Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 01:03 PM EDT

PDB ID	:	2GRV
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:

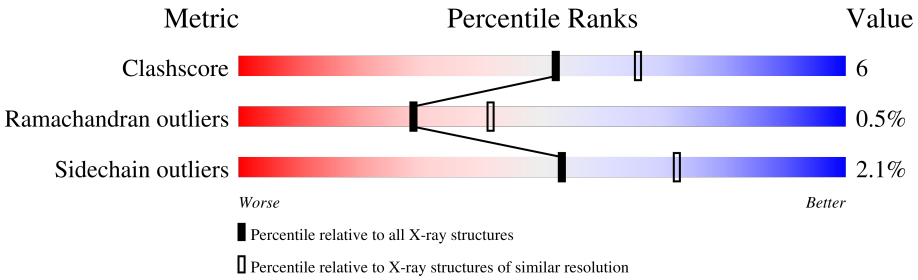
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	621	71% 11% • 17%
1	B	621	72% 9% • 18%
1	C	621	72% 9% • 18%

2 Entry composition (i)

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		

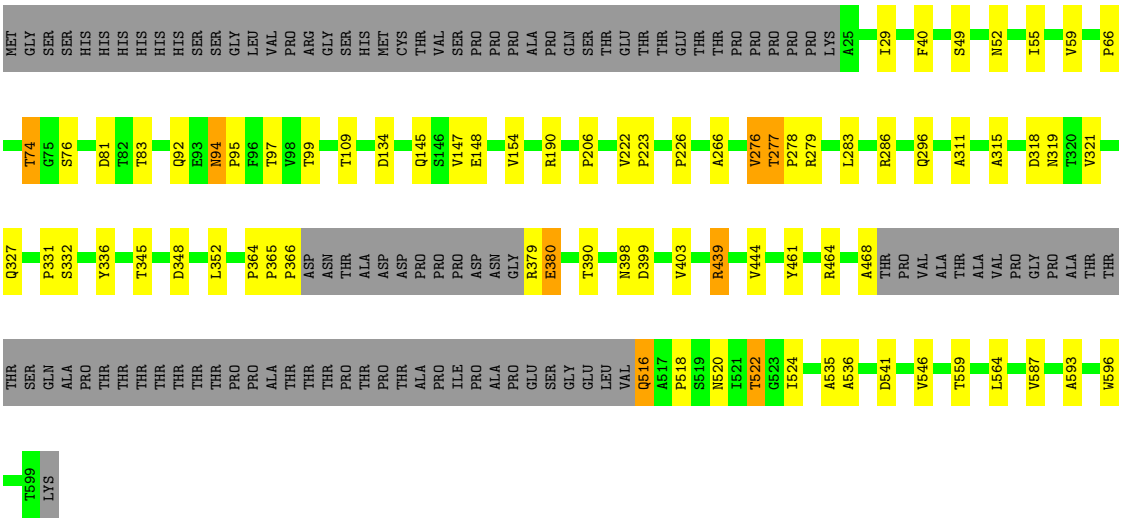
3 Residue-property plots (i)

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.

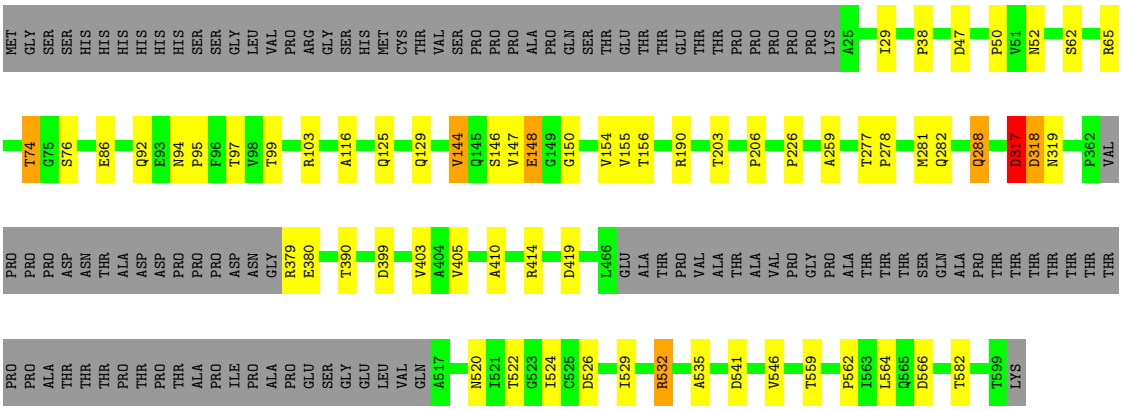
• Molecule 1: LpqW

Chain A:



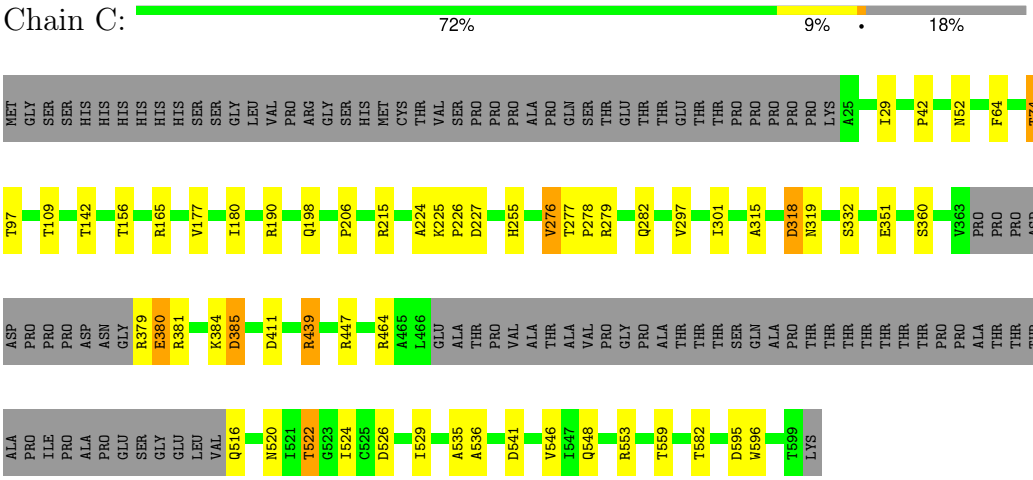
• Molecule 1: LpqW

Chain B:



• Molecule 1: LpqW

Chain C:


72%
9%
18%
MET GLY SER SER HIS 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 GLU THR THR PRO PRO PRO PRO LYS A25 I29 P42 N52 F64 T74 N94 P95 F96
T97 T109 T142 T156 R165 V177 I180 R190 Q198 P206 R215 A224 K225 P226 D227 H255 V276 T277 P278 R279 Q282 V297 I301 A315 D318 N319 S332 E351 S360 V363 PRO PRO PRO ASP ASN THR ALA ASP
ASP PRO PRO PRO ASP ASN GLY R379 E380 R381 K384 D385 D411 R439 R447 R464 A465 L466 GLU ALA THR PRO VAL ALA THR ALA VAL PRO GLY PRO ALA THR THR THR SER GLN ALA PRO THR THR THR THR THR THR THR PRO PRO ALA THR THR THR PRO THR PRO THR
ALA PRO ILE PRO ALA PRO GLU SER GLY GLU LEU VAL Q516 N520 I521 T522 G523 I524 C525 D526 I529 A535 A536 D541 V546 I547 Q548 R553 T559 T582 D595 W596 T599 LYS

4 Data and refinement statistics (i)

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	0.39	1/3937 (0.0%)	0.61	3/5405 (0.1%)
1	B	0.80	7/3883 (0.2%)	0.58	6/5328 (0.1%)
1	C	0.74	6/3899 (0.2%)	0.69	6/5350 (0.1%)
All	All	0.67	14/11719 (0.1%)	0.63	15/16083 (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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	380	GLU	CB-CG	33.94	2.16	1.52
1	B	148	GLU	CG-CD	-27.89	1.10	1.51
1	B	532	ARG	CZ-NH1	19.78	1.58	1.33
1	B	379	ARG	CB-CG	-17.65	1.04	1.52
1	C	516	GLN	CA-CB	16.70	1.90	1.53
1	B	317	ASP	CA-CB	-12.41	1.26	1.53
1	B	532	ARG	CD-NE	11.62	1.66	1.46
1	B	532	ARG	CZ-NH2	11.51	1.48	1.33
1	B	380	GLU	CB-CG	9.37	1.70	1.52
1	A	516	GLN	CA-CB	7.34	1.70	1.53
1	C	516	GLN	N-CA	6.63	1.59	1.46
1	C	439	ARG	CD-NE	5.97	1.56	1.46
1	C	385	ASP	CG-OD1	5.54	1.38	1.25
1	C	385	ASP	CG-OD2	5.28	1.37	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	516	GLN	N-CA-CB	-26.18	63.47	110.60
1	A	516	GLN	N-CA-CB	14.16	136.10	110.60
1	A	464	ARG	NE-CZ-NH1	-11.55	114.52	120.30
1	A	464	ARG	NE-CZ-NH2	10.35	125.47	120.30
1	B	532	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	B	532	ARG	CD-NE-CZ	-7.69	112.83	123.60
1	C	516	GLN	CB-CA-C	-7.66	95.08	110.40
1	B	148	GLU	CB-CG-CD	7.63	134.80	114.20
1	B	317	ASP	N-CA-CB	7.17	123.51	110.60
1	B	380	GLU	CA-CB-CG	-6.70	98.67	113.40
1	C	380	GLU	CA-CB-CG	6.21	127.06	113.40
1	C	439	ARG	CD-NE-CZ	-6.19	114.93	123.60
1	B	532	ARG	NH1-CZ-NH2	5.58	125.54	119.40
1	C	379	ARG	CB-CA-C	-5.46	99.49	110.40
1	C	380	GLU	CB-CG-CD	5.31	128.53	114.20

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
1	C	464	ARG	Sidechain

5.2 Too-close contacts (i)

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	51	0
1	B	3804	0	3792	37	1
1	C	3820	0	3809	39	0
2	A	231	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	82	0	0	0	0
2	C	223	0	0	5	0
All	All	12015	0	11442	126	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 (126) 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: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
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:281:MET:HE3	1:B:405:VAL:HG11	1.79	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:281:MET:CE	1:B:405:VAL:HG21	2.38	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:29:ILE:HD12	1:B:226:PRO:HB3	1.99	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:318:ASP:O	1:B:319:ASN:HB2	2.21	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: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 (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	510/621 (82%)	493 (97%)	14 (3%)	3 (1%)	25	36
1	B	503/621 (81%)	487 (97%)	15 (3%)	1 (0%)	47	62
1	C	505/621 (81%)	490 (97%)	12 (2%)	3 (1%)	25	36
All	All	1518/1863 (82%)	1470 (97%)	41 (3%)	7 (0%)	29	41

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 (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	412/502 (82%)	401 (97%)	11 (3%)	44	65
1	B	406/502 (81%)	399 (98%)	7 (2%)	60	78
1	C	408/502 (81%)	400 (98%)	8 (2%)	55	74
All	All	1226/1506 (81%)	1200 (98%)	26 (2%)	53	72

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	74	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	A	564	LEU
1	B	74	THR
1	B	144	VAL
1	B	203	THR
1	B	288	GLN
1	B	317	ASP

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Mol	Chain	Res	Type
1	B	564	LEU
1	B	582	THR
1	C	74	THR
1	C	109	THR
1	C	142	THR
1	C	276	VAL
1	C	351	GLU
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	207	GLN
1	A	296	GLN
1	A	327	GLN
1	B	288	GLN
1	B	296	GLN
1	B	577	GLN
1	C	52	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.