Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 12:38 PM EST

PDB ID	:	1AVH
Title	:	CRYSTAL AND MOLECULAR STRUCTURE OF HUMAN ANNEXIN V AFTER REFINEMENT. IMPLICATIONS FOR STRUCTURE, MEMBRANE BINDING AND ION CHANNEL FORMATION OF THE ANNEXIN FAMILY OF PROTEINS
Authors	:	Huber, R.; Berendes, R.; Burger, A.; Schneider, M.; Karshikov, A.; Luecke, H.; Roemisch, J.; Paques, E.
Deposited on	:	1991-10-17
Resolution	:	2.30 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:

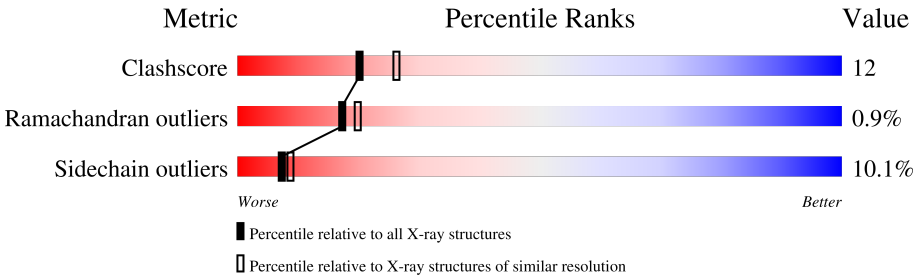
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	320	65% 27% 7%
1	B	320	64% 28% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5326 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.

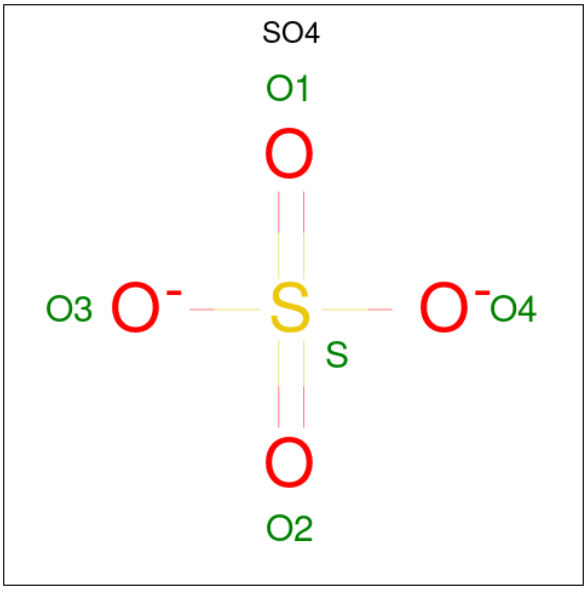
- Molecule 1 is a protein called ANNEXIN V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	22	0	0
			2513	1582	422	501	8			
1	B	318	Total	C	N	O	S	34	0	0
			2513	1582	422	501	8			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	128	Total O 128 128	1	0
4	B	147	Total O 147 147	0	0

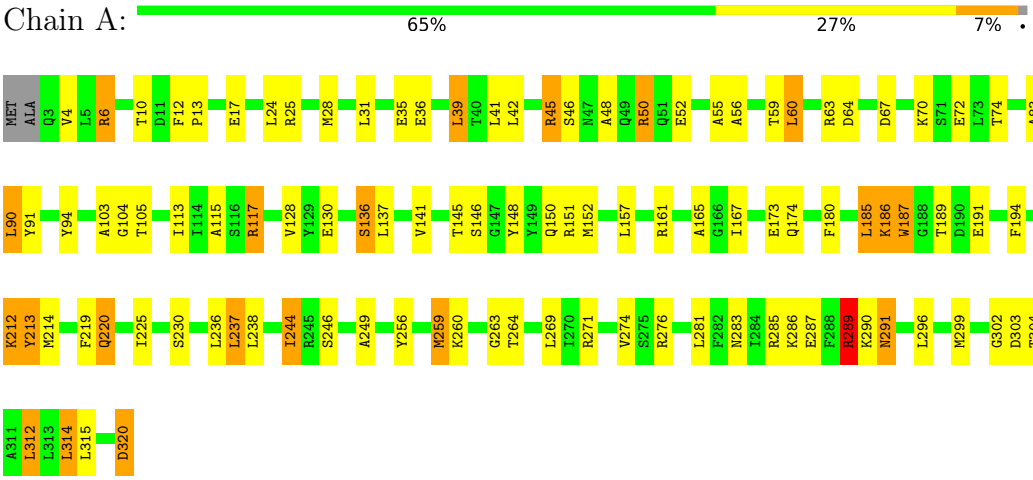
3 Residue-property plots (i)

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.

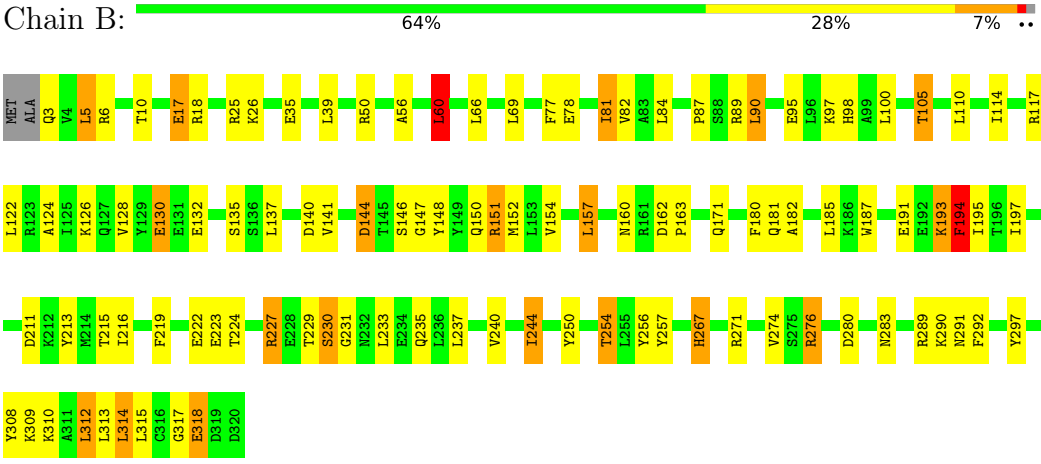
• Molecule 1: ANNEXIN V

Chain A:



• Molecule 1: ANNEXIN V

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	98.80Å 98.80Å 129.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5326	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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: SO4, CA

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	0.88	1/2547 (0.0%)	1.42	10/3427 (0.3%)
1	B	0.89	1/2547 (0.0%)	1.41	11/3427 (0.3%)
All	All	0.88	2/5094 (0.0%)	1.41	21/6854 (0.3%)

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	18
1	B	0	12
All	All	0	30

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	TRP	NE1-CE2	-7.81	1.27	1.37
1	B	187	TRP	NE1-CE2	-7.19	1.28	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	A	117	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	B	194	PHE	CB-CA-C	-9.92	90.57	110.40
1	B	201	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	161	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	B	227	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	25	ARG	NE-CZ-NH2	-7.37	116.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	50	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	227	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	271	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	117	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	B	271	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	213	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	A	39	LEU	N-CA-CB	-5.82	98.76	110.40
1	A	50	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	257	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	B	256	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	201	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	256	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	B	227	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	115	ALA	N-CA-CB	5.06	117.19	110.10

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	SER	Mainchain
1	A	165	ALA	Mainchain
1	A	187	TRP	Mainchain
1	A	212	LYS	Mainchain
1	A	244	ILE	Mainchain
1	A	259	MET	Mainchain
1	A	263	GLY	Mainchain
1	A	264	THR	Mainchain
1	A	276	ARG	Mainchain
1	A	286	LYS	Mainchain
1	A	289	ARG	Mainchain
1	A	303	ASP	Mainchain
1	A	304	THR	Mainchain
1	A	36	GLU	Mainchain
1	A	6	ARG	Mainchain
1	A	70	LYS	Mainchain
1	A	87	PRO	Mainchain
1	A	90	LEU	Mainchain
1	B	119	PRO	Mainchain
1	B	146	SER	Mainchain
1	B	194	PHE	Mainchain
1	B	229	THR	Mainchain
1	B	230	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	B	231	GLY	Peptide,Mainchain
1	B	276	ARG	Mainchain
1	B	303	ASP	Mainchain
1	B	317	GLY	Mainchain
1	B	318	GLU	Mainchain
1	B	60	LEU	Mainchain

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	2513	0	2514	60	1
1	B	2513	0	2514	64	1
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	128	0	0	2	1
4	B	147	0	0	3	2
All	All	5326	0	5028	124	4

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 12.

All (124) 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:185:LEU:HD23	1:A:189:THR:HB	1.45	0.97
1:A:24:LEU:HD13	1:A:41:LEU:HD13	1.64	0.80
1:B:6:ARG:H	1:B:283:ASN:HD21	1.36	0.72
1:A:6:ARG:H	1:A:283:ASN:HD21	1.36	0.72
1:A:225:ILE:HD12	1:A:238:LEU:HD13	1.72	0.71
1:B:39:LEU:HD12	1:B:77:PHE:CE1	2.29	0.67
1:B:126:LYS:HG2	1:B:137:LEU:HD23	1.76	0.66
1:B:307:ASP:HA	1:B:310:LYS:HD2	1.79	0.64
1:A:39:LEU:CD2	1:A:314:LEU:HD23	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:OG1	1:A:150:GLN:HG3	1.98	0.63
1:B:193:LYS:HE3	1:B:193:LYS:N	2.16	0.61
1:A:55:ALA:O	1:A:59:THR:HG23	2.01	0.60
1:A:6:ARG:H	1:A:283:ASN:ND2	1.98	0.60
1:A:24:LEU:HD21	1:A:42:LEU:HD21	1.82	0.59
1:A:90:LEU:HD23	1:A:128:VAL:CG1	2.34	0.57
1:A:64:ASP:HB3	1:A:67:ASP:HB2	1.85	0.56
1:A:285:ARG:HH21	1:A:320:ASP:C	2.09	0.56
1:B:130:GLU:HA	1:B:135:SER:O	2.05	0.56
1:A:214:MET:HA	1:A:219:PHE:O	2.05	0.56
1:B:297:TYR:CD2	1:B:313:LEU:HD22	2.42	0.55
1:A:308:TYR:O	1:A:312:LEU:HB2	2.08	0.54
1:B:120:GLU:HB2	4:B:880:HOH:O	2.06	0.54
1:A:35:GLU:O	1:A:39:LEU:HB2	2.09	0.53
1:B:193:LYS:HE3	1:B:193:LYS:H	1.72	0.53
1:A:302:GLY:HA3	4:A:854:HOH:O	2.08	0.52
1:B:308:TYR:O	1:B:312:LEU:HB2	2.10	0.52
1:B:87:PRO:HG2	1:B:90:LEU:HD12	1.91	0.51
1:B:90:LEU:HD21	1:B:132:GLU:HG2	1.91	0.51
1:A:46:SER:O	1:A:50:ARG:HG3	2.10	0.51
1:A:214:MET:HE2	1:A:220:GLN:HB3	1.92	0.51
1:B:213:TYR:OH	1:B:224:THR:HG21	2.10	0.51
1:A:269:LEU:HD23	1:A:312:LEU:HD21	1.93	0.51
1:A:83:ALA:HB1	1:A:274:VAL:HG11	1.92	0.50
1:B:150:GLN:O	1:B:154:VAL:HG23	2.11	0.50
1:A:12:PHE:HB2	1:A:45:ARG:HD2	1.93	0.49
1:B:84:LEU:HD23	1:B:274:VAL:HG22	1.93	0.49
1:B:78:GLU:O	1:B:82:VAL:HG23	2.13	0.48
1:A:180:PHE:HA	1:A:213:TYR:CE2	2.49	0.48
1:B:87:PRO:HG2	1:B:90:LEU:CD1	2.43	0.48
1:A:249:ALA:HA	1:A:287:GLU:HG2	1.96	0.48
1:A:152:MET:HE3	1:A:237:LEU:HD13	1.95	0.48
1:A:220:GLN:H	1:A:220:GLN:HG3	1.57	0.48
1:B:6:ARG:H	1:B:283:ASN:ND2	2.08	0.48
1:A:130:GLU:HG3	1:A:136:SER:HA	1.96	0.47
1:B:197:ILE:O	1:B:201:ARG:HG2	2.14	0.47
1:B:219:PHE:HE1	1:B:224:THR:HG22	1.80	0.47
1:A:12:PHE:CB	1:A:45:ARG:HD2	2.44	0.47
1:B:147:GLY:HA2	4:B:875:HOH:O	2.14	0.47
1:A:152:MET:HG2	1:A:236:LEU:HD21	1.97	0.47
1:A:312:LEU:HD12	1:A:312:LEU:HA	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLN:O	1:B:185:LEU:HB2	2.14	0.47
1:A:39:LEU:HD11	1:A:310:LYS:CB	2.45	0.46
1:A:152:MET:CE	1:A:237:LEU:HD13	2.44	0.46
1:B:304:THR:OG1	1:B:309:LYS:HB3	2.15	0.46
1:B:162:ASP:HA	1:B:163:PRO:HD3	1.66	0.46
1:B:250:TYR:O	1:B:254:THR:HG23	2.14	0.46
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.77	0.46
1:A:91:TYR:O	1:A:94:TYR:HB3	2.16	0.45
1:B:5:LEU:HG	1:B:280:ASP:HB3	1.98	0.45
1:A:28:MET:SD	1:A:72:GLU:HG3	2.56	0.45
1:A:39:LEU:HD11	1:A:310:LYS:HB2	1.98	0.45
1:A:214:MET:CE	1:A:220:GLN:HB3	2.46	0.45
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.80	0.45
1:B:39:LEU:HD12	1:B:77:PHE:CZ	2.52	0.45
1:B:110:LEU:O	1:B:114:ILE:HB	2.17	0.45
1:B:124:ALA:O	1:B:128:VAL:HG23	2.17	0.44
1:B:283:ASN:ND2	1:B:283:ASN:H	2.15	0.44
1:B:182:ALA:HB1	1:B:194:PHE:HE1	1.82	0.44
1:B:240:VAL:O	1:B:244:ILE:HD13	2.18	0.44
1:B:152:MET:HE3	1:B:237:LEU:HD12	1.98	0.44
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.75	0.44
1:A:4:VAL:HG12	1:A:6:ARG:HG3	1.99	0.44
1:A:289:ARG:HE	1:A:289:ARG:HB2	1.57	0.44
1:B:56:ALA:O	1:B:60:LEU:HB2	2.18	0.44
1:B:152:MET:O	1:B:152:MET:HG3	2.18	0.44
1:B:283:ASN:H	1:B:283:ASN:HD22	1.66	0.44
1:A:56:ALA:O	1:A:60:LEU:HB2	2.18	0.43
1:A:152:MET:CE	1:A:237:LEU:CD1	2.95	0.43
1:A:173:GLU:HG3	1:A:212:LYS:HE2	2.00	0.43
1:B:128:VAL:O	1:B:132:GLU:HB2	2.19	0.43
1:B:35:GLU:O	1:B:39:LEU:HB2	2.18	0.43
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.66	0.43
1:B:66:LEU:HD12	1:B:69:LEU:HB2	1.99	0.43
1:B:297:TYR:CE2	1:B:313:LEU:HB3	2.54	0.43
1:A:186:LYS:O	1:A:186:LYS:HE3	2.19	0.43
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.77	0.43
1:A:113:ILE:O	1:A:117:ARG:HD3	2.19	0.43
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.87	0.43
1:A:12:PHE:HA	1:A:13:PRO:HD3	1.84	0.42
1:B:276:ARG:HA	1:B:276:ARG:HD2	1.91	0.42
1:A:152:MET:HE3	1:A:237:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:O	1:A:291:ASN:HB2	2.19	0.42
1:B:211:ASP:O	1:B:215:THR:HG23	2.19	0.42
1:A:207:ARG:HG3	1:A:244:ILE:HG22	2.00	0.42
1:A:285:ARG:HG3	1:A:296:LEU:HD23	2.00	0.42
1:A:25:ARG:NE	4:A:807:HOH:O	2.52	0.42
1:A:152:MET:O	1:A:152:MET:HG3	2.20	0.42
1:B:151:ARG:HH11	1:B:151:ARG:HD3	1.62	0.42
1:B:314:LEU:HD12	1:B:314:LEU:HA	1.86	0.42
1:A:137:LEU:O	1:A:141:VAL:HG23	2.20	0.42
1:B:137:LEU:O	1:B:141:VAL:HG23	2.20	0.42
1:A:174:GLN:HE21	1:A:174:GLN:HB3	1.35	0.41
1:A:191:GLU:HG3	1:A:194:PHE:CZ	2.55	0.41
1:B:26:LYS:HE2	1:B:26:LYS:HB3	1.83	0.41
1:B:81:ILE:HD12	1:B:81:ILE:HA	1.89	0.41
1:B:194:PHE:HE2	1:B:233:LEU:HD21	1.86	0.41
1:B:17:GLU:H	1:B:17:GLU:HG3	1.45	0.41
1:B:18:ARG:HH11	1:B:18:ARG:HD3	1.70	0.41
1:A:48:ALA:O	1:A:52:GLU:HG2	2.20	0.41
1:B:191:GLU:O	1:B:195:ILE:HG13	2.21	0.41
1:B:201:ARG:HB2	1:B:206:LEU:HG	2.02	0.41
1:B:180:PHE:HA	1:B:213:TYR:CE1	2.56	0.41
1:B:100:LEU:HD22	1:B:144:ASP:HB2	2.03	0.41
1:A:148:TYR:HA	1:A:151:ARG:HB2	2.03	0.40
1:A:312:LEU:O	1:A:315:LEU:HB2	2.21	0.40
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.83	0.40
1:B:148:TYR:HA	1:B:151:ARG:HB2	2.03	0.40
1:B:216:ILE:HD13	1:B:216:ILE:HG21	1.90	0.40
1:B:100:LEU:HD23	1:B:105:THR:HG23	2.04	0.40
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.90	0.40
1:B:291:ASN:HD22	1:B:291:ASN:HA	1.34	0.40
1:B:100:LEU:HD13	1:B:140:ASP:HB3	2.02	0.40
1:B:180:PHE:HA	1:B:213:TYR:HE1	1.86	0.40
1:B:267:HIS:HD2	4:B:790:HOH:O	2.03	0.40

All (4) 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)
4:B:867:HOH:O	4:B:884:HOH:O[2_665]	0.98	1.22
4:A:848:HOH:O	4:B:651:HOH:O[2_665]	1.35	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:NH1	1:A:151:ARG:NH2[3_565]	2.01	0.19
1:B:181:GLN:NE2	1:B:292:PHE:O[2_675]	2.03	0.17

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	316/320 (99%)	299 (95%)	13 (4%)	4 (1%)	12 12
1	B	316/320 (99%)	301 (95%)	13 (4%)	2 (1%)	25 31
All	All	632/640 (99%)	600 (95%)	26 (4%)	6 (1%)	17 20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ALA
1	A	104	GLY
1	B	318	GLU
1	A	230	SER
1	A	246	SER
1	B	230	SER

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	271/272 (100%)	249 (92%)	22 (8%)	11 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	271/272 (100%)	238 (88%)	33 (12%)	5 5
All	All	542/544 (100%)	487 (90%)	55 (10%)	7 9

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

Mol	Chain	Res	Type
1	A	10	THR
1	A	17	GLU
1	A	45	ARG
1	A	60	LEU
1	A	74	THR
1	A	105	THR
1	A	136	SER
1	A	157	LEU
1	A	167	ILE
1	A	185	LEU
1	A	186	LYS
1	A	220	GLN
1	A	237	LEU
1	A	259	MET
1	A	260	LYS
1	A	289	ARG
1	A	290	LYS
1	A	291	ASN
1	A	299	MET
1	A	312	LEU
1	A	314	LEU
1	A	320	ASP
1	B	3	GLN
1	B	5	LEU
1	B	10	THR
1	B	17	GLU
1	B	60	LEU
1	B	81	ILE
1	B	89	ARG
1	B	90	LEU
1	B	95	GLU
1	B	97	LYS
1	B	98	HIS
1	B	105	THR
1	B	130	GLU
1	B	144	ASP

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Mol	Chain	Res	Type
1	B	151	ARG
1	B	157	LEU
1	B	160	ASN
1	B	171	GLN
1	B	193	LYS
1	B	200	THR
1	B	222	GLU
1	B	223	GLU
1	B	227	ARG
1	B	235	GLN
1	B	244	ILE
1	B	254	THR
1	B	267	HIS
1	B	289	ARG
1	B	290	LYS
1	B	303	ASP
1	B	312	LEU
1	B	314	LEU
1	B	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	174	GLN
1	A	181	GLN
1	A	283	ASN
1	B	3	GLN
1	B	51	GLN
1	B	106	ASN
1	B	127	GLN
1	B	232	ASN
1	B	235	GLN
1	B	283	ASN
1	B	291	ASN

5.3.3 RNA

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 (i)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	542	-	4,4,4	0.95	0	6,6,6	0.17	0
3	SO4	A	543	-	4,4,4	1.04	0	6,6,6	0.40	0
3	SO4	B	545	-	4,4,4	1.21	0	6,6,6	0.15	0
3	SO4	A	541	-	4,4,4	0.72	0	6,6,6	0.29	0

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 (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.