



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:01 PM UTC

PDB ID : 2GRV / pdb_00002grv
Title : Crystal Structure of LpqW
Authors : Marland, Z.; Rossjohn, J.
Deposited on : 2006-04-25
Resolution : 2.40 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

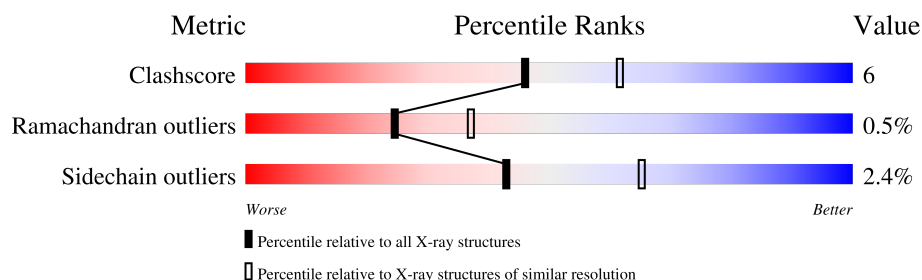
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	621	
1	B	621	
1	C	621	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12015 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 LpqW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	13	0	0
			3855	2427	675	745	8			
1	B	509	Total	C	N	O	S	21	0	0
			3804	2394	667	735	8			
1	C	511	Total	C	N	O	S	27	0	0
			3820	2404	670	738	8			

- Molecule 2 is water.

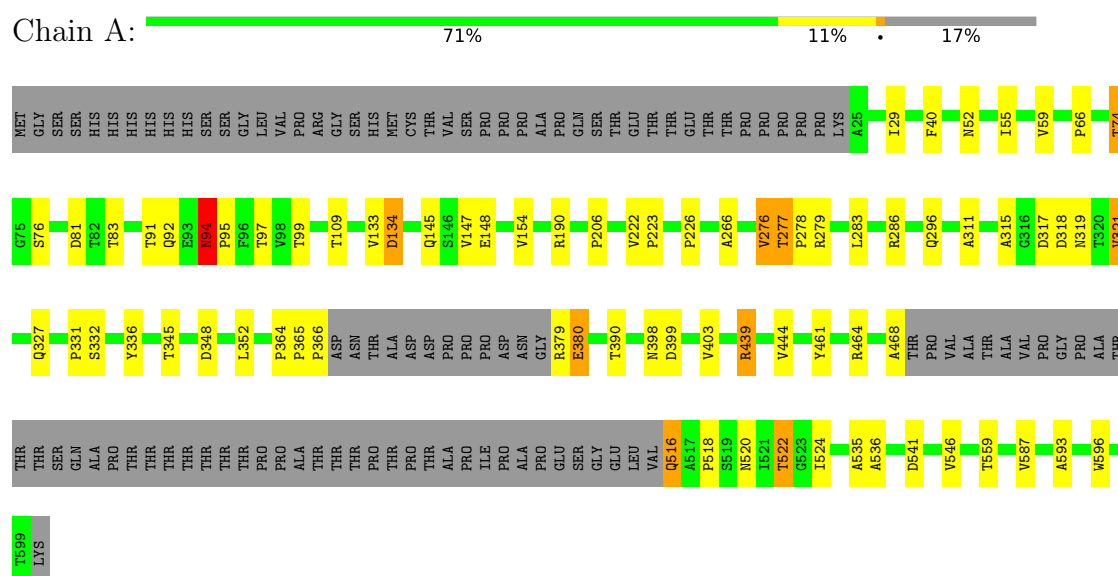
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	231	Total	O	0	0
			231	231		
2	B	82	Total	O	0	0
			82	82		
2	C	223	Total	O	0	0
			223	223		

3 Residue-property plots [i](#)

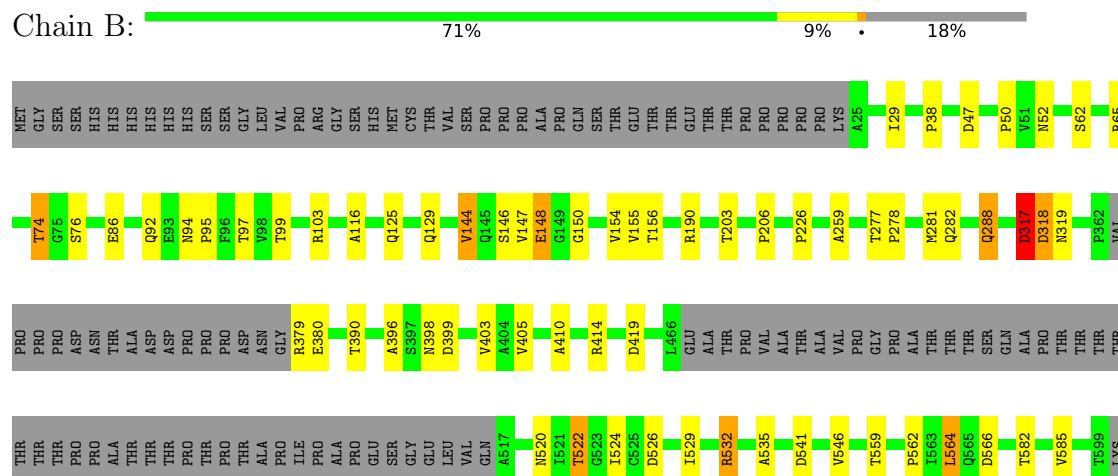
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: LpqW



- Molecule 1: LpqW



- Molecule 1: LpqW

Chain C: 71% 9% 18%

PRO	ALA	THR	THR	THR	PRO	PRO	THR	ALA	ALA	ILE	PRO	ALA	PRO	GLU	PRO	GLU	SER	GLY	LEU	VAL	Q516	N520	T522	G523	T524	G525	D526	I529	A535	A536	D541	V546	T547	Q548	R553	T559	T582	D595	V596	T599	LYS								
PRO	ALA	THR	THR	THR	PRO	PRO	THR	ALA	ALA	ILE	PRO	ALA	PRO	GLY	R379	E380	R381	S382	V383	K384	D385	D411	V436	R439	R447	R464	A465	L466	GLU	ALA	THR	PRO	VAL	ALA	THR	PRO	GLY	PRO	ALA	THR	THR	THR	THR	THR	THR	PRO			
ASP	ASN	THR	ALA	ASP	PRO	PRO	PRO	PRO	ASP	ASN	GLY	E380	R381	S382	V383	K384	D385	D411	V436	R439	R447	R464	A465	L466	GLU	ALA	THR	PRO	VAL	ALA	THR	PRO	GLY	PRO	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO				
T97	E105	T109	V133	D134	T142	T156	R165	V177	I180	R190	Q198	P206	R215	A224	K225	P226	D227	H255	V276	T277	P278	R279	Q282	V297	I301	A315	G316	D317	D318	N319	S332	E351	S360	V363	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO			
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	CYS	THR	VAL	SER	PRO	PRO	PRO	ALA	PRO	GLN	SER	THR	GLU	THR	THR	THR	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	188.57Å 312.04Å 104.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.6 (100.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12015	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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	0.53	2/3937 (0.1%)	0.87	9/5405 (0.2%)
1	B	0.80	8/3883 (0.2%)	0.87	6/5328 (0.1%)
1	C	0.73	7/3899 (0.2%)	0.95	9/5350 (0.2%)
All	All	0.70	17/11719 (0.1%)	0.90	24/16083 (0.1%)

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	1	0
1	B	1	0
1	C	0	2
All	All	2	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	380	GLU	CB-CG	21.39	2.16	1.52
1	C	516	GLN	CA-CB	18.61	1.90	1.53
1	B	532	ARG	CZ-NH1	18.58	1.58	1.32
1	B	317	ASP	CA-CB	-17.16	1.26	1.53
1	B	148	GLU	CG-CD	-16.77	1.10	1.52
1	B	379	ARG	CB-CG	-15.86	1.04	1.52
1	B	532	ARG	CD-NE	14.26	1.66	1.46
1	B	532	ARG	CZ-NH2	11.21	1.48	1.33
1	A	516	GLN	CA-CB	8.32	1.70	1.53
1	C	439	ARG	CD-NE	7.39	1.56	1.46
1	C	516	GLN	N-CA	7.04	1.59	1.46
1	C	385	ASP	CG-OD1	6.71	1.38	1.25
1	C	385	ASP	CG-OD2	6.38	1.37	1.25
1	B	380	GLU	CB-CG	5.84	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	464	ARG	CD-NE	-5.79	1.38	1.46
1	B	585	VAL	CA-CB	5.59	1.56	1.54
1	A	516	GLN	N-CA	5.26	1.56	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	516	GLN	N-CA-CB	-27.67	63.47	110.50
1	A	516	GLN	N-CA-CB	15.06	136.10	110.50
1	B	148	GLU	CB-CG-CD	13.06	134.80	112.60
1	A	516	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	C	516	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	C	380	GLU	CB-CG-CD	9.37	128.53	112.60
1	B	317	ASP	N-CA-CB	8.86	123.51	109.51
1	B	317	ASP	CA-CB-CG	8.28	120.88	112.60
1	B	532	ARG	CD-NE-CZ	-8.27	112.83	124.40
1	C	516	GLN	CB-CA-C	-7.90	95.08	110.10
1	B	380	GLU	CA-CB-CG	-7.72	98.67	114.10
1	A	464	ARG	NE-CZ-NH1	-6.98	114.52	121.50
1	A	464	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	C	439	ARG	CD-NE-CZ	-6.76	114.93	124.40
1	C	516	GLN	CG-CD-NE2	6.66	126.40	116.40
1	A	516	GLN	CG-CD-NE2	6.66	126.38	116.40
1	B	317	ASP	CB-CA-C	6.49	119.50	110.16
1	C	380	GLU	CA-CB-CG	6.48	127.06	114.10
1	A	94	ASN	CA-C-N	-5.78	112.61	119.84
1	A	94	ASN	C-N-CA	-5.78	112.61	119.84
1	C	379	ARG	CB-CA-C	-5.58	99.49	110.10
1	A	317	ASP	N-CA-C	-5.22	105.28	110.97
1	C	317	ASP	N-CA-C	-5.08	105.64	111.07
1	A	321	VAL	N-CA-C	5.05	115.96	108.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	516	GLN	CA
1	B	317	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	439	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	464	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	3855	0	3841	52	0
1	B	3804	0	3792	40	1
1	C	3820	0	3809	40	0
2	A	231	0	0	7	0
2	B	82	0	0	0	0
2	C	223	0	0	5	0
All	All	12015	0	11442	131	1

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 6.

All (131) 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:74:THR:HG21	2:A:654:HOH:O	1.73	0.88
1:B:281:MET:HE1	1:B:405:VAL:HG21	1.58	0.86
1:C:522:THR:HG21	2:C:660:HOH:O	1.79	0.82
1:C:94:ASN:HB3	1:C:95:PRO:CD	2.12	0.79
1:C:94:ASN:HB3	1:C:95:PRO:HD3	1.63	0.77
1:A:94:ASN:HB3	1:A:95:PRO:CD	2.14	0.77
1:A:439:ARG:NH1	2:A:827:HOH:O	2.18	0.75
1:A:522:THR:HG21	2:A:679:HOH:O	1.89	0.72
1:A:94:ASN:HB3	1:A:95:PRO:HD2	1.70	0.72
1:C:522:THR:HG22	1:C:524:ILE:H	1.55	0.72
1:C:315:ALA:O	1:C:319:ASN:HB2	1.93	0.69
1:B:94:ASN:HB2	1:B:95:PRO:HD3	1.73	0.69
1:A:74:THR:HG22	1:A:76:SER:H	1.59	0.68
1:B:520:ASN:OD1	1:B:522:THR:HB	1.93	0.67
1:B:522:THR:HG22	1:B:524:ILE:H	1.60	0.67
1:A:522:THR:HG22	1:A:524:ILE:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:HG12	1:A:148:GLU:HG2	1.78	0.65
1:C:74:THR:HG21	2:C:642:HOH:O	1.96	0.64
1:A:92:GLN:HB3	1:A:97:THR:CG2	2.27	0.64
1:A:92:GLN:HB3	1:A:97:THR:HG22	1.78	0.64
1:C:315:ALA:O	1:C:319:ASN:CB	2.45	0.64
1:B:277:THR:HB	1:B:566:ASP:HB3	1.81	0.63
1:A:520:ASN:OD1	1:A:522:THR:HB	1.97	0.63
1:C:277:THR:HG22	1:C:279:ARG:HG2	1.81	0.62
1:A:277:THR:HG22	1:A:279:ARG:HG2	1.81	0.62
1:B:526:ASP:HB3	1:B:529:ILE:HG12	1.82	0.62
2:A:825:HOH:O	1:C:318:ASP:HB2	2.00	0.61
1:C:42:PRO:HA	1:C:52:ASN:HD21	1.66	0.60
1:C:97:THR:HG22	1:C:156:THR:HA	1.84	0.60
1:B:92:GLN:HG3	1:B:95:PRO:HD2	1.85	0.59
1:B:146:SER:HB2	1:B:150:GLY:HA2	1.85	0.58
1:A:345:THR:HG23	1:A:348:ASP:H	1.67	0.58
1:A:283:LEU:HD23	1:A:444:VAL:HG22	1.87	0.57
1:B:288:GLN:HE21	1:B:288:GLN:H	1.51	0.57
1:C:215:ARG:NH2	1:C:227:ASP:OD1	2.38	0.56
1:C:360:SER:HA	1:C:381:ARG:O	2.06	0.56
1:C:520:ASN:OD1	1:C:522:THR:HB	2.05	0.56
1:C:215:ARG:NH1	1:C:224:ALA:O	2.39	0.55
1:B:522:THR:HG23	1:B:559:THR:HG21	1.88	0.54
1:B:74:THR:HG22	1:B:76:SER:H	1.71	0.53
1:A:81:ASP:OD1	1:A:83:THR:HB	2.08	0.53
1:B:190:ARG:HD2	1:B:206:PRO:HG3	1.91	0.53
1:A:29:ILE:HD12	1:A:226:PRO:HB3	1.89	0.53
1:A:277:THR:HG23	2:A:770:HOH:O	2.07	0.53
1:A:40:PHE:HA	1:A:52:ASN:HD22	1.74	0.52
1:A:190:ARG:HD2	1:A:206:PRO:HG3	1.91	0.52
1:C:225:LYS:HD3	1:C:595:ASP:HA	1.92	0.52
1:C:536:ALA:HB2	1:C:546:VAL:HG21	1.91	0.52
1:A:319:ASN:ND2	2:A:814:HOH:O	2.42	0.52
1:C:276:VAL:HG11	1:C:332:SER:HB3	1.92	0.52
1:C:535:ALA:HB1	1:C:541:ASP:HB2	1.91	0.52
1:C:526:ASP:OD2	1:C:553:ARG:HD2	2.10	0.51
1:B:99:THR:HG22	1:B:154:VAL:HG22	1.92	0.51
1:B:281:MET:CE	1:B:405:VAL:HG21	2.38	0.51
1:C:190:ARG:HD2	1:C:206:PRO:HG3	1.93	0.51
1:A:318:ASP:O	1:A:319:ASN:HB2	2.10	0.51
1:A:379:ARG:O	1:A:380:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:PHE:CZ	1:C:165:ARG:HG2	2.46	0.50
1:B:282:GLN:HG2	1:B:562:PRO:HA	1.93	0.50
1:B:410:ALA:O	1:B:414:ARG:HG3	2.11	0.50
1:C:29:ILE:HD13	1:C:596:TRP:HB3	1.93	0.50
1:C:255:HIS:HD2	1:C:319:ASN:HD21	1.60	0.50
1:B:532:ARG:HD2	1:B:546:VAL:HG22	1.93	0.49
1:A:522:THR:HG23	1:A:559:THR:HG21	1.95	0.49
1:B:62:SER:HB2	1:B:65:ARG:NH1	2.27	0.49
1:B:288:GLN:H	1:B:288:GLN:NE2	2.10	0.49
1:C:318:ASP:O	1:C:319:ASN:HB2	2.13	0.49
1:C:522:THR:HG23	1:C:559:THR:HG21	1.95	0.49
1:A:315:ALA:O	1:A:319:ASN:HB2	2.13	0.49
1:B:281:MET:HE2	1:B:564:LEU:CD2	2.43	0.49
1:B:277:THR:HG23	1:B:278:PRO:HD2	1.94	0.48
1:C:277:THR:HG23	1:C:278:PRO:HD2	1.94	0.48
1:C:177:VAL:HA	1:C:180:ILE:HG12	1.96	0.48
1:A:276:VAL:HG11	1:A:332:SER:HB3	1.95	0.48
1:A:94:ASN:CB	1:A:95:PRO:CD	2.90	0.47
1:A:277:THR:HG23	1:A:278:PRO:HD2	1.95	0.47
1:B:50:PRO:HD3	1:B:277:THR:HG21	1.97	0.47
1:B:125:GLN:O	1:B:129:GLN:HB2	2.15	0.47
1:C:384:LYS:HG2	1:C:385:ASP:OD2	2.14	0.47
1:B:277:THR:CG2	1:B:278:PRO:HD2	2.44	0.47
1:A:536:ALA:HB2	1:A:546:VAL:HG21	1.97	0.47
1:A:398:ASN:ND2	2:A:730:HOH:O	2.47	0.46
1:A:99:THR:HG22	1:A:154:VAL:HG13	1.98	0.45
1:A:296:GLN:HE21	1:A:352:LEU:HD22	1.81	0.45
1:B:86:GLU:HG3	1:B:103:ARG:HG2	1.98	0.45
1:C:297:VAL:O	1:C:301:ILE:HG12	2.17	0.45
1:C:526:ASP:HB3	1:C:529:ILE:HG12	1.98	0.45
1:A:311:ALA:HB1	1:A:321:VAL:HG21	1.99	0.45
1:B:396:ALA:C	1:B:398:ASN:H	2.25	0.45
1:B:62:SER:HB2	1:B:65:ARG:HH12	1.83	0.44
1:B:97:THR:HG22	1:B:156:THR:HG23	1.98	0.44
1:A:55:ILE:O	1:A:59:VAL:HG22	2.18	0.44
1:B:94:ASN:CB	1:B:95:PRO:HD3	2.43	0.44
1:A:266:ALA:O	1:C:411:ASP:HB3	2.17	0.44
1:A:327:GLN:NE2	1:A:461:TYR:OH	2.50	0.44
1:A:315:ALA:O	1:A:319:ASN:CB	2.66	0.43
1:B:535:ALA:HB1	1:B:541:ASP:HB2	2.00	0.43
1:A:318:ASP:CB	2:C:823:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ILE:HD12	1:B:226:PRO:HB3	1.99	0.43
1:B:396:ALA:C	1:B:398:ASN:N	2.77	0.43
1:C:94:ASN:CB	1:C:95:PRO:HD3	2.41	0.43
1:C:198:GLN:HG2	1:C:224:ALA:HB2	2.00	0.43
1:C:29:ILE:HD12	1:C:226:PRO:HB3	2.01	0.43
1:A:40:PHE:HA	1:A:52:ASN:ND2	2.34	0.43
1:C:133:VAL:O	1:C:134:ASP:C	2.62	0.42
1:A:535:ALA:HB1	1:A:541:ASP:HB2	2.01	0.42
1:A:593:ALA:HA	1:A:596:TRP:CE2	2.54	0.42
1:B:390:THR:HG22	1:B:419:ASP:HB3	2.00	0.42
1:A:133:VAL:O	1:A:134:ASP:C	2.63	0.42
1:A:318:ASP:HB2	2:C:823:HOH:O	2.19	0.42
1:A:439:ARG:HH11	1:A:439:ARG:HG2	1.85	0.42
1:A:66:PRO:HG2	1:A:587:VAL:HG23	2.01	0.42
1:B:399:ASP:O	1:B:403:VAL:HG23	2.19	0.42
1:C:553:ARG:HG2	2:C:602:HOH:O	2.19	0.42
1:A:399:ASP:O	1:A:403:VAL:HG23	2.19	0.42
1:C:94:ASN:CB	1:C:95:PRO:CD	2.90	0.41
1:B:47:ASP:HB3	1:B:52:ASN:ND2	2.35	0.41
1:B:144:VAL:HG12	1:B:155:VAL:HG13	2.03	0.41
1:A:365:PRO:HA	1:A:366:PRO:HD3	1.88	0.41
1:B:38:PRO:HG2	1:B:47:ASP:HA	2.01	0.41
1:A:222:VAL:HA	1:A:223:PRO:HD3	1.91	0.41
1:A:439:ARG:NH1	1:A:439:ARG:HG2	2.36	0.41
1:B:116:ALA:HB3	1:B:146:SER:HB3	2.02	0.41
1:A:331:PRO:HA	1:A:336:TYR:CG	2.56	0.40
1:A:468:ALA:CB	1:A:518:PRO:HD3	2.51	0.40
1:B:318:ASP:O	1:B:319:ASN:HB2	2.21	0.40
1:A:145:GLN:HG3	1:A:154:VAL:HB	2.04	0.40
1:B:147:VAL:HG12	1:B:148:GLU:H	1.86	0.40
1:C:282:GLN:OE1	1:C:447:ARG:HD2	2.22	0.40
1:C:315:ALA:O	1:C:319:ASN:HB3	2.21	0.40
1:A:364:PRO:HA	1:A:365:PRO:HD3	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ALA:CB	1:B:317:ASP:OD1[3_555]	1.79	0.41

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	510/621 (82%)	493 (97%)	14 (3%)	3 (1%)	21	32
1	B	503/621 (81%)	487 (97%)	15 (3%)	1 (0%)	43	58
1	C	505/621 (81%)	490 (97%)	12 (2%)	3 (1%)	21	32
All	All	1518/1863 (82%)	1470 (97%)	41 (3%)	7 (0%)	24	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	GLU
1	A	94	ASN
1	B	318	ASP
1	C	94	ASN
1	C	380	GLU
1	C	318	ASP
1	A	134	ASP

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	412/502 (82%)	402 (98%)	10 (2%)	43	65
1	B	406/502 (81%)	398 (98%)	8 (2%)	48	70
1	C	408/502 (81%)	396 (97%)	12 (3%)	37	60
All	All	1226/1506 (81%)	1196 (98%)	30 (2%)	43	65

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	91	THR
1	A	109	THR
1	A	276	VAL
1	A	277	THR
1	A	286	ARG
1	A	390	THR
1	A	439	ARG
1	A	516	GLN
1	A	522	THR
1	B	74	THR
1	B	144	VAL
1	B	203	THR
1	B	288	GLN
1	B	317	ASP
1	B	522	THR
1	B	564	LEU
1	B	582	THR
1	C	74	THR
1	C	105	GLU
1	C	109	THR
1	C	142	THR
1	C	276	VAL
1	C	277	THR
1	C	351	GLU
1	C	383	VAL
1	C	436	VAL
1	C	522	THR
1	C	548	GLN
1	C	582	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	125	GLN
1	A	152	GLN
1	A	207	GLN
1	A	296	GLN
1	A	319	ASN
1	A	325	GLN

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Mol	Chain	Res	Type
1	A	327	GLN
1	A	548	GLN
1	B	125	GLN
1	B	288	GLN
1	B	296	GLN
1	B	325	GLN
1	C	52	ASN
1	C	94	ASN
1	C	125	GLN
1	C	145	GLN
1	C	327	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.