



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:15 PM UTC

PDB ID : 1QAT / pdb_00001qat
Title : 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODI-
ESTERASE DELTA COMPLEX WITH SAMARIUM (III) CHLORIDE
Authors : Grobler, J.A.; Hurley, J.H.
Deposited on : 1996-08-02
Resolution : 3.00 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
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

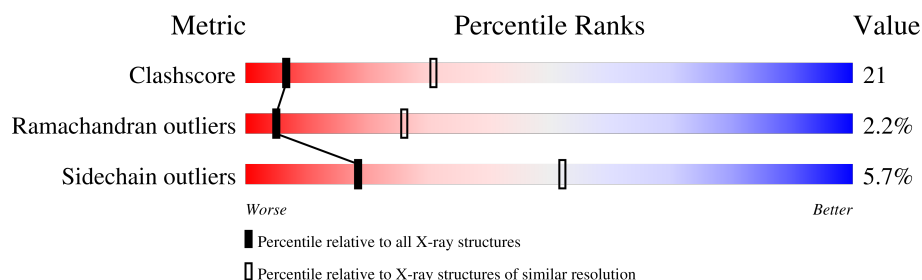
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	622	
1	B	622	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8022 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 PHOSPHOLIPASE C DELTA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4018	2536	704	756	22			
1	B	507	Total	C	N	O	S	0	0	0
			3999	2526	701	750	22			

- Molecule 2 is SAMARIUM (III) ION (CCD ID: SM) (formula: Sm).

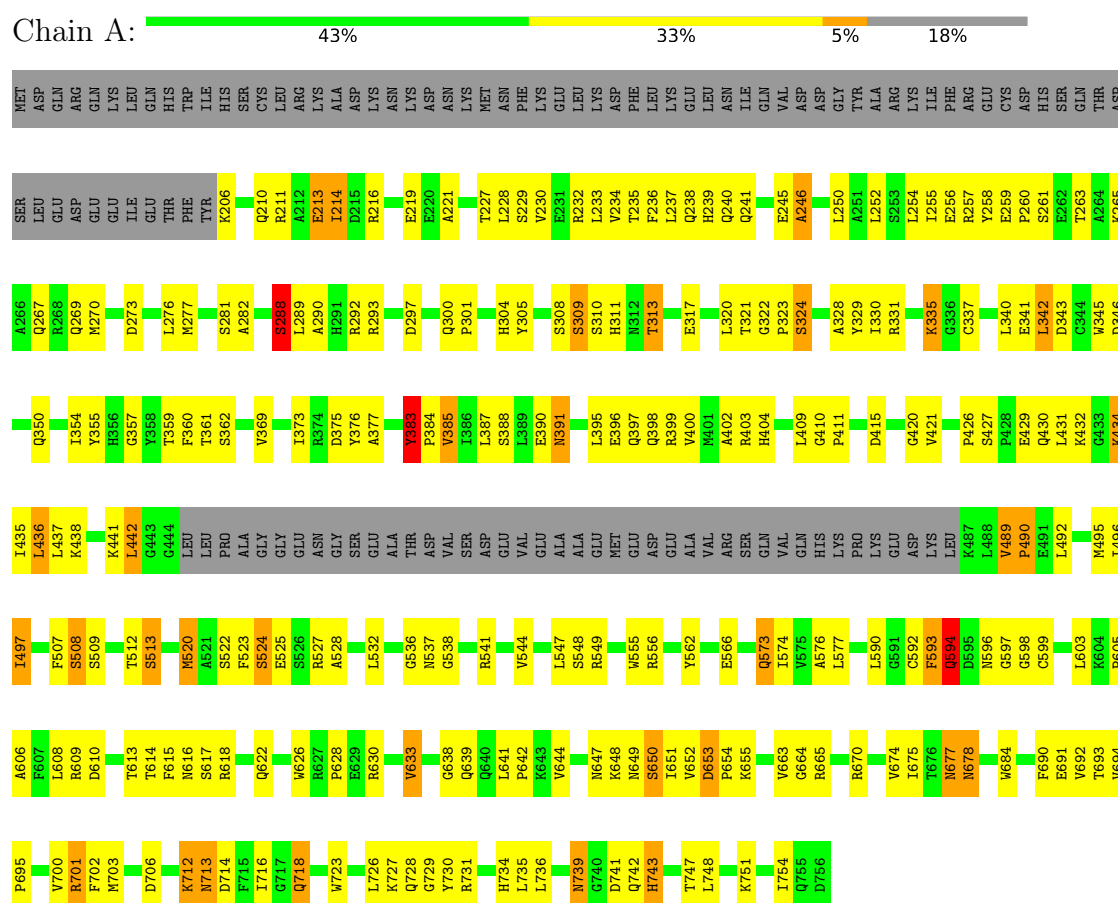
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Sm	0	0
			2	2		
2	B	3	Total	Sm	0	0
			3	3		

3 Residue-property plots

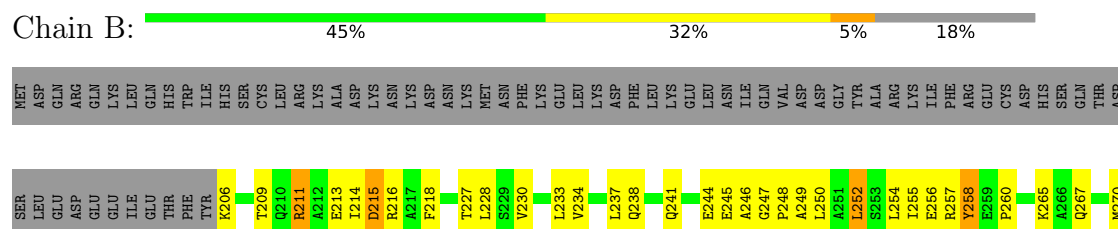
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PHOSPHOLIPASE C DELTA-1



• Molecule 1: PHOSPHOLIPASE C DELTA-1





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	61.60Å 75.10Å 86.40Å 66.40° 85.60° 89.80°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8022	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: SM

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	0.57	0/4111	1.10	32/5568 (0.6%)
1	B	0.56	0/4090	1.10	29/5539 (0.5%)
All	All	0.57	0/8201	1.10	61/11107 (0.5%)

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
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	649	ASN	N-CA-C	9.51	124.02	110.23
1	B	309	SER	N-CA-C	8.59	123.41	109.40
1	A	309	SER	N-CA-C	8.33	122.98	109.40
1	A	489	VAL	N-CA-C	7.96	115.48	108.63
1	A	497	ILE	N-CA-C	7.03	117.60	111.56
1	B	383	TYR	CA-C-N	7.01	127.05	119.90
1	B	383	TYR	C-N-CA	7.01	127.05	119.90
1	B	244	GLU	N-CA-C	-6.93	101.92	110.65
1	B	573	GLN	N-CA-C	6.80	121.90	112.45
1	B	594	GLN	N-CA-C	-6.79	104.47	112.89
1	B	497	ILE	N-CA-C	6.68	117.31	111.56
1	A	694	VAL	CA-C-N	6.64	126.42	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	694	VAL	C-N-CA	6.64	126.42	119.05
1	A	331	ARG	CD-NE-CZ	6.56	133.59	124.40
1	A	594	GLN	N-CA-C	-6.56	104.76	112.89
1	A	331	ARG	NE-CZ-NH2	-6.48	113.36	119.20
1	A	653	ASP	CA-C-N	6.47	126.39	119.85
1	A	653	ASP	C-N-CA	6.47	126.39	119.85
1	A	383	TYR	CA-C-N	6.47	126.50	119.90
1	A	383	TYR	C-N-CA	6.47	126.50	119.90
1	B	398	GLN	N-CA-C	-6.46	104.32	111.36
1	B	653	ASP	CA-C-N	6.35	126.26	119.85
1	B	653	ASP	C-N-CA	6.35	126.26	119.85
1	A	573	GLN	N-CA-C	6.33	121.25	112.45
1	A	335	LYS	N-CA-C	-6.32	105.44	113.02
1	B	331	ARG	CD-NE-CZ	6.32	133.24	124.40
1	A	398	GLN	N-CA-C	-6.20	104.62	111.82
1	B	538	GLY	N-CA-C	-6.05	105.02	112.77
1	A	538	GLY	N-CA-C	-6.04	105.04	112.77
1	A	524	SER	N-CA-C	-6.03	102.41	110.55
1	B	258	TYR	N-CA-C	5.99	120.32	112.89
1	A	331	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	B	743	HIS	CA-C-N	5.93	125.41	119.24
1	B	743	HIS	C-N-CA	5.93	125.41	119.24
1	A	513	SER	N-CA-C	5.88	123.31	110.80
1	B	694	VAL	CA-C-N	5.86	125.56	119.05
1	B	694	VAL	C-N-CA	5.86	125.56	119.05
1	A	391	ASN	N-CA-C	5.72	118.86	109.76
1	B	331	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	B	335	LYS	N-CA-C	-5.70	106.17	113.02
1	A	593	PHE	N-CA-C	5.58	119.95	113.20
1	B	215	ASP	N-CA-C	-5.55	105.31	111.36
1	B	520	MET	N-CA-C	5.54	117.39	107.80
1	B	544	VAL	CB-CA-C	-5.50	104.94	111.97
1	B	391	ASN	N-CA-C	5.49	118.48	109.76
1	A	743	HIS	CA-C-N	5.48	124.94	119.24
1	A	743	HIS	C-N-CA	5.48	124.94	119.24
1	B	324	SER	N-CA-C	-5.33	100.71	109.40
1	A	324	SER	N-CA-C	-5.31	100.74	109.40
1	B	593	PHE	N-CA-C	5.28	119.59	113.20
1	A	442	LEU	N-CA-C	5.27	122.03	110.80
1	B	639	GLN	N-CA-C	5.22	117.67	108.75
1	B	644	VAL	N-CA-C	5.18	120.12	109.34
1	A	520	MET	N-CA-C	5.17	116.75	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	617	SER	N-CA-C	5.16	118.36	111.75
1	A	544	VAL	CB-CA-C	-5.13	105.40	111.97
1	B	375	ASP	N-CA-C	5.12	116.54	111.07
1	A	617	SER	N-CA-C	5.09	118.26	111.75
1	A	375	ASP	N-CA-C	5.07	116.50	111.07
1	A	735	LEU	N-CA-C	5.07	117.01	109.25
1	A	701	ARG	N-CA-C	5.03	116.89	107.99

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	TYR	Sidechain
1	B	305	TYR	Sidechain
1	B	383	TYR	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	4018	0	3941	172	0
1	B	3999	0	3916	171	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
All	All	8022	0	7857	341	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 21.

All (341) 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:206:LYS:HA	1:A:210:GLN:HG3	1.49	0.93
1:A:438:LYS:HE3	1:A:520:MET:HE2	1.59	0.85
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LYS:HE3	1:B:520:MET:HE2	1.61	0.83
1:A:537:ASN:HD22	1:A:614:THR:HA	1.43	0.81
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.62	0.81
1:B:537:ASN:HD22	1:B:614:THR:HA	1.46	0.79
1:B:206:LYS:HA	1:B:209:THR:OG1	1.83	0.78
1:B:241:GLN:HE22	1:B:730:TYR:H	1.32	0.78
1:A:211:ARG:HB2	1:A:214:ILE:HB	1.65	0.76
1:B:309:SER:OG	1:B:574:ILE:HG23	1.86	0.76
1:A:350:GLN:HE22	1:A:396:GLU:HG3	1.52	0.75
1:B:350:GLN:HE22	1:B:396:GLU:HG3	1.52	0.74
1:B:648:LYS:HE2	1:B:648:LYS:HA	1.70	0.73
1:B:442:LEU:HG	1:B:488:LEU:HD23	1.69	0.72
1:B:245:GLU:HA	1:B:250:LEU:HD22	1.69	0.72
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.36	0.72
1:B:548:SER:H	1:B:573:GLN:HE21	1.38	0.71
1:B:289:LEU:HD12	1:B:292:ARG:HG3	1.73	0.71
1:B:335:LYS:HD3	1:B:590:LEU:HD11	1.71	0.71
1:A:230:VAL:O	1:A:234:VAL:HG23	1.90	0.71
1:B:644:VAL:CG1	1:B:716:ILE:HG12	2.19	0.70
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.72	0.69
1:A:335:LYS:HD3	1:A:590:LEU:HD11	1.74	0.69
1:B:211:ARG:NH1	1:B:276:LEU:HD11	2.07	0.69
1:B:566:GLU:HG2	1:B:618:ARG:HH21	1.56	0.69
1:B:321:THR:HG22	1:B:360:PHE:HB2	1.72	0.69
1:A:385:VAL:HG22	1:A:435:ILE:HG12	1.75	0.68
1:B:644:VAL:HG12	1:B:716:ILE:HG12	1.74	0.68
1:A:309:SER:OG	1:A:574:ILE:HG23	1.92	0.68
1:B:644:VAL:HG11	1:B:706:ASP:HB2	1.76	0.68
1:B:734:HIS:HA	1:B:747:THR:HG22	1.74	0.68
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.24	0.68
1:A:228:LEU:HB2	1:A:270:MET:HB3	1.76	0.68
1:B:610:ASP:HB3	1:B:613:THR:HB	1.76	0.68
1:A:536:GLY:HA3	1:A:616:ASN:HD22	1.59	0.67
1:B:399:ARG:O	1:B:403:ARG:HG2	1.95	0.67
1:B:385:VAL:HG22	1:B:435:ILE:HG12	1.77	0.67
1:A:610:ASP:HB3	1:A:613:THR:HB	1.77	0.67
1:B:605:PRO:HD2	1:B:608:LEU:HD12	1.76	0.67
1:A:701:ARG:HE	1:A:718:GLN:HE21	1.42	0.66
1:A:548:SER:H	1:A:573:GLN:HE21	1.43	0.66
1:A:566:GLU:HG2	1:A:618:ARG:HH21	1.61	0.65
1:B:652:VAL:O	1:B:677:ASN:HA	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:HB3	1:A:246:ALA:HB3	1.79	0.65
1:B:536:GLY:HA3	1:B:616:ASN:HD22	1.61	0.65
1:A:395:LEU:O	1:A:399:ARG:HG3	1.97	0.64
1:A:399:ARG:O	1:A:403:ARG:HG2	1.98	0.64
1:A:734:HIS:HA	1:A:747:THR:HG22	1.78	0.64
1:B:324:SER:H	1:B:362:SER:HB3	1.62	0.64
1:A:324:SER:H	1:A:362:SER:HB3	1.61	0.64
1:B:395:LEU:O	1:B:399:ARG:HG3	1.98	0.64
1:B:652:VAL:HG12	1:B:653:ASP:N	2.13	0.64
1:B:703:MET:HG2	1:B:718:GLN:HB3	1.79	0.64
1:A:605:PRO:HD2	1:A:608:LEU:HD12	1.80	0.64
1:B:228:LEU:HB2	1:B:270:MET:HB3	1.79	0.64
1:B:593:PHE:O	1:B:598:GLY:HA2	1.98	0.63
1:B:437:LEU:HD12	1:B:495:MET:HB3	1.80	0.63
1:A:651:ILE:HB	1:A:677:ASN:OD1	1.98	0.63
1:A:238:GLN:HB3	1:A:246:ALA:CB	2.29	0.62
1:A:236:PHE:CD1	1:A:240:GLN:HG3	2.35	0.61
1:A:228:LEU:HD13	1:A:233:LEU:HD13	1.81	0.61
1:A:593:PHE:O	1:A:598:GLY:HA2	2.00	0.61
1:B:292:ARG:O	1:B:597:GLY:HA2	2.01	0.61
1:A:437:LEU:HD12	1:A:495:MET:HB3	1.82	0.61
1:A:236:PHE:HD1	1:A:240:GLN:HG3	1.66	0.61
1:B:300:GLN:HB2	1:B:305:TYR:CE1	2.36	0.61
1:B:373:ILE:O	1:B:377:ALA:HB2	2.01	0.61
1:B:256:GLU:HA	1:B:265:LYS:HE3	1.82	0.60
1:B:301:PRO:HD2	1:B:304:HIS:ND1	2.17	0.60
1:A:373:ILE:O	1:A:377:ALA:HB2	2.01	0.59
1:A:256:GLU:HA	1:A:265:LYS:HE3	1.82	0.59
1:A:350:GLN:NE2	1:A:396:GLU:HG3	2.16	0.59
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.84	0.59
1:A:642:PRO:HD2	1:A:716:ILE:HG22	1.84	0.59
1:A:227:THR:HG22	1:A:269:GLN:HB3	1.84	0.59
1:A:642:PRO:HG2	1:A:743:HIS:CE1	2.37	0.59
1:B:350:GLN:NE2	1:B:396:GLU:HG3	2.17	0.59
1:B:701:ARG:HE	1:B:718:GLN:NE2	2.00	0.59
1:B:536:GLY:HA3	1:B:616:ASN:ND2	2.17	0.58
1:A:300:GLN:HB2	1:A:305:TYR:CE2	2.38	0.58
1:A:692:VAL:HG21	1:A:723:TRP:CZ3	2.38	0.58
1:A:411:PRO:O	1:A:434:LYS:HE2	2.03	0.58
1:A:537:ASN:ND2	1:A:614:THR:HA	2.17	0.58
1:A:395:LEU:HD22	1:A:489:VAL:HG13	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:LEU:O	1:A:594:GLN:HG2	2.03	0.58
1:A:594:GLN:HA	1:A:594:GLN:HE21	1.69	0.58
1:A:729:GLY:O	1:A:751:LYS:HA	2.03	0.58
1:B:729:GLY:O	1:B:751:LYS:HA	2.02	0.58
1:A:652:VAL:O	1:A:677:ASN:HA	2.04	0.58
1:A:630:ARG:NH1	1:A:630:ARG:HB2	2.20	0.57
1:B:590:LEU:O	1:B:594:GLN:HG2	2.03	0.57
1:A:492:LEU:HD23	1:A:495:MET:HE3	1.87	0.57
1:A:596:ASN:ND2	1:A:599:CYS:SG	2.77	0.57
1:B:311:HIS:HB2	1:B:576:ALA:HB1	1.86	0.57
1:B:594:GLN:HA	1:B:594:GLN:HE21	1.69	0.57
1:B:218:PHE:CE1	1:B:228:LEU:HG	2.40	0.57
1:B:411:PRO:O	1:B:434:LYS:HE2	2.04	0.57
1:B:728:GLN:NE2	1:B:754:ILE:H	2.03	0.57
1:A:263:THR:O	1:A:267:GLN:HG3	2.05	0.57
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.87	0.57
1:B:610:ASP:O	1:B:613:THR:HG22	2.04	0.57
1:A:237:LEU:HD11	1:A:254:LEU:HD12	1.86	0.57
1:B:644:VAL:C	1:B:646:LYS:H	2.13	0.57
1:A:292:ARG:O	1:A:597:GLY:HA2	2.05	0.57
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.87	0.56
1:A:313:THR:HB	1:A:329:TYR:CE1	2.40	0.56
1:A:536:GLY:HA3	1:A:616:ASN:ND2	2.20	0.56
1:A:323:PRO:HA	1:A:362:SER:HB2	1.86	0.56
1:B:320:LEU:HD11	1:B:557:THR:HG21	1.88	0.56
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.88	0.55
1:B:548:SER:N	1:B:573:GLN:HE21	2.03	0.55
1:A:214:ILE:HG13	1:A:276:LEU:HD13	1.88	0.55
1:B:652:VAL:HG12	1:B:653:ASP:H	1.69	0.55
1:B:701:ARG:NE	1:B:718:GLN:HE21	2.03	0.55
1:A:429:GLU:O	1:A:432:LYS:HG3	2.05	0.55
1:B:429:GLU:O	1:B:432:LYS:HG3	2.05	0.55
1:B:633:VAL:HG11	1:B:702:PHE:HE2	1.73	0.54
1:A:400:VAL:HG12	1:A:404:HIS:CD2	2.42	0.54
1:A:301:PRO:HD2	1:A:304:HIS:ND1	2.23	0.54
1:B:537:ASN:ND2	1:B:614:THR:HA	2.20	0.54
1:B:323:PRO:HA	1:B:362:SER:HB2	1.89	0.54
1:B:492:LEU:HD23	1:B:495:MET:HE3	1.90	0.54
1:B:537:ASN:O	1:B:541:ARG:HG3	2.09	0.53
1:B:728:GLN:HE21	1:B:754:ILE:H	1.56	0.53
1:B:727:LYS:HE3	1:B:731:ARG:NH2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.89	0.53
1:B:246:ALA:H	1:B:250:LEU:HB2	1.73	0.53
1:A:549:ARG:HG2	1:A:549:ARG:NH1	2.23	0.53
1:B:354:ILE:HD12	1:B:369:VAL:HG21	1.89	0.53
1:A:701:ARG:HE	1:A:718:GLN:NE2	2.06	0.53
1:B:258:TYR:OH	1:B:283:ASP:HB2	2.08	0.53
1:A:610:ASP:O	1:A:613:THR:HG22	2.08	0.53
1:B:400:VAL:HG12	1:B:404:HIS:CD2	2.43	0.53
1:B:444:GLY:HA2	1:B:500:LYS:HZ1	1.73	0.53
1:B:313:THR:HB	1:B:329:TYR:CE2	2.43	0.53
1:A:346:ASP:HA	1:A:397:GLN:OE1	2.09	0.53
1:A:420:GLY:H	1:B:349:ASN:ND2	2.07	0.53
1:A:537:ASN:O	1:A:541:ARG:HG3	2.09	0.53
1:B:230:VAL:O	1:B:234:VAL:HG23	2.09	0.53
1:B:630:ARG:NH1	1:B:630:ARG:HB2	2.25	0.52
1:B:596:ASN:ND2	1:B:599:CYS:SG	2.82	0.52
1:A:728:GLN:NE2	1:A:754:ILE:H	2.08	0.52
1:A:297:ASP:OD1	1:A:300:GLN:HG2	2.09	0.52
1:A:282:ALA:HB1	1:A:289:LEU:HD13	1.91	0.52
1:B:436:LEU:N	1:B:436:LEU:HD23	2.24	0.52
1:A:648:LYS:HA	1:A:648:LYS:HE2	1.90	0.52
1:A:237:LEU:HD23	1:A:241:GLN:HG3	1.92	0.52
1:B:692:VAL:HG21	1:B:723:TRP:CZ3	2.45	0.51
1:B:330:ILE:HG12	1:B:376:TYR:CD2	2.45	0.51
1:A:549:ARG:HG2	1:A:549:ARG:HH11	1.76	0.51
1:B:304:HIS:O	1:B:603:LEU:HD12	2.10	0.51
1:B:346:ASP:HA	1:B:397:GLN:OE1	2.11	0.51
1:B:402:ALA:HA	1:B:495:MET:HE1	1.91	0.51
1:B:736:LEU:HA	1:B:742:GLN:HA	1.91	0.51
1:A:206:LYS:HA	1:A:210:GLN:CG	2.30	0.51
1:A:311:HIS:HB2	1:A:576:ALA:HB1	1.93	0.51
1:A:703:MET:HG2	1:A:718:GLN:HB3	1.91	0.51
1:A:736:LEU:HA	1:A:742:GLN:HA	1.91	0.51
1:B:292:ARG:C	1:B:597:GLY:HA2	2.35	0.51
1:A:548:SER:N	1:A:573:GLN:HE21	2.07	0.51
1:B:644:VAL:HG21	1:B:706:ASP:OD2	2.10	0.51
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.36	0.51
1:A:211:ARG:HB3	1:A:213:GLU:OE2	2.10	0.51
1:A:638:GLY:HA2	1:A:748:LEU:HA	1.93	0.51
1:B:211:ARG:HB2	1:B:213:GLU:OE2	2.10	0.51
1:B:355:TYR:CZ	1:B:357:GLY:HA2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ARG:HD2	1:B:258:TYR:CZ	2.45	0.51
1:A:354:ILE:HD12	1:A:369:VAL:HG21	1.93	0.50
1:A:675:ILE:HG12	1:A:684:TRP:NE1	2.26	0.50
1:A:523:PHE:HD1	1:A:527:ARG:HD3	1.76	0.50
1:B:650:SER:O	1:B:651:ILE:HG13	2.11	0.50
1:B:395:LEU:HD22	1:B:489:VAL:HG13	1.94	0.50
1:A:300:GLN:HG3	1:A:603:LEU:HD11	1.94	0.50
1:A:727:LYS:HE3	1:A:731:ARG:NH2	2.27	0.50
1:B:415:ASP:C	1:B:497:ILE:HD11	2.37	0.50
1:A:396:GLU:O	1:A:400:VAL:HG23	2.11	0.49
1:B:297:ASP:OD1	1:B:300:GLN:HG2	2.12	0.49
1:A:402:ALA:HA	1:A:495:MET:HE1	1.93	0.49
1:A:421:VAL:HG11	1:A:426:PRO:HD3	1.94	0.49
1:B:438:LYS:CE	1:B:520:MET:HE2	2.38	0.49
1:B:429:GLU:HA	1:B:432:LYS:HG3	1.93	0.49
1:A:355:TYR:CZ	1:A:357:GLY:HA2	2.48	0.49
1:A:429:GLU:HA	1:A:432:LYS:HG3	1.92	0.49
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.38	0.49
1:A:313:THR:O	1:A:328:ALA:HB1	2.12	0.49
1:A:436:LEU:N	1:A:436:LEU:HD23	2.28	0.49
1:B:396:GLU:O	1:B:400:VAL:HG23	2.12	0.49
1:A:618:ARG:HH11	1:A:618:ARG:HG3	1.76	0.49
1:A:290:ALA:O	1:A:293:ARG:HG2	2.13	0.48
1:B:427:SER:OG	1:B:430:GLN:HG3	2.13	0.48
1:B:739:ASN:ND2	1:B:741:ASP:CG	2.72	0.48
1:A:258:TYR:CE1	1:A:281:SER:HB2	2.48	0.48
1:A:630:ARG:HB2	1:A:630:ARG:HH11	1.78	0.48
1:A:633:VAL:HG11	1:A:702:PHE:HE2	1.78	0.48
1:B:234:VAL:O	1:B:238:GLN:HG2	2.13	0.48
1:B:549:ARG:NH1	1:B:549:ARG:HG2	2.28	0.48
1:B:523:PHE:HD1	1:B:527:ARG:HD3	1.78	0.48
1:B:548:SER:H	1:B:573:GLN:NE2	2.10	0.48
1:A:701:ARG:NE	1:A:718:GLN:HE21	2.10	0.48
1:B:555:TRP:HE3	1:B:555:TRP:O	1.96	0.48
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.44	0.48
1:B:245:GLU:HA	1:B:250:LEU:CD2	2.43	0.48
1:B:675:ILE:HG12	1:B:684:TRP:NE1	2.29	0.48
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.48	0.47
1:B:256:GLU:O	1:B:265:LYS:HE3	2.13	0.47
1:A:728:GLN:HE21	1:A:754:ILE:H	1.62	0.47
1:B:341:GLU:C	1:B:342:LEU:HD12	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:MET:HE3	1:B:549:ARG:CB	2.45	0.47
1:B:528:ALA:O	1:B:532:LEU:HG	2.14	0.47
1:B:643:LYS:O	1:B:645:ASN:N	2.47	0.47
1:A:628:PRO:HB3	1:A:693:THR:HA	1.97	0.47
1:B:652:VAL:CG1	1:B:653:ASP:N	2.78	0.47
1:A:259:GLU:OE2	1:A:261:SER:HB3	2.15	0.47
1:A:341:GLU:C	1:A:342:LEU:HD12	2.41	0.46
1:B:594:GLN:HE21	1:B:594:GLN:CA	2.28	0.46
1:A:739:ASN:ND2	1:A:741:ASP:CG	2.74	0.46
1:A:292:ARG:C	1:A:597:GLY:HA2	2.39	0.46
1:B:643:LYS:H	1:B:643:LYS:HD2	1.81	0.46
1:A:562:TYR:CE1	1:A:577:LEU:HD23	2.51	0.46
1:A:520:MET:HE3	1:A:549:ARG:CB	2.45	0.46
1:A:594:GLN:HE21	1:A:594:GLN:CA	2.28	0.46
1:B:241:GLN:HE21	1:B:241:GLN:N	2.14	0.46
1:B:300:GLN:HB2	1:B:305:TYR:CZ	2.51	0.46
1:A:388:SER:HA	1:A:438:LYS:HB3	1.98	0.46
1:B:258:TYR:O	1:B:260:PRO:HD3	2.15	0.46
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.81	0.46
1:B:618:ARG:HG3	1:B:618:ARG:HH11	1.78	0.46
1:A:555:TRP:HE3	1:A:555:TRP:O	1.98	0.46
1:A:330:ILE:HG12	1:A:376:TYR:CD2	2.51	0.45
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.51	0.45
1:B:228:LEU:HD12	1:B:270:MET:HB3	1.97	0.45
1:B:313:THR:O	1:B:328:ALA:HB1	2.15	0.45
1:B:369:VAL:O	1:B:373:ILE:HG13	2.16	0.45
1:A:415:ASP:C	1:A:497:ILE:HD11	2.40	0.45
1:A:427:SER:OG	1:A:430:GLN:HG3	2.16	0.45
1:B:525:GLU:OE2	1:B:556:ARG:NE	2.49	0.45
1:B:289:LEU:HA	1:B:292:ARG:HG2	1.98	0.45
1:A:441:LYS:HD2	1:A:496:ILE:O	2.17	0.45
1:B:630:ARG:HB2	1:B:630:ARG:HH11	1.82	0.45
1:B:638:GLY:HA2	1:B:748:LEU:HA	1.99	0.45
1:A:508:SER:O	1:A:509:SER:HB2	2.16	0.45
1:B:642:PRO:HD3	1:B:746:ALA:HB2	1.97	0.45
1:B:707:TYR:CE2	1:B:709:SER:HA	2.51	0.45
1:B:606:ALA:HA	1:B:609:ARG:HE	1.82	0.45
1:B:290:ALA:O	1:B:293:ARG:HG2	2.17	0.45
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.99	0.45
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.99	0.44
1:A:438:LYS:CE	1:A:520:MET:HE2	2.40	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:HG13	1:B:276:LEU:HD13	1.99	0.44
1:B:317:GLU:HB2	1:B:323:PRO:HD2	1.98	0.44
1:B:403:ARG:HG3	1:B:403:ARG:HH11	1.82	0.44
1:A:256:GLU:HA	1:A:265:LYS:CE	2.47	0.44
1:A:525:GLU:OE2	1:A:556:ARG:NE	2.49	0.44
1:A:235:THR:O	1:A:239:HIS:HB3	2.18	0.44
1:A:277:MET:O	1:A:281:SER:HB3	2.17	0.44
1:A:712:LYS:HG2	1:A:713:ASN:H	1.81	0.44
1:A:706:ASP:O	1:A:713:ASN:HA	2.17	0.44
1:B:388:SER:HA	1:B:438:LYS:HB3	2.00	0.44
1:B:652:VAL:CG1	1:B:653:ASP:H	2.28	0.44
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.53	0.44
1:B:324:SER:N	1:B:362:SER:HB3	2.32	0.44
1:B:364:ILE:HD12	1:B:369:VAL:HG22	1.99	0.44
1:B:228:LEU:HD13	1:B:233:LEU:HD13	2.00	0.44
1:B:489:VAL:HG23	1:B:492:LEU:H	1.81	0.44
1:B:248:PRO:O	1:B:252:LEU:HD12	2.16	0.44
1:A:214:ILE:HD13	1:A:214:ILE:HA	1.88	0.43
1:A:221:ALA:HB1	1:A:228:LEU:HD21	2.01	0.43
1:B:227:THR:HG22	1:B:271:THR:HG22	1.99	0.43
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.71	0.43
1:A:300:GLN:HB2	1:A:305:TYR:CZ	2.54	0.43
1:B:347:GLY:HA3	1:B:351:GLU:O	2.18	0.43
1:B:487:LYS:HG2	1:B:487:LYS:O	2.17	0.43
1:A:320:LEU:O	1:A:359:THR:HB	2.17	0.43
1:A:237:LEU:O	1:A:241:GLN:HB2	2.19	0.43
1:A:257:ARG:O	1:A:257:ARG:HG2	2.18	0.43
1:B:323:PRO:HA	1:B:362:SER:CB	2.48	0.43
1:A:308:SER:OG	1:A:337:CYS:HA	2.19	0.43
1:A:317:GLU:HB2	1:A:323:PRO:HD2	2.00	0.43
1:A:644:VAL:O	1:A:644:VAL:HG22	2.18	0.43
1:A:654:PRO:HD2	1:A:675:ILE:O	2.17	0.43
1:B:237:LEU:HD13	1:B:250:LEU:HD23	2.01	0.43
1:B:343:ASP:HA	1:B:390:GLU:HB3	2.01	0.43
1:B:652:VAL:HG13	1:B:706:ASP:CG	2.44	0.43
1:A:343:ASP:HA	1:A:390:GLU:HB3	2.01	0.43
1:A:492:LEU:HD23	1:A:495:MET:CE	2.48	0.43
1:A:663:VAL:O	1:A:664:GLY:C	2.61	0.43
1:A:700:VAL:HG21	1:A:726:LEU:HD22	2.00	0.43
1:B:700:VAL:HG21	1:B:726:LEU:HD22	2.00	0.43
1:A:490:PRO:HD2	1:B:327:GLU:OE2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ARG:HG2	1:B:549:ARG:HH11	1.84	0.43
1:A:258:TYR:CE1	1:A:281:SER:CB	3.02	0.42
1:A:507:PHE:O	1:A:508:SER:HB3	2.18	0.42
1:B:246:ALA:CB	1:B:249:ALA:HB3	2.49	0.42
1:A:229:SER:OG	1:A:232:ARG:HB2	2.20	0.42
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.66	0.42
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.54	0.42
1:B:245:GLU:C	1:B:247:GLY:H	2.27	0.42
1:B:592:CYS:HB2	1:B:699:LEU:HD21	2.00	0.42
1:B:674:VAL:HG21	1:B:707:TYR:CG	2.54	0.42
1:A:618:ARG:HG3	1:A:618:ARG:NH1	2.34	0.42
1:A:650:SER:C	1:A:651:ILE:HG13	2.44	0.42
1:B:296:GLN:HG3	1:B:596:ASN:OD1	2.20	0.42
1:B:507:PHE:O	1:B:508:SER:HB2	2.20	0.42
1:B:562:TYR:CE1	1:B:577:LEU:HD23	2.55	0.42
1:B:701:ARG:HH21	1:B:718:GLN:HG2	1.84	0.42
1:A:245:GLU:HB2	1:A:250:LEU:HD22	2.02	0.42
1:A:324:SER:HB2	1:A:362:SER:O	2.20	0.42
1:A:340:LEU:HB2	1:A:387:LEU:CD2	2.50	0.41
1:B:537:ASN:HB3	1:B:615:PHE:O	2.20	0.41
1:A:260:PRO:HG3	1:A:273:ASP:CB	2.50	0.41
1:A:528:ALA:O	1:A:532:LEU:HG	2.19	0.41
1:B:442:LEU:HD21	1:B:488:LEU:HB3	2.02	0.41
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.89	0.41
1:A:522:SER:HA	1:A:549:ARG:O	2.20	0.41
1:B:421:VAL:HG11	1:B:426:PRO:HD3	2.02	0.41
1:B:310:SER:HB2	1:B:337:CYS:SG	2.60	0.41
1:A:606:ALA:HA	1:A:609:ARG:HE	1.86	0.41
1:A:255:ILE:O	1:A:259:GLU:HB3	2.21	0.41
1:A:304:HIS:O	1:A:603:LEU:HD12	2.21	0.41
1:A:693:THR:C	1:A:695:PRO:HD3	2.46	0.41
1:B:618:ARG:HG3	1:B:618:ARG:NH1	2.35	0.41
1:B:645:ASN:O	1:B:647:ASN:N	2.53	0.41
1:A:288:SER:HA	1:A:727:LYS:HD2	2.02	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.86	0.41
1:A:652:VAL:HG12	1:A:653:ASP:N	2.35	0.41
1:B:218:PHE:HE1	1:B:228:LEU:HG	1.84	0.41
1:B:709:SER:C	1:B:711:SER:H	2.28	0.41
1:A:655:LYS:HB3	1:A:674:VAL:HG22	2.02	0.41
1:A:310:SER:HB2	1:A:337:CYS:SG	2.61	0.40
1:A:322:GLY:O	1:A:361:THR:HA	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:GLY:HA3	1:A:411:PRO:HD2	1.87	0.40
1:A:537:ASN:HB3	1:A:615:PHE:O	2.21	0.40
1:B:492:LEU:HD23	1:B:495:MET:CE	2.50	0.40
1:B:555:TRP:O	1:B:555:TRP:CE3	2.74	0.40
1:A:626:TRP:HH2	1:A:665:ARG:CZ	2.34	0.40
1:B:654:PRO:HD2	1:B:675:ILE:O	2.21	0.40
1:A:323:PRO:HA	1:A:362:SER:CB	2.50	0.40
1:A:654:PRO:HG2	1:A:678:ASN:O	2.20	0.40
1:B:255:ILE:HD13	1:B:255:ILE:HG21	1.85	0.40
1:B:730:TYR:CZ	1:B:751:LYS:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	505/622 (81%)	457 (90%)	37 (7%)	11 (2%)	5	26
1	B	501/622 (80%)	452 (90%)	38 (8%)	11 (2%)	5	26
All	All	1006/1244 (81%)	909 (90%)	75 (8%)	22 (2%)	5	26

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	THR
1	A	513	SER
1	A	647	ASN
1	B	444	GLY
1	B	644	VAL
1	B	646	LYS
1	A	508	SER
1	A	246	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	650	SER
1	A	677	ASN
1	A	678	ASN
1	B	677	ASN
1	B	678	ASN
1	B	709	SER
1	B	710	SER
1	A	442	LEU
1	A	288	SER
1	A	712	LYS
1	B	281	SER
1	B	288	SER
1	B	650	SER
1	B	443	GLY

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	441/544 (81%)	417 (95%)	24 (5%)	20	53
1	B	437/544 (80%)	411 (94%)	26 (6%)	18	50
All	All	878/1088 (81%)	828 (94%)	50 (6%)	18	52

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
1	A	214	ILE
1	A	216	ARG
1	A	219	GLU
1	A	288	SER
1	A	313	THR
1	A	342	LEU
1	A	385	VAL
1	A	391	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	434	LYS
1	A	436	LEU
1	A	490	PRO
1	A	524	SER
1	A	592	CYS
1	A	594	GLN
1	A	622	GLN
1	A	633	VAL
1	A	639	GLN
1	A	641	LEU
1	A	691	GLU
1	A	713	ASN
1	A	714	ASP
1	A	718	GLN
1	A	739	ASN
1	B	211	ARG
1	B	215	ASP
1	B	216	ARG
1	B	252	LEU
1	B	254	LEU
1	B	267	GLN
1	B	277	MET
1	B	283	ASP
1	B	342	LEU
1	B	385	VAL
1	B	391	ASN
1	B	434	LYS
1	B	436	LEU
1	B	490	PRO
1	B	524	SER
1	B	592	CYS
1	B	594	GLN
1	B	622	GLN
1	B	633	VAL
1	B	639	GLN
1	B	641	LEU
1	B	643	LYS
1	B	691	GLU
1	B	708	ASP
1	B	718	GLN
1	B	739	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	350	GLN
1	A	430	GLN
1	A	503	HIS
1	A	515	GLN
1	A	573	GLN
1	A	594	GLN
1	A	718	GLN
1	A	724	ASN
1	A	728	GLN
1	A	734	HIS
1	A	743	HIS
1	B	241	GLN
1	B	267	GLN
1	B	349	ASN
1	B	350	GLN
1	B	430	GLN
1	B	503	HIS
1	B	573	GLN
1	B	594	GLN
1	B	718	GLN
1	B	728	GLN
1	B	743	HIS

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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.