



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:56 am BST

PDB ID : 1KXV
Title : Camelid VHH Domains in Complex with Porcine Pancreatic alpha-Amylase
Authors : Desmyter, A.; Spinelli, S.; Payan, F.; Lauwereys, M.; Wyns, L.; Muyldermans, S.; Cambillau, C.
Deposited on : 2002-02-01
Resolution : 1.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

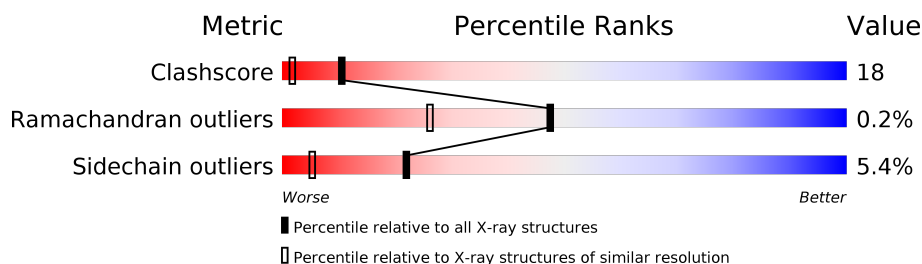
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 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	496	77% 19% .
1	B	496	76% 19% .
2	C	121	82% 15% ...
2	D	121	72% 18% 8% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10951 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 ALPHA-AMYLASE, PANCREATIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3900	2465	684	730	21			
1	B	496	Total	C	N	O	S	0	0	0
			3894	2459	685	729	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	LYS	GLN	SEE REMARK 999	UNP P00690
A	310	SER	ALA	SEE REMARK 999	UNP P00690
A	323	ILE	VAL	SEE REMARK 999	UNP P00690
A	404	GLN	GLU	SEE REMARK 999	UNP P00690
B	243	LYS	GLN	SEE REMARK 999	UNP P00690
B	310	SER	ALA	SEE REMARK 999	UNP P00690
B	323	ILE	VAL	SEE REMARK 999	UNP P00690
B	404	GLN	GLU	SEE REMARK 999	UNP P00690

- Molecule 2 is a protein called CAMELID VHH DOMAIN CAB10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	119	Total	C	N	O	S	0	0	0
			882	548	152	175	7			
2	D	121	Total	C	N	O	S	0	0	0
			898	556	155	180	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	590	Total	O	0	0
			590	590		
3	B	484	Total	O	0	0
			484	484		

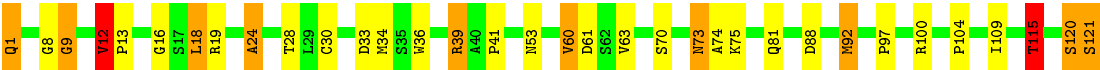
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	147	Total 147	O 147	0	0
3	D	156	Total 156	O 156	0	0



● Molecule 2: CAMELID VHH DOMAIN CAB10



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.57 Å 60.99 Å 107.33 Å 98.78° 100.88° 101.14°	Depositor
Resolution (Å)	29.34 – 1.60	Depositor
% Data completeness (in resolution range)	95.1 (29.34-1.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.205 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10951	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.93	2/4010 (0.0%)	1.34	35/5450 (0.6%)
1	B	0.88	3/4003 (0.1%)	1.16	25/5439 (0.5%)
2	C	0.82	0/901	1.06	3/1225 (0.2%)
2	D	1.67	5/917 (0.5%)	1.56	18/1245 (1.4%)
All	All	0.99	10/9831 (0.1%)	1.27	81/13359 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	2
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	121	SER	C-OXT	33.39	1.86	1.23
2	D	8	GLY	C-N	-23.54	0.90	1.33
2	D	1	GLN	C-N	-6.71	1.18	1.34
2	D	121	SER	N-CA	5.68	1.57	1.46
1	B	421	ARG	CD-NE	-5.67	1.36	1.46
1	A	252	ARG	CG-CD	5.37	1.65	1.51
1	B	282	GLU	CD-OE2	5.37	1.31	1.25
1	A	421	ARG	CZ-NH1	-5.22	1.26	1.33
2	D	8	GLY	C-O	-5.11	1.15	1.23
1	B	395	VAL	CB-CG2	-5.02	1.42	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	60	VAL	CG1-CB-CG2	21.17	144.77	110.90
1	A	195	ARG	NE-CZ-NH1	-21.02	109.79	120.30
1	A	195	ARG	NE-CZ-NH2	20.61	130.61	120.30
2	D	121	SER	N-CA-CB	20.05	140.58	110.50
1	A	252	ARG	NE-CZ-NH2	19.88	130.24	120.30
1	B	252	ARG	NE-CZ-NH1	-19.40	110.60	120.30
1	B	252	ARG	NE-CZ-NH2	19.30	129.95	120.30
1	A	252	ARG	NE-CZ-NH1	-19.19	110.70	120.30
1	B	176	ARG	NE-CZ-NH2	18.86	129.73	120.30
1	A	176	ARG	NE-CZ-NH1	-17.06	111.77	120.30
1	A	10	ARG	NE-CZ-NH1	-16.78	111.91	120.30
1	A	72	ARG	NE-CZ-NH1	-16.70	111.95	120.30
1	A	72	ARG	NE-CZ-NH2	16.21	128.40	120.30
1	A	176	ARG	NE-CZ-NH2	16.19	128.40	120.30
1	A	10	ARG	NE-CZ-NH2	15.67	128.14	120.30
1	A	92	ARG	NE-CZ-NH1	-15.20	112.70	120.30
1	B	176	ARG	NE-CZ-NH1	-15.15	112.73	120.30
1	A	92	ARG	NE-CZ-NH2	14.63	127.61	120.30
2	D	8	GLY	C-N-CA	14.51	152.78	122.30
1	B	72	ARG	NE-CZ-NH1	-13.68	113.46	120.30
1	B	72	ARG	NE-CZ-NH2	13.13	126.87	120.30
1	A	389	ARG	NE-CZ-NH1	-12.77	113.92	120.30
1	A	421	ARG	NE-CZ-NH2	12.74	126.67	120.30
1	B	290	ASP	CB-CG-OD2	12.53	129.57	118.30
1	B	195	ARG	NE-CZ-NH2	11.94	126.27	120.30
1	A	421	ARG	NE-CZ-NH1	-11.77	114.41	120.30
1	A	389	ARG	NE-CZ-NH2	11.73	126.17	120.30
2	D	8	GLY	O-C-N	-11.16	104.22	123.20
1	B	389	ARG	NE-CZ-NH1	-11.09	114.75	120.30
1	B	10	ARG	NE-CZ-NH2	10.89	125.75	120.30
1	B	195	ARG	NE-CZ-NH1	-10.87	114.87	120.30
1	B	290	ASP	CB-CG-OD1	-10.47	108.87	118.30
1	B	389	ARG	NE-CZ-NH2	9.89	125.25	120.30
1	A	252	ARG	CD-NE-CZ	9.82	137.35	123.60
1	A	293	LEU	CA-CB-CG	-9.16	94.24	115.30
1	B	293	LEU	CA-CB-CG	-8.72	95.24	115.30
1	A	224	ALA	C-N-CA	-8.67	104.09	122.30
1	B	252	ARG	CD-NE-CZ	8.52	135.52	123.60
1	A	176	ARG	CB-CG-CD	8.09	132.63	111.60
2	D	8	GLY	CA-C-N	7.90	132.00	116.20
1	A	252	ARG	CB-CG-CD	7.86	132.04	111.60
1	B	10	ARG	NE-CZ-NH1	-7.79	116.41	120.30
2	D	39	ARG	NE-CZ-NH2	7.75	124.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ARG	CG-CD-NE	-7.50	96.05	111.80
1	A	195	ARG	CD-NE-CZ	7.43	134.00	123.60
2	C	39	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	B	252	ARG	CB-CG-CD	7.22	130.36	111.60
1	A	92	ARG	CB-CG-CD	7.18	130.26	111.60
2	D	12	VAL	N-CA-CB	-7.18	95.71	111.50
1	A	92	ARG	CD-NE-CZ	7.04	133.45	123.60
2	D	12	VAL	CG1-CB-CG2	6.79	121.76	110.90
1	A	72	ARG	CD-NE-CZ	6.73	133.03	123.60
1	B	176	ARG	CB-CG-CD	6.67	128.94	111.60
1	A	395	VAL	CG1-CB-CG2	6.61	121.47	110.90
1	B	70	CYS	CA-CB-SG	6.58	125.85	114.00
2	D	120	SER	C-N-CA	-6.49	105.48	121.70
1	B	176	ARG	CD-NE-CZ	6.46	132.65	123.60
2	D	121	SER	N-CA-C	-6.35	93.86	111.00
2	D	115	THR	CB-CA-C	-6.31	94.57	111.60
2	C	45	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	159	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	10	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	176	ARG	CD-NE-CZ	5.74	131.64	123.60
2	D	24	ALA	N-CA-C	-5.55	96.02	111.00
1	B	227	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	D	34	MET	CG-SD-CE	5.43	108.88	100.20
2	D	60	VAL	CA-CB-CG2	-5.39	102.81	110.90
2	D	8	GLY	N-CA-C	5.38	126.54	113.10
1	B	72	ARG	CD-NE-CZ	5.35	131.09	123.60
2	D	115	THR	N-CA-CB	5.28	120.33	110.30
1	B	153	ASP	CB-CG-OD2	5.27	123.04	118.30
2	D	92	MET	CA-CB-CG	5.26	122.25	113.30
1	A	30	ARG	NE-CZ-NH1	-5.23	117.69	120.30
2	C	92	MET	CG-SD-CE	-5.18	91.91	100.20
1	B	291	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	70	CYS	N-CA-CB	-5.10	101.43	110.60
1	A	224	ALA	O-C-N	-5.09	114.55	123.20
1	B	158	ARG	NE-CZ-NH2	5.07	122.83	120.30
2	D	115	THR	CA-CB-CG2	5.06	119.48	112.40
1	A	186	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	178	MET	CG-SD-CE	5.03	108.24	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	TYR	Sidechain
2	C	39	ARG	Sidechain
2	C	45	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	3900	0	3671	143	0
1	B	3894	0	3666	164	0
2	C	882	0	848	16	0
2	D	898	0	862	21	0
3	A	590	0	0	27	0
3	B	484	0	0	24	0
3	C	147	0	0	4	0
3	D	156	0	0	8	0
All	All	10951	0	9047	344	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 18.

All (344) 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:B:1:GLN:H1	1:B:1:GLN:NE2	1.19	1.40
1:B:1:GLN:NE2	1:B:1:GLN:N	1.90	1.19
1:B:282:GLU:OE1	3:B:626:HOH:O	1.66	1.14
1:A:1:GLN:OE1	1:A:1:GLN:CA	2.00	1.09
1:B:15:HIS:HB3	1:B:339:MET:HE3	1.31	1.08
1:A:409:TRP:CH2	1:A:417:VAL:HG11	1.90	1.06
1:B:341:SER:O	1:B:383:VAL:HG22	1.55	1.05
1:B:339:MET:HE2	1:B:340:SER:H	1.19	1.05
1:A:229:PHE:HE2	1:A:252:ARG:HD3	1.17	1.04
1:B:170:LEU:O	1:B:176:ARG:HD3	1.58	1.04
1:B:229:PHE:HE2	1:B:252:ARG:HD3	1.19	1.01
1:B:157:VAL:HG21	1:B:242:ILE:HD11	1.42	1.01
1:B:484:GLU:HG2	1:B:485:ASP:N	1.77	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:TRP:CH2	1:B:417:VAL:HG11	1.96	0.99
1:A:1:GLN:OE1	1:A:1:GLN:HA	1.13	0.99
1:A:207:ILE:O	1:A:211:LEU:HD13	1.63	0.98
1:B:266:VAL:HG13	1:B:323:ILE:HD12	1.45	0.98
1:B:2:TYR:O	1:B:252:ARG:HD2	1.64	0.97
1:B:69:LEU:HD21	1:B:185:LYS:HE3	1.48	0.96
1:B:320:LEU:O	1:B:323:ILE:HG13	1.63	0.96
1:A:341:SER:O	1:A:383:VAL:HG22	1.66	0.95
1:A:2:TYR:O	1:A:252:ARG:HD2	1.68	0.94
1:B:358:ILE:HB	3:B:826:HOH:O	1.66	0.94
1:B:170:LEU:O	1:B:176:ARG:CD	2.15	0.94
1:B:1:GLN:HE21	1:B:1:GLN:H1	1.05	0.93
2:D:61:ASP:OD2	3:D:159:HOH:O	1.87	0.92
2:D:16:GLY:HA3	3:D:226:HOH:O	1.68	0.92
1:B:1:GLN:CD	1:B:1:GLN:N	2.23	0.92
1:A:170:LEU:O	1:A:176:ARG:HD3	1.68	0.91
1:A:170:LEU:O	1:A:176:ARG:CD	2.19	0.91
1:A:1:GLN:N	1:A:228:PRO:O	2.03	0.91
1:A:229:PHE:CE2	1:A:252:ARG:HD3	2.05	0.90
1:A:325:VAL:O	1:A:329:LEU:HD23	1.71	0.89
1:B:154:PRO:HA	1:B:157:VAL:HG22	1.55	0.88
1:B:339:MET:HE2	1:B:340:SER:N	1.90	0.86
1:A:100:ASN:HD22	1:A:101:HIS:HD2	1.23	0.85
1:B:49:ILE:HG21	1:B:103:CYS:CB	2.08	0.83
1:B:100:ASN:HD22	1:B:101:HIS:HD2	1.23	0.82
1:A:484:GLU:N	1:A:484:GLU:OE2	2.13	0.82
1:B:392:ARG:O	1:B:395:VAL:HG22	1.80	0.82
1:A:484:GLU:CD	1:A:485:ASP:H	1.83	0.82
2:C:12:VAL:HG23	2:C:13:PRO:HD2	1.62	0.81
1:B:229:PHE:CE2	1:B:252:ARG:HD3	2.10	0.81
1:B:1:GLN:H3	1:B:1:GLN:CD	1.83	0.80
1:B:157:VAL:HG21	1:B:242:ILE:CD1	2.12	0.80
1:B:266:VAL:CG1	1:B:323:ILE:HD12	2.11	0.80
1:A:300:ASP:HB2	3:A:737:HOH:O	1.80	0.80
1:A:349:VAL:HG13	3:A:838:HOH:O	1.82	0.79
1:A:72:ARG:CD	3:A:545:HOH:O	2.28	0.79
1:B:355:ASN:ND2	3:B:805:HOH:O	2.15	0.78
1:B:5:GLN:HE21	1:B:5:GLN:HA	1.48	0.78
1:A:157:VAL:HG11	1:A:242:ILE:HD11	1.64	0.77
2:D:13:PRO:HD2	3:D:226:HOH:O	1.86	0.75
1:B:157:VAL:HG23	1:B:158:ARG:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HA	1:A:5:GLN:HE21	1.50	0.75
1:A:323:ILE:HD11	1:A:486:PRO:HG2	1.68	0.75
1:B:439:THR:C	1:B:440:LEU:HD12	2.08	0.74
1:B:49:ILE:HG22	1:B:65:VAL:CG1	2.16	0.74
1:A:72:ARG:HD3	3:A:545:HOH:O	1.88	0.74
1:B:154:PRO:HA	1:B:157:VAL:CG2	2.18	0.74
1:B:69:LEU:N	1:B:69:LEU:HD22	2.02	0.74
1:A:319:ARG:HH21	1:A:319:ARG:HG2	1.53	0.74
2:D:12:VAL:HG13	3:D:226:HOH:O	1.86	0.74
2:C:12:VAL:CG2	2:C:13:PRO:HD2	2.18	0.73
1:A:383:VAL:HG23	1:A:385:GLU:OE2	1.88	0.73
1:A:72:ARG:HD2	3:A:545:HOH:O	1.88	0.73
1:A:207:ILE:O	1:A:211:LEU:CD1	2.36	0.73
1:B:313:LEU:HD11	3:B:831:HOH:O	1.87	0.73
1:B:72:ARG:HD2	3:B:566:HOH:O	1.87	0.73
1:B:440:LEU:N	1:B:440:LEU:HD12	2.04	0.72
1:B:383:VAL:HG23	1:B:385:GLU:OE2	1.89	0.72
1:B:49:ILE:HG21	1:B:103:CYS:HB2	1.71	0.72
1:B:266:VAL:CG1	1:B:323:ILE:CD1	2.67	0.72
1:A:288:PRO:HG3	3:C:208:HOH:O	1.88	0.72
1:B:69:LEU:HD21	1:B:185:LYS:CE	2.19	0.72
1:B:347:ASN:HB2	3:B:805:HOH:O	1.89	0.72
1:B:409:TRP:CH2	1:B:417:VAL:CG1	2.71	0.72
1:A:5:GLN:O	1:A:92:ARG:CD	2.38	0.71
1:A:5:GLN:O	1:A:92:ARG:HD2	1.91	0.71
1:B:267:ARG:HG3	3:B:831:HOH:O	1.89	0.70
1:B:341:SER:C	1:B:383:VAL:HG22	2.11	0.70
1:B:446:GLY:HA2	1:B:469:VAL:HG13	1.73	0.70
1:B:266:VAL:HG13	1:B:323:ILE:CD1	2.21	0.70
1:A:447:GLY:HA3	1:A:495:LYS:HZ2	1.55	0.70
1:A:417:VAL:HG12	1:A:418:ALA:N	2.06	0.70
1:A:208:LYS:HE3	3:C:205:HOH:O	1.92	0.70
1:B:274:MET:HE3	1:B:429:PHE:HB2	1.73	0.70
1:B:484:GLU:CG	1:B:485:ASP:N	2.53	0.69
1:B:319:ARG:HG2	1:B:319:ARG:HH21	1.57	0.69
1:A:447:GLY:HA3	1:A:495:LYS:NZ	2.07	0.69
1:B:227:ARG:CD	3:B:799:HOH:O	2.40	0.69
1:A:154:PRO:HA	1:A:157:VAL:HG12	1.74	0.68
1:A:383:VAL:CG2	1:A:385:GLU:OE2	2.41	0.68
1:A:154:PRO:HA	1:A:157:VAL:CG1	2.24	0.68
1:B:279:ASN:HD22	1:B:279:ASN:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:VAL:HB	3:C:208:HOH:O	1.93	0.68
1:A:389:ARG:HD2	1:A:453:ILE:O	1.94	0.68
1:B:392:ARG:O	1:B:395:VAL:CG2	2.41	0.68
1:B:438:SER:HB2	1:B:440:LEU:HD11	1.76	0.68
1:B:363:ASN:O	1:B:366:VAL:HG22	1.94	0.68
1:B:49:ILE:CG2	1:B:103:CYS:CB	2.72	0.67
1:A:274:MET:HE2	1:A:415:ASN:O	1.93	0.67
1:A:157:VAL:HG11	1:A:242:ILE:CD1	2.25	0.67
1:B:72:ARG:CD	3:B:566:HOH:O	2.43	0.67
1:A:170:LEU:O	1:A:176:ARG:HD2	1.94	0.67
1:A:409:TRP:CH2	1:A:417:VAL:CG1	2.75	0.66
1:B:320:LEU:O	1:B:323:ILE:CG1	2.39	0.66
2:C:13:PRO:HA	2:C:120:SER:HA	1.77	0.66
1:A:447:GLY:O	1:A:469:VAL:HG22	1.96	0.66
2:C:47:PHE:HD2	3:C:208:HOH:O	1.79	0.65
1:B:320:LEU:HA	1:B:323:ILE:HG12	1.78	0.65
2:D:33:ASP:OD2	2:D:100:ARG:HD2	1.96	0.65
1:A:279:ASN:H	1:A:279:ASN:HD22	1.45	0.65
1:B:2:TYR:O	1:B:252:ARG:CD	2.43	0.65
1:B:1:GLN:NE2	3:B:799:HOH:O	2.29	0.65
1:B:320:LEU:HA	1:B:323:ILE:HD11	1.80	0.64
1:B:170:LEU:O	1:B:176:ARG:HD2	1.96	0.64
1:A:449:TYR:HE2	1:A:469:VAL:HG21	1.62	0.64
1:B:320:LEU:HA	1:B:323:ILE:CG1	2.27	0.64
1:A:439:THR:C	1:A:440:LEU:HD12	2.19	0.63
1:B:227:ARG:HD3	3:B:799:HOH:O	1.95	0.63
1:B:346:ARG:C	3:B:805:HOH:O	2.37	0.63
1:B:320:LEU:HA	1:B:323:ILE:CD1	2.29	0.63
1:A:349:VAL:O	1:A:349:VAL:HG23	1.99	0.62
1:B:100:ASN:HD22	1:B:101:HIS:CD2	2.12	0.62
2:D:28:THR:HG22	3:D:138:HOH:O	1.97	0.62
1:B:49:ILE:HD11	1:B:63:GLN:OE1	2.00	0.62
1:A:20:ARG:CZ	3:A:673:HOH:O	2.47	0.62
1:B:462:CYS:SG	1:B:496:LEU:HD11	2.40	0.61
1:A:484:GLU:CG	3:A:745:HOH:O	2.48	0.61
1:B:355:ASN:O	3:B:826:HOH:O	2.15	0.61
1:B:458:VAL:HG23	1:B:458:VAL:O	2.01	0.61
1:A:496:LEU:HD12	1:A:496:LEU:N	2.16	0.60
1:B:449:TYR:HE2	1:B:469:VAL:HG11	1.64	0.60
1:A:266:VAL:HG12	1:A:320:LEU:HG	1.84	0.60
1:A:100:ASN:HD22	1:A:101:HIS:CD2	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HG12	3:A:971:HOH:O	2.02	0.60
2:D:19:ARG:HE	2:D:81:GLN:HE21	1.49	0.59
1:A:446:GLY:HA2	1:A:469:VAL:HG23	1.84	0.59
1:B:49:ILE:CD1	3:B:817:HOH:O	2.50	0.59
1:A:484:GLU:HG2	3:A:745:HOH:O	2.02	0.59
1:A:5:GLN:O	1:A:92:ARG:HD3	2.02	0.59
1:B:154:PRO:CA	1:B:157:VAL:HG22	2.30	0.59
1:B:389:ARG:HD2	1:B:453:ILE:O	2.02	0.59
1:B:49:ILE:CG2	1:B:103:CYS:HB3	2.32	0.59
1:A:347:ASN:OD1	3:A:838:HOH:O	2.16	0.58
1:B:383:VAL:CG2	1:B:385:GLU:OE2	2.51	0.58
1:A:323:ILE:HD11	1:A:486:PRO:CG	2.32	0.58
1:B:237:LEU:HD21	1:B:307:ALA:HB1	1.84	0.58
1:B:69:LEU:H	1:B:69:LEU:HD22	1.67	0.58
1:A:290:ASP:HB3	3:A:772:HOH:O	2.02	0.58
1:A:449:TYR:CE2	1:A:469:VAL:HG21	2.38	0.58
1:B:227:ARG:HG3	1:B:228:PRO:HD2	1.84	0.58
2:D:24:ALA:HB1	2:D:109:ILE:HD11	1.84	0.58
1:A:129:VAL:CG1	1:A:178:MET:HG2	2.33	0.58
2:D:30:CYS:O	2:D:75:LYS:HE2	2.02	0.58
2:D:19:ARG:HE	2:D:81:GLN:NE2	2.03	0.57
1:B:31:TYR:OH	1:B:392:ARG:HG3	2.04	0.57
1:B:320:LEU:N	1:B:320:LEU:HD12	2.19	0.57
1:B:417:VAL:HG12	1:B:418:ALA:N	2.19	0.57
1:A:323:ILE:HG23	1:A:429:PHE:CD2	2.39	0.57
2:D:33:ASP:OD1	3:D:128:HOH:O	2.18	0.57
1:B:447:GLY:O	1:B:469:VAL:HG12	2.04	0.57
1:B:450:CYS:SG	1:B:496:LEU:HD11	2.45	0.57
1:B:282:GLU:OE2	1:B:288:PRO:HA	2.05	0.57
1:B:440:LEU:CD1	1:B:440:LEU:N	2.68	0.56
1:B:157:VAL:CG2	1:B:242:ILE:HD11	2.27	0.56
1:A:211:LEU:HD12	1:A:211:LEU:N	2.21	0.56
1:A:341:SER:C	1:A:383:VAL:HG22	2.24	0.56
2:C:12:VAL:CG2	2:C:13:PRO:CD	2.84	0.56
1:A:409:TRP:CZ3	1:A:417:VAL:HG11	2.39	0.56
1:A:483:ALA:HB1	1:A:484:GLU:OE2	2.05	0.56
1:A:63:GLN:HG2	1:A:165:LEU:HD21	1.88	0.56
1:B:447:GLY:H	1:B:469:VAL:HG13	1.71	0.56
2:D:120:SER:O	2:D:121:SER:C	2.40	0.56
1:A:14:VAL:HG11	1:A:37:PHE:CE2	2.41	0.56
1:A:349:VAL:CG1	3:A:838:HOH:O	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:CE	1:A:415:ASN:O	2.53	0.56
1:A:438:SER:CB	1:A:440:LEU:HD11	2.36	0.56
1:B:274:MET:CE	1:B:429:PHE:HB2	2.36	0.56
2:D:97:PRO:HB2	2:D:109:ILE:HD12	1.88	0.55
1:B:447:GLY:N	1:B:469:VAL:HG13	2.20	0.55
1:B:462:CYS:HB2	1:B:466:LYS:HZ1	1.72	0.55
1:B:15:HIS:CB	1:B:339:MET:HE3	2.20	0.55
1:B:75:ASN:HB2	1:B:77:ASN:OD1	2.06	0.55
2:D:60:VAL:HG12	2:D:63:VAL:HG22	1.87	0.55
1:B:341:SER:HB2	1:B:383:VAL:HG21	1.88	0.55
1:A:22:VAL:HG12	3:A:769:HOH:O	2.08	0.54
1:B:460:ASN:CG	1:B:460:ASN:O	2.44	0.54
2:C:119:VAL:O	2:C:120:SER:HB2	2.07	0.54
1:A:447:GLY:H	1:A:469:VAL:HG23	1.73	0.54
1:B:49:ILE:CD1	1:B:63:GLN:OE1	2.56	0.53
1:A:438:SER:HB2	1:A:440:LEU:HD11	1.89	0.53
1:B:154:PRO:O	1:B:157:VAL:HG22	2.09	0.53
1:B:349:VAL:HG22	1:B:354:VAL:HG13	1.90	0.53
1:A:172:LYS:HD2	3:A:775:HOH:O	2.07	0.53
2:C:12:VAL:HG21	2:C:16:GLY:HA3	1.91	0.53
1:A:458:VAL:HG23	1:A:458:VAL:O	2.08	0.53
1:A:476:GLN:HG3	3:A:722:HOH:O	2.09	0.53
1:B:157:VAL:HG23	1:B:158:ARG:CD	2.39	0.53
1:B:366:VAL:HG23	1:B:366:VAL:O	2.09	0.53
1:B:14:VAL:HG11	1:B:37:PHE:CE2	2.44	0.53
1:A:323:ILE:HG23	1:A:429:PHE:HD2	1.74	0.52
1:A:374:ALA:C	1:A:376:THR:H	2.11	0.52
1:A:476:GLN:CD	3:A:640:HOH:O	2.47	0.52
1:B:200:LYS:HE3	3:B:703:HOH:O	2.08	0.52
2:C:12:VAL:HG22	2:C:13:PRO:N	2.24	0.52
1:B:392:ARG:HD2	3:B:637:HOH:O	2.09	0.52
1:A:157:VAL:CG1	1:A:242:ILE:HD11	2.38	0.52
1:A:469:VAL:O	1:A:469:VAL:HG23	2.09	0.52
1:A:129:VAL:HG13	1:A:178:MET:HG2	1.92	0.52
1:B:449:TYR:CE2	1:B:469:VAL:HG11	2.44	0.51
1:A:349:VAL:O	1:A:349:VAL:CG2	2.57	0.51
1:B:1:GLN:HB3	3:B:731:HOH:O	2.10	0.51
1:A:2:TYR:O	1:A:252:ARG:CD	2.52	0.51
2:C:39:ARG:NH2	2:C:94:TYR:OH	2.43	0.51
1:A:227:ARG:NH2	3:A:713:HOH:O	2.44	0.50
1:A:417:VAL:CG1	1:A:418:ALA:N	2.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:CYS:SG	1:A:496:LEU:HD11	2.52	0.50
1:B:319:ARG:NH2	1:B:319:ARG:HG2	2.23	0.50
1:A:170:LEU:CD2	1:A:202:MET:SD	2.99	0.50
1:A:299:HIS:HE1	3:A:694:HOH:O	1.95	0.50
1:B:11:THR:H	1:B:399:ASN:HD21	1.60	0.49
1:B:15:HIS:HB3	1:B:339:MET:CE	2.23	0.49
2:C:13:PRO:HA	2:C:120:SER:CA	2.42	0.49
1:A:409:TRP:CZ2	1:A:417:VAL:HG11	2.45	0.49
2:C:74:ALA:O	2:C:77:THR:OG1	2.23	0.49
1:A:389:ARG:CD	1:A:453:ILE:O	2.60	0.49
1:A:178:MET:HA	1:A:178:MET:CE	2.41	0.49
1:A:319:ARG:NH2	1:A:319:ARG:HG2	2.26	0.49
1:B:349:VAL:O	1:B:349:VAL:HG23	2.13	0.48
1:A:383:VAL:HG23	1:A:384:CYS:N	2.28	0.48
1:A:484:GLU:CG	1:A:485:ASP:N	2.76	0.48
1:B:435:GLN:HG2	1:B:480:SER:HA	1.95	0.48
1:B:428:VAL:O	1:B:428:VAL:HG13	2.12	0.48
1:A:157:VAL:HG13	1:A:158:ARG:HD2	1.95	0.48
1:A:349:VAL:HG22	1:A:354:VAL:HG13	1.95	0.48
1:A:375:ASP:O	1:A:376:THR:OG1	2.22	0.48
1:B:47:GLU:HG2	1:B:65:VAL:CG2	2.43	0.48
2:D:73:ASN:HD22	2:D:74:ALA:N	2.11	0.48
1:A:409:TRP:CZ2	1:A:417:VAL:CG1	2.97	0.48
1:B:5:GLN:O	1:B:92:ARG:HD2	2.14	0.48
2:D:9:GLY:HA3	2:D:115:THR:CG2	2.44	0.48
1:A:440:LEU:N	1:A:440:LEU:HD12	2.29	0.47
1:A:7:GLN:OE1	1:A:10:ARG:HD2	2.14	0.47
1:B:170:LEU:CD2	1:B:202:MET:SD	3.02	0.47
1:A:153:ASP:HB3	1:A:156:GLN:HG2	1.96	0.47
1:B:154:PRO:C	1:B:157:VAL:HG22	2.34	0.47
1:B:62:TYR:O	1:B:101:HIS:HE1	1.98	0.47
1:B:227:ARG:NE	3:B:691:HOH:O	2.45	0.47
1:A:348:PHE:C	3:A:838:HOH:O	2.52	0.47
1:B:170:LEU:HD21	1:B:202:MET:SD	2.55	0.46
1:B:5:GLN:NE2	1:B:5:GLN:HA	2.24	0.46
1:A:229:PHE:HE2	1:A:252:ARG:CD	2.06	0.46
1:A:237:LEU:N	1:A:237:LEU:HD22	2.30	0.46
1:A:348:PHE:HA	1:A:352:GLU:O	2.15	0.46
1:B:374:ALA:C	1:B:376:THR:H	2.16	0.46
1:B:69:LEU:N	1:B:69:LEU:CD2	2.74	0.46
1:A:476:GLN:CG	3:A:722:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:GLN:HA	3:D:192:HOH:O	2.14	0.46
2:C:73:ASN:OD1	2:C:74:ALA:N	2.48	0.46
1:B:49:ILE:HD13	1:B:103:CYS:HB2	1.97	0.46
1:B:49:ILE:HG23	1:B:103:CYS:HB3	1.96	0.46
1:B:22:VAL:HG13	3:B:591:HOH:O	2.16	0.46
1:B:266:VAL:CG1	1:B:323:ILE:HD11	2.45	0.45
1:A:447:GLY:N	1:A:469:VAL:HG23	2.31	0.45
1:B:279:ASN:N	1:B:279:ASN:HD22	2.09	0.45
1:A:374:ALA:C	1:A:376:THR:N	2.70	0.45
1:A:496:LEU:CD1	1:A:496:LEU:N	2.80	0.45
1:A:349:VAL:HG22	1:A:354:VAL:CG1	2.46	0.45
1:A:31:TYR:OH	1:A:392:ARG:HG3	2.16	0.45
1:B:262:LEU:HD13	1:B:324:ALA:HB1	1.99	0.45
1:B:28:CYS:HA	1:B:32:LEU:HB2	1.98	0.45
2:D:104:PRO:HG2	3:D:243:HOH:O	2.17	0.45
1:B:447:GLY:N	1:B:469:VAL:CG1	2.80	0.45
1:A:319:ARG:HD2	3:A:809:HOH:O	2.17	0.45
1:A:7:GLN:HB3	1:A:10:ARG:HD3	1.98	0.45
1:B:9:GLY:HA2	3:B:729:HOH:O	2.16	0.45
1:A:154:PRO:CA	1:A:157:VAL:HG12	2.45	0.45
2:D:88:ASP:C	2:D:88:ASP:OD1	2.55	0.45
1:B:354:VAL:HA	3:B:954:HOH:O	2.17	0.44
1:A:211:LEU:H	1:A:211:LEU:CD1	2.30	0.44
1:B:320:LEU:CA	1:B:323:ILE:HG12	2.46	0.44
1:A:216:ASN:OD1	1:A:227:ARG:HD2	2.18	0.44
1:A:440:LEU:CD1	1:A:440:LEU:N	2.80	0.44
1:B:15:HIS:HD2	3:B:671:HOH:O	2.00	0.44
1:A:1:GLN:NE2	3:A:633:HOH:O	2.51	0.44
1:B:107:ALA:HB3	1:B:121:PRO:HG2	2.00	0.44
1:B:14:VAL:CG1	1:B:37:PHE:CE2	3.01	0.44
1:B:72:ARG:HD3	3:B:566:HOH:O	2.16	0.44
1:B:63:GLN:HG2	1:B:165:LEU:CD2	2.47	0.43
1:B:409:TRP:CZ2	1:B:417:VAL:CG1	3.01	0.43
1:B:462:CYS:HB2	1:B:466:LYS:NZ	2.33	0.43
1:A:211:LEU:CD1	1:A:211:LEU:N	2.81	0.43
1:A:22:VAL:HG11	3:A:944:HOH:O	2.18	0.43
1:A:323:ILE:CD1	1:A:486:PRO:HG2	2.45	0.43
1:B:428:VAL:CG1	1:B:488:ILE:HB	2.48	0.43
1:A:347:ASN:C	3:A:838:HOH:O	2.55	0.43
1:A:435:GLN:HG2	3:A:940:HOH:O	2.18	0.43
1:A:9:GLY:HA2	3:A:818:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:VAL:O	1:B:469:VAL:HG13	2.17	0.43
1:A:468:TYR:C	1:A:468:TYR:CD1	2.90	0.43
1:A:484:GLU:CG	1:A:485:ASP:H	2.31	0.43
2:C:6:GLU:OE2	2:C:95:CYS:HB3	2.18	0.43
1:B:355:ASN:HB3	1:B:358:ILE:HD12	2.00	0.43
1:A:170:LEU:HD21	1:A:202:MET:SD	2.59	0.43
1:B:417:VAL:CG1	1:B:418:ALA:N	2.82	0.43
2:D:12:VAL:HG21	2:D:18:LEU:HG	2.01	0.42
1:B:69:LEU:HD21	1:B:185:LYS:NZ	2.34	0.42
2:C:73:ASN:OD1	2:C:77:THR:HG21	2.19	0.42
1:A:383:VAL:HG21	1:A:385:GLU:OE2	2.16	0.42
1:B:409:TRP:CZ3	1:B:417:VAL:HG11	2.52	0.42
1:B:435:GLN:HE21	1:B:435:GLN:HB3	1.52	0.42
1:B:449:TYR:HE2	1:B:469:VAL:CG1	2.29	0.42
1:B:162:LEU:HD22	1:B:163:VAL:HG13	2.02	0.42
1:B:339:MET:HA	1:B:339:MET:CE	2.49	0.42
1:A:120:ASN:HB3	1:A:125:GLU:HB2	2.00	0.42
2:D:53:ASN:HA	2:D:53:ASN:HD22	1.55	0.42
1:A:211:LEU:H	1:A:211:LEU:HD12	1.85	0.42
1:A:329:LEU:N	1:A:329:LEU:HD22	2.35	0.42
1:A:11:THR:H	1:A:399:ASN:HD21	1.67	0.42
1:B:49:ILE:HD11	3:B:817:HOH:O	2.18	0.42
1:A:14:VAL:CG1	1:A:37:PHE:CE2	3.02	0.41
1:A:450:CYS:SG	1:A:496:LEU:HD11	2.60	0.41
1:B:49:ILE:CG2	1:B:65:VAL:CG1	2.95	0.41
1:A:438:SER:HB3	1:A:440:LEU:HD11	2.01	0.41
1:B:409:TRP:CZ2	1:B:417:VAL:HG13	2.56	0.41
2:C:12:VAL:CG2	2:C:16:GLY:HA3	2.50	0.41
1:A:101:HIS:CE1	1:A:165:LEU:HD13	2.55	0.41
1:B:320:LEU:CA	1:B:323:ILE:CG1	2.99	0.41
1:A:319:ARG:CG	1:A:319:ARG:HH21	2.21	0.41
1:B:458:VAL:CG2	1:B:458:VAL:O	2.65	0.41
1:B:49:ILE:HG21	1:B:103:CYS:SG	2.61	0.41
1:A:5:GLN:HA	1:A:5:GLN:NE2	2.28	0.41
1:B:63:GLN:HG2	1:B:165:LEU:HD21	2.03	0.40
1:B:49:ILE:HG22	1:B:65:VAL:HG11	2.02	0.40
1:B:7:GLN:OE1	1:B:10:ARG:HD2	2.20	0.40
1:A:207:ILE:C	1:A:211:LEU:HD13	2.35	0.40
1:A:402:ASP:HA	3:A:652:HOH:O	2.20	0.40
1:B:266:VAL:HG11	1:B:323:ILE:CD1	2.50	0.40
1:B:69:LEU:H	1:B:69:LEU:CD2	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:OD1	1:A:77:ASN:OD1	2.39	0.40
1:B:320:LEU:CD1	1:B:320:LEU:N	2.83	0.40
1:A:355:ASN:HB3	1:A:358:ILE:HD12	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	
1	A	494/496 (100%)	482 (98%)	12 (2%)	0	100	100
1	B	494/496 (100%)	480 (97%)	13 (3%)	1 (0%)	47	26
2	C	117/121 (97%)	112 (96%)	5 (4%)	0	100	100
2	D	119/121 (98%)	114 (96%)	4 (3%)	1 (1%)	19	6
All	All	1224/1234 (99%)	1188 (97%)	34 (3%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	ALA
2	D	9	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	
1	A	411/413 (100%)	391 (95%)	20 (5%)	25	6
1	B	410/413 (99%)	388 (95%)	22 (5%)	22	5
2	C	95/97 (98%)	91 (96%)	4 (4%)	30	9
2	D	97/97 (100%)	88 (91%)	9 (9%)	9	1
All	All	1013/1020 (99%)	958 (95%)	55 (5%)	22	5

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

Mol	Chain	Res	Type
1	A	1	GLN
1	A	5	GLN
1	A	35	LYS
1	A	69	LEU
1	A	77	ASN
1	A	92	ARG
1	A	115	CYS
1	A	162	LEU
1	A	168	LEU
1	A	178	MET
1	A	186	LEU
1	A	262	LEU
1	A	279	ASN
1	A	293	LEU
1	A	319	ARG
1	A	320	LEU
1	A	395	VAL
1	A	421	ARG
1	A	444	LEU
1	A	484	GLU
1	B	1	GLN
1	B	5	GLN
1	B	77	ASN
1	B	92	ARG
1	B	115	CYS
1	B	162	LEU
1	B	168	LEU
1	B	186	LEU
1	B	211	LEU
1	B	227	ARG
1	B	262	LEU
1	B	279	ASN
1	B	293	LEU

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Mol	Chain	Res	Type
1	B	305	HIS
1	B	319	ARG
1	B	329	LEU
1	B	375	ASP
1	B	435	GLN
1	B	440	LEU
1	B	444	LEU
1	B	460	ASN
1	B	484	GLU
2	C	27	ASN
2	C	35	SER
2	C	36	TRP
2	C	88	ASP
2	D	12	VAL
2	D	18	LEU
2	D	36	TRP
2	D	39	ARG
2	D	41	PRO
2	D	70	SER
2	D	73	ASN
2	D	92	MET
2	D	115	THR

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	15	HIS
1	A	101	HIS
1	A	161	GLN
1	A	201	HIS
1	A	279	ASN
1	A	299	HIS
1	A	350	ASN
1	A	364	ASN
1	A	399	ASN
1	B	1	GLN
1	B	5	GLN
1	B	15	HIS
1	B	75	ASN
1	B	101	HIS
1	B	161	GLN

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Mol	Chain	Res	Type
1	B	201	HIS
1	B	279	ASN
1	B	299	HIS
1	B	350	ASN
1	B	399	ASN
1	B	435	GLN
1	B	476	GLN
2	C	27	ASN
2	C	81	GLN
2	D	53	ASN
2	D	73	ASN
2	D	81	GLN

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](#)

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
2	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1:GLN	C	2:VAL	N	1.18
1	D	8:GLY	C	9:GLY	N	0.90

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.