	GLY	N-CA-C	-5.34	100.52	113.18
1	A	266	VAL	CA-CB-CG1	5.33	119.46	110.40
1	A	59	THR	O-C-N	5.30	127.53	122.07
1	A	70	GLY	O-C-N	5.30	127.36	122.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	TYR	CA-CB-CG	5.29	123.42	113.90
1	A	271	PRO	CA-C-N	5.28	129.23	120.94
1	A	271	PRO	C-N-CA	5.28	129.23	120.94
1	B	148	THR	N-CA-C	-5.26	106.55	113.17
1	A	79	PRO	N-CA-C	5.25	121.48	114.18
1	A	67	GLY	N-CA-C	-5.22	106.10	112.68
1	A	418	ARG	CG-CD-NE	5.21	123.45	112.00
1	A	354	GLU	CB-CG-CD	5.19	121.42	112.60
1	B	432	LEU	O-C-N	5.17	129.11	123.27
1	A	323	GLY	N-CA-C	-5.16	100.96	113.18
1	B	302	MET	CA-C-N	5.16	127.19	120.28
1	B	302	MET	C-N-CA	5.16	127.19	120.28
1	B	309	LEU	CB-CA-C	5.14	118.96	110.88
1	A	261	ASP	O-C-N	5.13	127.63	122.09
1	A	3	GLU	N-CA-CB	5.12	119.14	110.49
1	B	13	GLN	N-CA-C	5.12	116.86	111.28
1	B	316	GLY	N-CA-C	-5.11	106.92	112.08
1	B	78	LEU	O-C-N	5.10	125.64	121.31
1	B	435	GLN	CB-CG-CD	-5.10	103.93	112.60
1	A	396	ALA	CA-C-N	-5.08	115.64	122.91
1	A	396	ALA	C-N-CA	-5.08	115.64	122.91
1	A	202	VAL	O-C-N	5.05	128.23	123.03
1	A	26	THR	CA-CB-OG1	-5.02	102.07	109.60
1	A	10	ARG	CD-NE-CZ	-5.01	117.39	124.40
1	B	80	LEU	CB-CA-C	5.00	118.29	110.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3304	0	3250	127	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3304	0	3250	135	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
All	All	6630	0	6500	251	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 19.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:THR:CG2	1:A:113:VAL:HG12	1.69	1.23
1:A:1:THR:N	1:A:2:PRO:HD3	1.67	1.09
1:A:111:THR:HG23	1:A:113:VAL:HG12	1.35	1.08
1:A:232:ARG:HB3	1:A:232:ARG:HH11	1.26	0.99
1:B:223:LYS:HG3	1:B:227:GLU:OE1	1.63	0.98
1:B:176:GLN:OE1	1:B:177:LYS:HE2	1.60	0.97
1:A:6:VAL:CG1	1:A:357:LYS:HD3	1.95	0.96
1:A:224:THR:OG1	1:A:227:GLU:HG3	1.66	0.94
1:A:289:ASN:O	1:A:292:ARG:HG2	1.68	0.94
1:A:274:THR:HG21	1:A:281:LYS:HE3	1.49	0.94
1:A:1:THR:H3	1:A:2:PRO:HD3	1.26	0.92
1:A:232:ARG:HH11	1:A:232:ARG:CB	1.82	0.92
1:A:1:THR:N	1:A:2:PRO:CD	2.32	0.90
1:A:2:PRO:O	1:A:3:GLU:HG2	1.71	0.90
1:B:279:ILE:HD11	1:B:382:LYS:HE2	1.53	0.89
1:A:12:ALA:HB1	1:A:16:ILE:HD11	1.53	0.88
1:A:220:TRP:HB3	1:A:223:LYS:HE2	1.56	0.86
1:A:292:ARG:O	1:A:293:ASN:HB2	1.77	0.84
1:A:6:VAL:HG11	1:A:357:LYS:HD3	1.59	0.83
1:A:449:LYS:HE3	1:A:449:LYS:N	1.94	0.82
1:B:6:VAL:HG12	1:B:77:ALA:HB1	1.62	0.81
1:B:228:GLU:O	1:B:232:ARG:HG3	1.80	0.80
1:A:38:SER:OG	1:A:40:LYS:HG2	1.80	0.80
1:A:92:LYS:HA	1:A:92:LYS:HE3	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:HG2	1:B:253:LYS:HZ1	1.46	0.79
1:A:6:VAL:HG13	1:A:357:LYS:HD3	1.63	0.79
1:A:12:ALA:CB	1:A:16:ILE:HD11	2.12	0.79
1:B:137:LYS:NZ	1:B:199:ARG:HB3	1.99	0.77
1:B:236:LEU:HD21	1:B:256:LEU:HD23	1.67	0.76
1:A:2:PRO:O	1:A:3:GLU:OE2	2.04	0.76
1:A:111:THR:CG2	1:A:113:VAL:CG1	2.59	0.76
1:B:279:ILE:HD11	1:B:382:LYS:CE	2.15	0.76
1:B:253:LYS:H	1:B:254:PRO:CD	1.99	0.76
1:B:408:ASP:OD1	1:B:409:SER:N	2.18	0.76
1:A:1:THR:H2	1:A:2:PRO:HD3	1.49	0.75
1:B:199:ARG:NH2	1:B:232:ARG:O	2.20	0.74
1:A:2:PRO:O	1:A:3:GLU:CG	2.35	0.74
1:B:199:ARG:NH1	1:B:251:GLN:O	2.20	0.74
1:A:220:TRP:HD1	1:A:223:LYS:HE3	1.52	0.73
1:B:279:ILE:CD1	1:B:382:LYS:HD3	2.19	0.73
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.24	0.72
1:A:252:GLN:HE21	1:A:252:GLN:H	1.38	0.72
1:A:1:THR:H2	1:A:2:PRO:CD	2.02	0.72
1:A:107:THR:O	1:A:111:THR:HB	1.90	0.71
1:B:281:LYS:HZ2	1:B:281:LYS:HB3	1.55	0.71
1:A:6:VAL:HG13	1:A:357:LYS:CD	2.20	0.70
1:A:111:THR:HG21	1:A:113:VAL:HG12	1.72	0.69
1:B:380:ASP:O	1:B:382:LYS:NZ	2.24	0.69
1:B:293:ASN:HB3	1:B:295:SER:H	1.57	0.68
1:A:448:LEU:O	1:A:449:LYS:HB2	1.95	0.67
1:B:226:ARG:O	1:B:230:GLU:HG3	1.95	0.67
1:B:418:ARG:HH11	1:B:420:ALA:CB	2.08	0.67
1:A:220:TRP:HA	1:A:223:LYS:NZ	2.09	0.66
1:A:449:LYS:HE3	1:A:449:LYS:CA	2.25	0.66
1:A:173:ALA:O	1:A:177:LYS:HE2	1.94	0.66
1:B:6:VAL:CG1	1:B:77:ALA:HB1	2.26	0.65
1:A:111:THR:HG22	1:A:113:VAL:H	1.61	0.65
1:A:228:GLU:O	1:A:232:ARG:HG2	1.97	0.65
1:B:199:ARG:HA	1:B:234:TYR:OH	1.97	0.65
1:A:440:TYR:CD2	1:B:23:ARG:HD3	2.32	0.64
1:A:2:PRO:C	1:A:3:GLU:HG2	2.22	0.64
1:B:313:ASN:HD21	1:B:315:LYS:HB2	1.62	0.64
1:B:298:THR:OG1	1:B:301:GLN:HG3	1.98	0.64
1:A:300:ALA:O	1:A:304:ASP:HB2	1.97	0.64
1:A:381:THR:HG23	1:B:411:GLU:OE1	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:HB2	1:B:296:VAL:HG23	1.80	0.63
1:B:267:ARG:NH2	1:B:347:GLU:OE2	2.30	0.62
1:A:220:TRP:CB	1:A:223:LYS:HE2	2.29	0.62
1:B:102:SER:OG	4:B:453:PO4:P	2.55	0.62
1:A:305:LYS:NZ	1:A:308:GLU:OE2	2.32	0.62
1:A:274:THR:HG21	1:A:281:LYS:CE	2.29	0.61
1:B:305:LYS:HD3	1:B:305:LYS:N	2.15	0.61
1:A:33:LEU:HD22	1:B:427:ALA:HB1	1.83	0.61
1:B:1:THR:O	1:B:3:GLU:N	2.34	0.61
1:B:171:PRO:HB2	1:B:213:GLU:HG2	1.83	0.60
1:A:406:GLU:OE1	1:B:276:HIS:HE1	1.84	0.60
1:A:252:GLN:HE21	1:A:252:GLN:N	1.99	0.60
1:B:133:LEU:HD23	1:B:133:LEU:C	2.26	0.60
1:A:121:GLY:O	1:A:162:HIS:HD2	1.83	0.59
1:B:151:LEU:HD21	1:B:203:THR:HG22	1.84	0.59
1:B:301:GLN:O	1:B:305:LYS:HG2	2.02	0.59
1:A:276:HIS:HE1	1:B:406:GLU:OE1	1.85	0.59
1:A:1:THR:H3	1:A:2:PRO:CD	2.03	0.58
1:A:248:GLU:OE1	1:A:312:LYS:HG3	2.03	0.58
1:B:221:GLN:HG3	1:B:222:GLY:N	2.17	0.58
1:A:15:ASN:HD21	1:A:17:THR:HB	1.68	0.58
1:A:220:TRP:CD1	1:A:223:LYS:HE3	2.37	0.58
1:A:232:ARG:HB3	1:A:232:ARG:NH1	2.08	0.58
1:B:253:LYS:N	1:B:254:PRO:CD	2.63	0.57
1:A:173:ALA:HB1	1:A:177:LYS:HE3	1.85	0.57
1:B:195:LEU:CD1	1:B:195:LEU:C	2.77	0.57
1:B:1:THR:HG23	1:B:2:PRO:HD2	1.85	0.57
1:A:12:ALA:HB1	1:A:16:ILE:CD1	2.30	0.56
1:A:248:GLU:HG2	1:A:312:LYS:HZ3	1.70	0.56
1:A:73:LYS:HZ2	1:A:73:LYS:HB2	1.70	0.56
1:B:313:ASN:ND2	1:B:315:LYS:H	2.04	0.56
1:B:253:LYS:H	1:B:254:PRO:HD3	1.71	0.56
1:B:393:LYS:O	1:B:393:LYS:HG3	2.05	0.56
1:A:6:VAL:CG1	1:A:357:LYS:CD	2.74	0.56
1:B:137:LYS:HZ1	1:B:199:ARG:HB3	1.70	0.56
1:A:438:LEU:O	1:A:442:MET:HG3	2.05	0.55
1:B:76:ASP:HA	1:B:418:ARG:HH22	1.71	0.55
1:A:248:GLU:HG2	1:A:312:LYS:NZ	2.22	0.55
1:A:269:LEU:HD13	1:A:289:ASN:HB2	1.86	0.55
1:B:359:GLU:OE1	1:B:361:ASN:N	2.39	0.55
1:A:15:ASN:ND2	1:A:17:THR:HB	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASP:OD2	1:A:351:ARG:HD2	2.08	0.54
1:A:267:ARG:HG2	1:A:292:ARG:NH2	2.22	0.54
1:B:279:ILE:CD1	1:B:382:LYS:CD	2.85	0.54
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.88	0.54
1:A:276:HIS:CE1	1:B:406:GLU:OE1	2.61	0.54
1:A:381:THR:CG2	1:B:411:GLU:OE1	2.55	0.54
1:A:15:ASN:C	1:A:15:ASN:HD22	2.17	0.53
1:A:359:GLU:OE1	1:A:361:ASN:N	2.35	0.53
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.44	0.53
1:A:232:ARG:HH11	1:A:232:ARG:CG	2.14	0.53
1:B:298:THR:H	1:B:301:GLN:HE21	1.56	0.53
1:B:45:ILE:CD1	1:B:442:MET:HB3	2.39	0.52
1:B:1:THR:CG2	1:B:2:PRO:HD2	2.38	0.52
1:B:354:GLU:O	1:B:358:LYS:NZ	2.41	0.52
1:B:182:ALA:HB1	1:B:184:GLU:OE2	2.09	0.52
1:B:195:LEU:C	1:B:195:LEU:HD12	2.35	0.52
1:B:4:MET:HG2	1:B:35:ASN:O	2.10	0.52
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.92	0.52
1:B:190:SER:OG	1:B:193:GLU:HG3	2.09	0.52
1:B:369:ASP:CG	1:B:370:HIS:CD2	2.88	0.52
1:A:116:TYR:CE2	1:A:119:ALA:HB2	2.45	0.51
1:A:417:LEU:C	1:A:417:LEU:HD12	2.34	0.51
1:B:121:GLY:O	1:B:162:HIS:HD2	1.93	0.51
1:B:73:LYS:H	1:B:73:LYS:HD2	1.75	0.51
1:B:418:ARG:HH11	1:B:420:ALA:HB3	1.74	0.51
1:B:351:ARG:NH2	1:B:354:GLU:OE1	2.34	0.51
1:B:281:LYS:HB3	1:B:281:LYS:NZ	2.25	0.51
1:B:354:GLU:HG2	1:B:358:LYS:HZ1	1.75	0.51
1:B:134:GLU:OE2	1:B:162:HIS:HE1	1.94	0.50
1:B:10:ARG:O	1:B:24:ARG:HD3	2.11	0.50
1:B:177:LYS:C	1:B:179:PRO:HD3	2.36	0.50
1:A:92:LYS:HE3	1:A:92:LYS:CA	2.29	0.50
1:B:137:LYS:NZ	1:B:198:ALA:O	2.42	0.50
1:B:46:ILE:HG22	1:B:48:LEU:HD22	1.93	0.50
1:B:424:PRO:O	1:B:425:HIS:HB2	2.12	0.50
1:B:131:THR:O	1:B:135:MET:HG3	2.12	0.49
1:B:15:ASN:O	1:B:21:GLY:HA3	2.12	0.49
1:B:149:ALA:HA	1:B:263:ASN:HD22	1.78	0.49
1:A:267:ARG:NH2	1:A:347:GLU:OE2	2.46	0.49
1:A:449:LYS:HE3	1:A:449:LYS:HA	1.95	0.48
1:A:128:ASP:OD2	1:A:188:LYS:NZ	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:HIS:ND1	1:A:410:GLN:O	2.41	0.48
1:B:351:ARG:HA	1:B:351:ARG:NE	2.28	0.48
1:B:380:ASP:O	1:B:382:LYS:CE	2.60	0.48
1:B:426:ALA:O	1:B:429:VAL:HG22	2.12	0.48
1:A:145:ASN:O	1:A:203:THR:HA	2.14	0.48
1:A:293:ASN:HB3	1:A:296:VAL:H	1.79	0.48
1:A:2:PRO:O	1:A:3:GLU:CD	2.56	0.48
1:B:313:ASN:HD22	1:B:315:LYS:N	2.12	0.48
1:A:149:ALA:HA	1:A:263:ASN:HD22	1.78	0.47
1:B:236:LEU:CD2	1:B:256:LEU:HD23	2.40	0.47
1:B:242:SER:O	1:B:246:VAL:HG23	2.14	0.47
1:A:274:THR:HG22	1:A:277:GLY:CA	2.45	0.47
1:B:176:GLN:OE1	1:B:177:LYS:CE	2.47	0.47
1:A:111:THR:HG21	1:A:113:VAL:CG1	2.39	0.47
1:A:33:LEU:HD23	1:B:37:LEU:HD11	1.97	0.47
1:B:152:GLN:NE2	1:B:210:THR:HB	2.30	0.47
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.45	0.47
1:A:432:LEU:O	1:B:10:ARG:HD2	2.15	0.47
1:A:293:ASN:HB2	1:A:296:VAL:HB	1.96	0.46
1:B:313:ASN:HD21	1:B:315:LYS:CB	2.26	0.46
1:B:221:GLN:C	1:B:223:LYS:H	2.23	0.46
1:A:178:CYS:N	1:A:179:PRO:CD	2.78	0.46
1:A:449:LYS:CA	1:A:449:LYS:CE	2.94	0.46
1:B:289:ASN:ND2	1:B:291:GLN:H	2.13	0.46
1:A:122:VAL:HA	1:A:127:LYS:O	2.16	0.46
1:B:10:ARG:HB2	1:B:71:PHE:CE1	2.51	0.46
1:B:214:THR:OG1	1:B:222:GLY:C	2.58	0.46
1:B:279:ILE:HD13	1:B:382:LYS:HD3	1.97	0.46
1:A:80:LEU:HD23	1:A:426:ALA:HB3	1.97	0.46
1:B:30:THR:O	1:B:34:ARG:HG3	2.16	0.46
1:B:253:LYS:N	1:B:254:PRO:HD2	2.30	0.46
1:B:4:MET:HA	1:B:5:PRO:HD3	1.66	0.46
1:A:80:LEU:HD23	1:A:426:ALA:CB	2.46	0.45
1:B:144:GLY:HA2	1:B:202:VAL:O	2.15	0.45
1:A:73:LYS:CB	1:A:73:LYS:NZ	2.79	0.45
1:A:315:LYS:HD2	1:A:315:LYS:HA	1.75	0.45
1:B:224:THR:OG1	1:B:227:GLU:HG3	2.16	0.45
1:B:48:LEU:HG	1:B:349:VAL:HG22	1.99	0.45
1:A:220:TRP:HA	1:A:223:LYS:HZ3	1.78	0.45
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.84	0.45
1:A:208:ALA:O	1:A:226:ARG:NH2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:NZ	1:B:126:GLU:OE2	2.33	0.45
1:A:313:ASN:OD1	1:A:315:LYS:N	2.50	0.45
1:B:281:LYS:NZ	1:B:281:LYS:CB	2.79	0.45
1:A:220:TRP:CD1	1:A:223:LYS:CE	3.00	0.45
1:A:293:ASN:CB	1:A:296:VAL:HB	2.47	0.45
1:B:213:GLU:HB3	1:B:225:LEU:HD22	1.98	0.45
1:B:279:ILE:CD1	1:B:382:LYS:CE	2.90	0.45
1:A:168:CYS:HB3	1:A:174:THR:OG1	2.18	0.44
1:B:354:GLU:HG2	1:B:358:LYS:NZ	2.33	0.44
1:A:406:GLU:OE1	1:B:276:HIS:CE1	2.66	0.44
1:A:220:TRP:HD1	1:A:223:LYS:CE	2.27	0.44
1:B:248:GLU:CG	1:B:253:LYS:HZ1	2.22	0.44
1:B:332:ALA:O	1:B:333:ALA:HB3	2.18	0.44
1:B:178:CYS:HB3	1:B:181:ASN:OD1	2.18	0.44
1:B:382:LYS:HE3	1:B:382:LYS:HB2	1.72	0.44
1:B:40:LYS:HA	1:B:40:LYS:HD2	1.79	0.43
1:B:142:ALA:HA	1:B:201:ASP:OD2	2.18	0.43
1:B:351:ARG:HA	1:B:351:ARG:HE	1.82	0.43
1:B:92:LYS:HD2	1:B:92:LYS:HA	1.33	0.43
1:B:255:LEU:HD12	1:B:309:LEU:CD1	2.49	0.43
1:B:280:ASP:C	1:B:281:LYS:CG	2.91	0.43
1:A:269:LEU:HD13	1:A:289:ASN:CB	2.49	0.43
1:A:91:LYS:HG3	1:A:116:TYR:CD1	2.54	0.43
1:B:248:GLU:HG2	1:B:253:LYS:NZ	2.26	0.43
1:B:331:HIS:ND1	1:B:410:GLN:O	2.44	0.43
1:A:272:LYS:HB3	1:A:272:LYS:HE3	1.35	0.43
1:A:33:LEU:HD22	1:B:427:ALA:CB	2.48	0.42
1:B:438:LEU:O	1:B:442:MET:HG3	2.20	0.42
1:B:196:LEU:HD12	1:B:196:LEU:HA	1.87	0.42
1:A:147:SER:O	1:A:205:GLY:HA2	2.20	0.42
1:B:289:ASN:HA	1:B:290:PRO:HD3	1.92	0.42
1:B:45:ILE:HD12	1:B:442:MET:HB3	2.01	0.42
1:A:337:GLY:O	1:A:341:GLU:HG2	2.20	0.42
1:B:48:LEU:HD13	1:B:321:VAL:HB	2.01	0.42
1:B:148:THR:OG1	1:B:324:ALA:HB3	2.20	0.42
1:A:7:LEU:HB2	1:A:77:ALA:O	2.19	0.42
1:A:48:LEU:HG	1:A:349:VAL:HG22	2.02	0.42
1:B:13:GLN:OE1	1:B:23:ARG:O	2.38	0.42
1:B:313:ASN:ND2	1:B:315:LYS:N	2.66	0.42
1:B:379:PRO:HA	1:B:399:VAL:HG21	2.02	0.42
1:A:220:TRP:HA	1:A:223:LYS:CE	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASN:HD22	1:B:315:LYS:H	1.68	0.41
1:B:206:GLY:HA3	1:B:262:GLY:O	2.20	0.41
1:A:16:ILE:HD12	1:A:16:ILE:HA	1.74	0.41
1:A:195:LEU:C	1:A:195:LEU:HD23	2.46	0.41
1:B:267:ARG:HH22	1:B:347:GLU:CD	2.25	0.41
1:A:402:TYR:HB3	1:A:410:GLN:HG3	2.02	0.41
1:A:48:LEU:HD13	1:A:321:VAL:HB	2.02	0.41
1:B:269:LEU:HD22	1:B:289:ASN:HA	2.02	0.41
1:A:274:THR:HG22	1:A:277:GLY:HA2	2.01	0.41
1:B:141:LEU:CD1	1:B:315:LYS:HD2	2.51	0.41
1:B:237:VAL:O	1:B:257:GLY:HA2	2.19	0.41
1:B:110:SER:O	1:B:132:ILE:N	2.53	0.41
1:B:151:LEU:HD12	1:B:151:LEU:HA	1.90	0.41
1:B:359:GLU:OE2	1:B:361:ASN:HB2	2.20	0.41
1:A:267:ARG:O	1:A:292:ARG:NH2	2.43	0.40
1:A:424:PRO:O	1:A:425:HIS:HB2	2.20	0.40
1:A:78:LEU:HB2	1:A:420:ALA:HB1	2.04	0.40
1:A:73:LYS:HB2	1:A:73:LYS:NZ	2.33	0.40
1:A:4:MET:HE3	1:A:4:MET:HB2	1.92	0.40
1:A:134:GLU:OE2	1:A:162:HIS:HE1	2.04	0.40
1:A:449:LYS:HA	1:A:449:LYS:CE	2.51	0.40
1:B:357:LYS:HZ3	1:B:357:LYS:HG3	1.79	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	
1	A	447/449 (100%)	431 (96%)	12 (3%)	4 (1%)	14	9
1	B	447/449 (100%)	424 (95%)	18 (4%)	5 (1%)	11	7
All	All	894/898 (100%)	855 (96%)	30 (3%)	9 (1%)	12	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	B	253	LYS
1	B	4	MET
1	B	2	PRO
1	B	293	ASN
1	A	2	PRO
1	A	408	ASP
1	A	293	ASN
1	B	171	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/340 (100%)	298 (88%)	42 (12%)	4	2
1	B	340/340 (100%)	298 (88%)	42 (12%)	4	2
All	All	680/680 (100%)	596 (88%)	84 (12%)	4	2

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	7	LEU
1	A	15	ASN
1	A	16	ILE
1	A	43	LYS
1	A	48	LEU
1	A	73	LYS
1	A	80	LEU
1	A	83	GLN
1	A	84	TYR
1	A	91	LYS
1	A	92	LYS
1	A	111	THR
1	A	127	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	LEU
1	A	167	LYS
1	A	185	LYS
1	A	196	LEU
1	A	232	ARG
1	A	244	ASN
1	A	245	SER
1	A	248	GLU
1	A	252	GLN
1	A	266	VAL
1	A	269	LEU
1	A	272	LYS
1	A	274	THR
1	A	279	ILE
1	A	294	ASP
1	A	310	LEU
1	A	314	GLU
1	A	315	LYS
1	A	353	LEU
1	A	354	GLU
1	A	357	LYS
1	A	358	LYS
1	A	406	GLU
1	A	429	VAL
1	A	443	LYS
1	A	446	LEU
1	A	448	LEU
1	A	449	LYS
1	B	8	GLU
1	B	13	GLN
1	B	37	LEU
1	B	47	LEU
1	B	48	LEU
1	B	84	TYR
1	B	92	LYS
1	B	151	LEU
1	B	155	THR
1	B	159	LEU
1	B	167	LYS
1	B	171	PRO
1	B	172	SER
1	B	176	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	184	GLU
1	B	188	LYS
1	B	195	LEU
1	B	196	LEU
1	B	209	LYS
1	B	213	GLU
1	B	221	GLN
1	B	223	LYS
1	B	225	LEU
1	B	235	GLN
1	B	242	SER
1	B	250	ASN
1	B	255	LEU
1	B	269	LEU
1	B	272	LYS
1	B	281	LYS
1	B	294	ASP
1	B	304	ASP
1	B	313	ASN
1	B	345	LEU
1	B	351	ARG
1	B	353	LEU
1	B	357	LYS
1	B	382	LYS
1	B	400	MET
1	B	443	LYS
1	B	448	LEU
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	35	ASN
1	A	83	GLN
1	A	162	HIS
1	A	194	GLN
1	A	244	ASN
1	A	252	GLN
1	A	263	ASN
1	A	276	HIS
1	A	301	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	329	GLN
1	A	375	GLN
1	A	391	ASN
1	A	435	GLN
1	B	35	ASN
1	B	83	GLN
1	B	145	ASN
1	B	162	HIS
1	B	194	GLN
1	B	235	GLN
1	B	263	ASN
1	B	276	HIS
1	B	289	ASN
1	B	301	GLN
1	B	313	ASN
1	B	338	GLN
1	B	350	GLN
1	B	391	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	A	453	2	4,4,4	0.25	0	6,6,6	0.34	0
4	PO4	B	453	2	4,4,4	1.44	1 (25%)	6,6,6	0.84	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	453	PO4	P-O1	2.02	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	453	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.