



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:48 PM UTC

PDB ID : 1KW2 / pdb_00001kw2
Title : CRYSTAL STRUCTURE OF UNCOMPLEXED VITAMIN D-BINDING PROTEIN
Authors : Otterbein, L.R.; Dominguez, R.
Deposited on : 2002-01-28
Resolution : 2.15 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
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

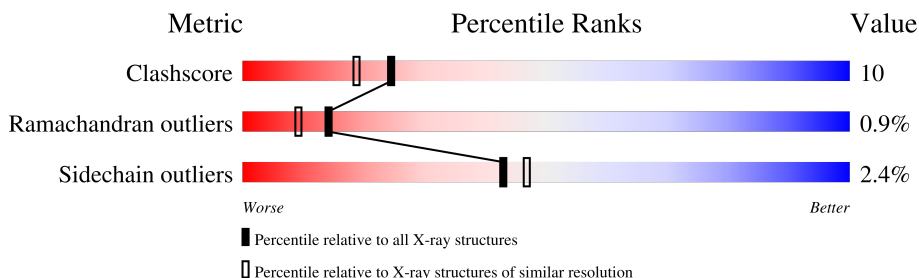
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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	458	 77% 20% ..
1	B	458	 77% 20% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7408 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 Vitamin D-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3547	2224	577	711	35			
1	B	453	Total	C	N	O	S	0	0	0
			3528	2213	571	709	35			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	149	Total	O	0	0
			149	149		
2	B	184	Total	O	0	0
			184	184		

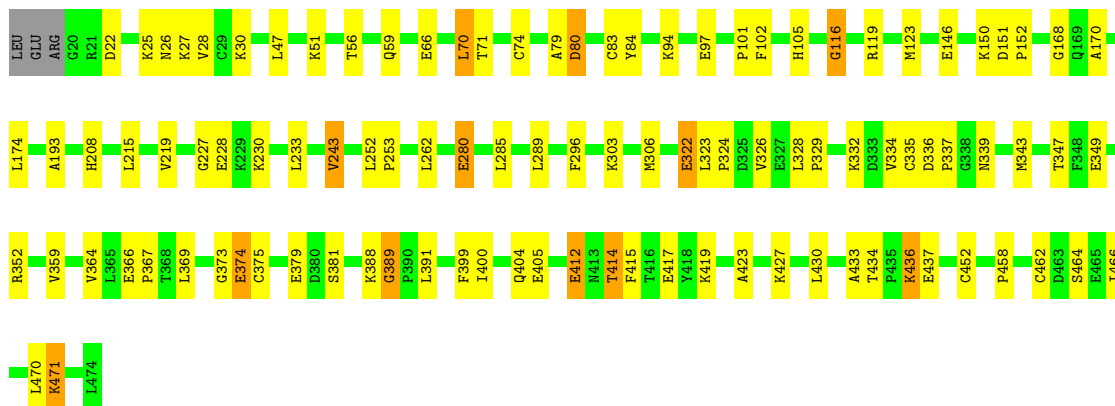
3 Residue-property plots

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.

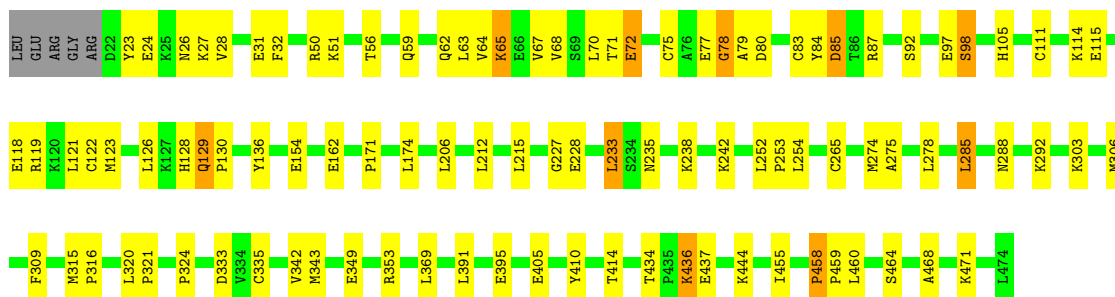
• Molecule 1: Vitamin D-binding protein

Chain A:  77% 20% ..



• Molecule 1: Vitamin D-binding protein

Chain B:  77% 20% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	133.93Å 133.93Å 73.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.15	Depositor
% Data completeness (in resolution range)	94.9 (60.00-2.15)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7408	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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	0.38	0/3614	0.87	13/4886 (0.3%)
1	B	0.40	0/3595	0.89	11/4863 (0.2%)
All	All	0.39	0/7209	0.88	24/9749 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	GLY	N-CA-C	-8.69	101.73	112.68
1	A	289	LEU	N-CA-C	7.38	123.31	113.72
1	B	335	CYS	N-CA-C	7.36	122.09	113.18
1	B	228	GLU	N-CA-C	7.11	119.65	111.11
1	A	227	GLY	N-CA-C	-7.00	103.86	112.68
1	A	303	LYS	N-CA-C	6.52	118.47	111.36
1	A	228	GLU	N-CA-C	6.47	118.88	111.11
1	A	458	PRO	CA-C-N	5.70	124.90	118.97
1	A	458	PRO	C-N-CA	5.70	124.90	118.97
1	B	265	CYS	N-CA-C	5.61	120.82	113.30
1	B	410	TYR	N-CA-C	5.58	117.04	111.07
1	A	414	THR	N-CA-C	-5.56	103.58	110.41
1	B	85	ASP	N-CA-C	-5.54	107.77	114.75
1	A	170	ALA	N-CA-C	-5.42	102.39	110.20
1	A	193	ALA	N-CA-C	-5.24	106.39	112.89
1	A	168	GLY	N-CA-C	5.22	120.20	114.40
1	A	452	CYS	N-CA-C	5.18	119.15	112.41
1	B	303	LYS	N-CA-C	5.16	116.90	111.28
1	B	414	THR	N-CA-C	-5.14	103.61	110.55
1	B	288	ASN	N-CA-C	5.12	118.68	112.23
1	A	430	LEU	CA-C-N	5.10	124.89	119.28
1	A	430	LEU	C-N-CA	5.10	124.89	119.28
1	B	458	PRO	CA-C-N	5.04	126.14	119.84
1	B	458	PRO	C-N-CA	5.04	126.14	119.84

There are no chirality outliers.

There are no planarity outliers.

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	3547	0	3481	77	0
1	B	3528	0	3454	63	0
2	A	149	0	0	3	0
2	B	184	0	0	2	0
All	All	7408	0	6935	138	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 10.

All (138) 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:332:LYS:HE2	1:A:381:SER:HB2	1.40	1.02
1:B:436:LYS:HE3	1:B:436:LYS:HA	1.48	0.93
1:B:343:MET:HE3	1:B:369:LEU:HD13	1.59	0.84
1:A:366:GLU:HB3	1:A:367:PRO:HD3	1.61	0.83
1:A:414:THR:HG23	1:A:417:GLU:H	1.47	0.80
1:A:243:VAL:HG22	1:A:296:PHE:CE1	2.18	0.78
1:A:94:LYS:HE2	1:A:101:PRO:HG3	1.69	0.75
1:A:94:LYS:O	1:A:97:GLU:HG2	1.87	0.73
1:B:436:LYS:HE3	1:B:436:LYS:CA	2.20	0.71
1:B:92:SER:HB3	1:B:123:MET:HE1	1.73	0.71
1:A:334:VAL:O	1:A:334:VAL:HG12	1.91	0.70
1:A:219:VAL:HG11	1:A:262:LEU:HD21	1.74	0.70
1:A:343:MET:SD	1:A:369:LEU:HD22	2.32	0.69
1:A:436:LYS:HE3	1:A:436:LYS:HA	1.73	0.69
1:A:252:LEU:HB3	1:A:253:PRO:HD3	1.75	0.69
1:B:254:LEU:HD13	1:B:285:LEU:HD12	1.74	0.69
1:B:83:CYS:C	1:B:85:ASP:H	2.00	0.68
1:A:27:LYS:HA	1:A:30:LYS:HE2	1.76	0.68
1:A:323:LEU:HD12	1:A:352:ARG:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:O	1:B:67:VAL:HG23	1.96	0.65
1:B:70:LEU:HD22	1:B:87:ARG:HB3	1.78	0.65
1:A:25:LYS:HG2	1:A:84:TYR:CD2	2.32	0.65
1:A:412:GLU:H	1:A:412:GLU:CD	2.06	0.64
1:B:83:CYS:SG	1:B:87:ARG:HD3	2.39	0.62
1:B:212:LEU:HD21	1:B:275:ALA:HB2	1.82	0.62
1:A:219:VAL:CG1	1:A:262:LEU:HD21	2.30	0.60
1:A:70:LEU:C	1:A:70:LEU:HD12	2.28	0.59
1:A:243:VAL:HG22	1:A:296:PHE:HE1	1.66	0.59
1:B:24:GLU:O	1:B:28:VAL:HG23	2.02	0.59
1:A:215:LEU:C	1:A:215:LEU:HD23	2.27	0.59
1:A:349:GLU:HA	1:A:352:ARG:HD2	1.85	0.58
1:B:242:LYS:HE2	1:B:315:MET:O	2.05	0.57
1:B:391:LEU:O	1:B:395:GLU:HG3	2.05	0.57
1:B:215:LEU:HD21	1:B:309:PHE:CD2	2.41	0.56
1:B:171:PRO:HD2	1:B:174:LEU:HD12	1.88	0.56
1:A:433:ALA:HA	1:A:437:GLU:OE1	2.06	0.56
1:B:434:THR:OG1	1:B:437:GLU:HG3	2.06	0.56
1:A:56:THR:OG1	1:A:59:GLN:HG3	2.06	0.55
1:B:333:ASP:HB3	1:B:342:VAL:HG21	1.88	0.55
1:A:471:LYS:HB3	1:A:471:LYS:NZ	2.21	0.55
1:A:47:LEU:C	1:A:47:LEU:HD23	2.32	0.54
1:B:97:GLU:HG2	1:B:98:SER:N	2.22	0.54
1:B:115:GLU:O	1:B:118:GLU:HB2	2.07	0.54
1:B:324:PRO:O	1:B:353:ARG:NH1	2.39	0.54
1:A:335:CYS:O	1:A:337:PRO:HD3	2.08	0.53
1:B:119:ARG:HG2	1:B:123:MET:HE2	1.89	0.53
1:A:373:GLY:C	1:A:375:CYS:H	2.17	0.53
1:B:252:LEU:HB3	1:B:253:PRO:HD3	1.89	0.53
1:A:399:PHE:CE1	1:A:470:LEU:HD11	2.43	0.53
1:B:27:LYS:O	1:B:31:GLU:HG2	2.09	0.52
1:A:336:ASP:HB2	1:A:339:ASN:HB3	1.91	0.52
1:B:114:LYS:O	1:B:119:ARG:HB2	2.10	0.52
1:A:334:VAL:HG11	1:A:343:MET:SD	2.50	0.51
1:A:322:GLU:HA	1:A:322:GLU:OE1	2.11	0.51
1:B:83:CYS:O	1:B:85:ASP:N	2.43	0.51
1:B:121:LEU:C	1:B:121:LEU:HD23	2.35	0.50
1:A:146:GLU:O	1:A:150:LYS:HG3	2.12	0.50
1:A:22:ASP:CG	1:A:25:LYS:HD2	2.37	0.49
1:B:56:THR:OG1	1:B:59:GLN:HG3	2.12	0.49
1:A:79:ALA:O	1:A:80:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HE2	2:A:610:HOH:O	2.13	0.48
1:B:306:MET:HA	1:B:306:MET:HE2	1.95	0.48
1:B:468:ALA:HA	1:B:471:LYS:HE2	1.96	0.48
1:B:65:LYS:NZ	1:B:65:LYS:HB2	2.28	0.48
1:A:119:ARG:HD2	1:A:123:MET:HE2	1.97	0.47
1:B:83:CYS:C	1:B:85:ASP:N	2.67	0.47
1:A:219:VAL:HG12	1:A:262:LEU:CD2	2.44	0.47
1:A:415:PHE:CE2	1:A:419:LYS:HE3	2.49	0.47
1:A:233:LEU:HD11	1:A:347:THR:HG21	1.97	0.47
1:A:388:LYS:O	1:A:389:GLY:C	2.57	0.47
1:B:62:GLN:O	1:B:65:LYS:HB3	2.14	0.46
1:B:71:THR:O	1:B:75:CYS:SG	2.74	0.46
1:A:379:GLU:HB2	1:B:126:LEU:O	2.16	0.46
1:A:233:LEU:CD1	1:A:347:THR:HG21	2.46	0.46
1:B:64:VAL:O	1:B:68:VAL:HG23	2.15	0.46
1:A:208:HIS:CE1	1:A:306:MET:HE2	2.51	0.46
1:B:444:LYS:HB3	2:B:658:HOH:O	2.15	0.46
1:B:458:PRO:HA	1:B:459:PRO:HD3	1.80	0.46
1:B:349:GLU:OE1	1:B:353:ARG:NH2	2.48	0.45
1:A:323:LEU:HB3	1:A:324:PRO:CD	2.46	0.45
1:B:235:ASN:ND2	2:B:508:HOH:O	2.44	0.45
1:A:208:HIS:ND1	1:A:306:MET:HE2	2.31	0.45
1:A:359:VAL:HG21	1:A:462:CYS:HB2	1.97	0.45
1:A:219:VAL:CG1	1:A:262:LEU:CD2	2.95	0.45
1:A:285:LEU:C	1:A:285:LEU:HD23	2.42	0.45
1:A:433:ALA:HB1	1:A:437:GLU:HG3	1.97	0.45
1:A:334:VAL:O	1:A:334:VAL:CG1	2.63	0.45
1:B:238:LYS:HE2	1:B:455:ILE:O	2.16	0.45
1:A:27:LYS:O	1:A:30:LYS:HG2	2.16	0.45
1:B:292:LYS:HA	1:B:292:LYS:HD3	1.80	0.45
1:B:50:ARG:O	1:B:128:HIS:CE1	2.70	0.45
1:B:111:CYS:SG	1:B:122:CYS:C	3.00	0.45
1:A:51:LYS:O	1:A:105:HIS:HE1	2.00	0.44
1:A:219:VAL:HG13	2:A:488:HOH:O	2.17	0.44
1:A:332:LYS:HE2	1:A:381:SER:CB	2.29	0.44
1:A:334:VAL:HG13	1:A:343:MET:HG2	1.98	0.44
1:A:434:THR:OG1	1:A:437:GLU:HG2	2.17	0.44
1:A:70:LEU:HD12	1:A:71:THR:N	2.32	0.44
1:A:326:VAL:HG21	1:A:349:GLU:HB3	1.99	0.44
1:A:399:PHE:HE1	1:A:470:LEU:HD11	1.83	0.43
1:A:116:GLY:O	1:A:119:ARG:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:HA	1:B:321:PRO:HD3	1.89	0.43
1:B:343:MET:HE3	1:B:369:LEU:HB3	2.01	0.43
1:A:423:ALA:O	1:A:427:LYS:HG3	2.19	0.43
1:A:243:VAL:CG2	1:A:296:PHE:CE1	2.95	0.43
1:A:280:GLU:HB3	2:A:554:HOH:O	2.18	0.43
1:B:343:MET:HG2	1:B:369:LEU:HD22	2.00	0.43
1:A:74:CYS:SG	1:A:83:CYS:C	3.01	0.43
1:A:366:GLU:HB3	1:A:367:PRO:CD	2.40	0.43
1:A:412:GLU:CD	1:A:412:GLU:N	2.75	0.43
1:B:77:GLU:O	1:B:78:GLY:C	2.62	0.43
1:A:388:LYS:HA	1:A:391:LEU:HD12	2.01	0.42
1:A:400:ILE:O	1:A:404:GLN:HG3	2.19	0.42
1:B:136:TYR:HD1	1:B:162:GLU:HG2	1.83	0.42
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.89	0.42
1:B:274:MET:HG3	1:B:278:LEU:HD11	2.01	0.42
1:B:130:PRO:HD2	1:B:460:LEU:CD1	2.49	0.42
1:B:333:ASP:CB	1:B:342:VAL:HG21	2.50	0.42
1:B:436:LYS:HA	1:B:436:LYS:CE	2.35	0.42
1:A:66:GLU:CD	1:A:102:PHE:HZ	2.27	0.42
1:A:334:VAL:CG1	1:A:343:MET:SD	3.08	0.42
1:A:434:THR:H	1:A:437:GLU:CD	2.27	0.42
1:B:79:ALA:O	1:B:80:ASP:C	2.63	0.42
1:A:364:VAL:HB	1:A:399:PHE:CE2	2.55	0.41
1:B:51:LYS:O	1:B:105:HIS:HE1	2.03	0.41
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.90	0.41
1:A:466:ILE:O	1:A:470:LEU:HG	2.21	0.41
1:B:212:LEU:CD2	1:B:275:ALA:HB2	2.49	0.41
1:B:306:MET:HE2	1:B:306:MET:CA	2.51	0.41
1:B:315:MET:HA	1:B:316:PRO:HD3	1.84	0.41
1:B:23:TYR:HA	1:B:26:ASN:HD22	1.84	0.41
1:B:119:ARG:C	1:B:121:LEU:H	2.28	0.41
1:A:28:VAL:HG12	1:A:71:THR:HG23	2.03	0.41
1:A:151:ASP:HA	1:A:152:PRO:HD2	1.95	0.41
1:A:391:LEU:CD1	1:B:121:LEU:HD12	2.51	0.40
1:B:32:PHE:CE2	1:B:72:GLU:HA	2.56	0.40
1:A:22:ASP:O	1:A:26:ASN:ND2	2.55	0.40
1:B:129:GLN:H	1:B:129:GLN:HG2	1.73	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	453/458 (99%)	435 (96%)	14 (3%)	4 (1%)	14	9
1	B	451/458 (98%)	429 (95%)	18 (4%)	4 (1%)	14	9
All	All	904/916 (99%)	864 (96%)	32 (4%)	8 (1%)	14	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY
1	B	72	GLU
1	B	78	GLY
1	B	84	TYR
1	A	374	GLU
1	B	98	SER
1	A	389	GLY
1	A	80	ASP

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	412/415 (99%)	401 (97%)	11 (3%)	39	41
1	B	410/415 (99%)	401 (98%)	9 (2%)	45	51
All	All	822/830 (99%)	802 (98%)	20 (2%)	43	47

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	174	LEU
1	A	243	VAL
1	A	280	GLU
1	A	322	GLU
1	A	374	GLU
1	A	405	GLU
1	A	412	GLU
1	A	436	LYS
1	A	464	SER
1	A	471	LYS
1	B	65	LYS
1	B	129	GLN
1	B	154	GLU
1	B	206	LEU
1	B	233	LEU
1	B	285	LEU
1	B	405	GLU
1	B	436	LYS
1	B	464	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	99	ASN
1	A	105	HIS
1	A	169	GLN
1	A	205	GLN
1	A	241	GLN
1	A	260	ASN
1	A	386	ASN
1	B	26	ASN
1	B	34	HIS
1	B	105	HIS
1	B	128	HIS
1	B	157	ASN
1	B	169	GLN
1	B	222	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 oligosaccharides 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](#)

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.