



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:41 AM UTC

PDB ID : 6GBH / pdb_00006gbh
Title : Helicobacter pylori adhesin HopQ type II bound to the N-terminal domain of human CEACAM1
Authors : Moonens, K.; Kruse, T.; Gerhard, M.; Remaut, H.
Deposited on : 2018-04-13
Resolution : 2.59 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

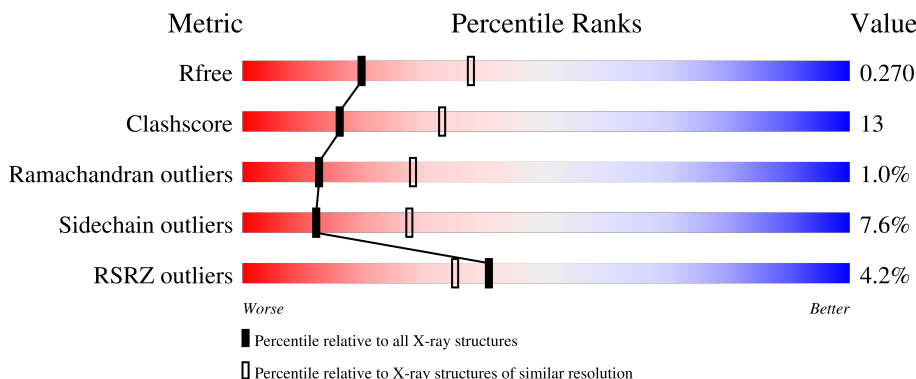
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	115	4% 60% 30% • 6%
1	D	115	2% 71% 18% • • 6%
2	A	425	3% 51% 21% • 25%
2	C	425	4% 52% 20% • 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6490 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 Carcinoembryonic antigen-related cell adhesion molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	108	Total	C	N	O	S	0	0	0
			847	537	143	166	1			
1	D	108	Total	C	N	O	S	0	1	0
			852	540	144	167	1			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P13688
B	109	HIS	-	expression tag	UNP P13688
B	110	HIS	-	expression tag	UNP P13688
B	111	HIS	-	expression tag	UNP P13688
B	112	HIS	-	expression tag	UNP P13688
B	113	HIS	-	expression tag	UNP P13688
B	114	HIS	-	expression tag	UNP P13688
D	0	MET	-	initiating methionine	UNP P13688
D	109	HIS	-	expression tag	UNP P13688
D	110	HIS	-	expression tag	UNP P13688
D	111	HIS	-	expression tag	UNP P13688
D	112	HIS	-	expression tag	UNP P13688
D	113	HIS	-	expression tag	UNP P13688
D	114	HIS	-	expression tag	UNP P13688

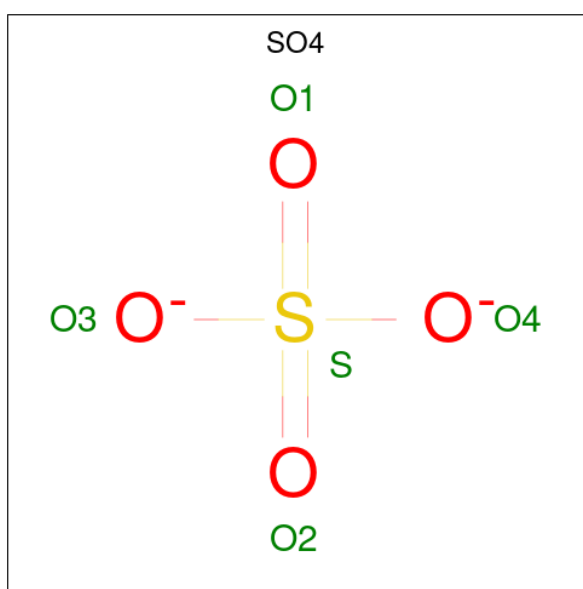
- Molecule 2 is a protein called HopQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	318	Total	C	N	O	S	0	0	0
			2367	1453	411	495	8			
2	A	318	Total	C	N	O	S	0	1	0
			2378	1461	414	495	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q8GDI6
C	435	HIS	-	expression tag	UNP Q8GDI6
C	436	HIS	-	expression tag	UNP Q8GDI6
C	437	HIS	-	expression tag	UNP Q8GDI6
C	438	HIS	-	expression tag	UNP Q8GDI6
C	439	HIS	-	expression tag	UNP Q8GDI6
C	440	HIS	-	expression tag	UNP Q8GDI6
A	16	MET	-	initiating methionine	UNP Q8GDI6
A	435	HIS	-	expression tag	UNP Q8GDI6
A	436	HIS	-	expression tag	UNP Q8GDI6
A	437	HIS	-	expression tag	UNP Q8GDI6
A	438	HIS	-	expression tag	UNP Q8GDI6
A	439	HIS	-	expression tag	UNP Q8GDI6
A	440	HIS	-	expression tag	UNP Q8GDI6

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

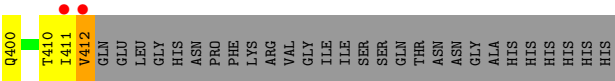
Continued on next page...

Continued from previous page...

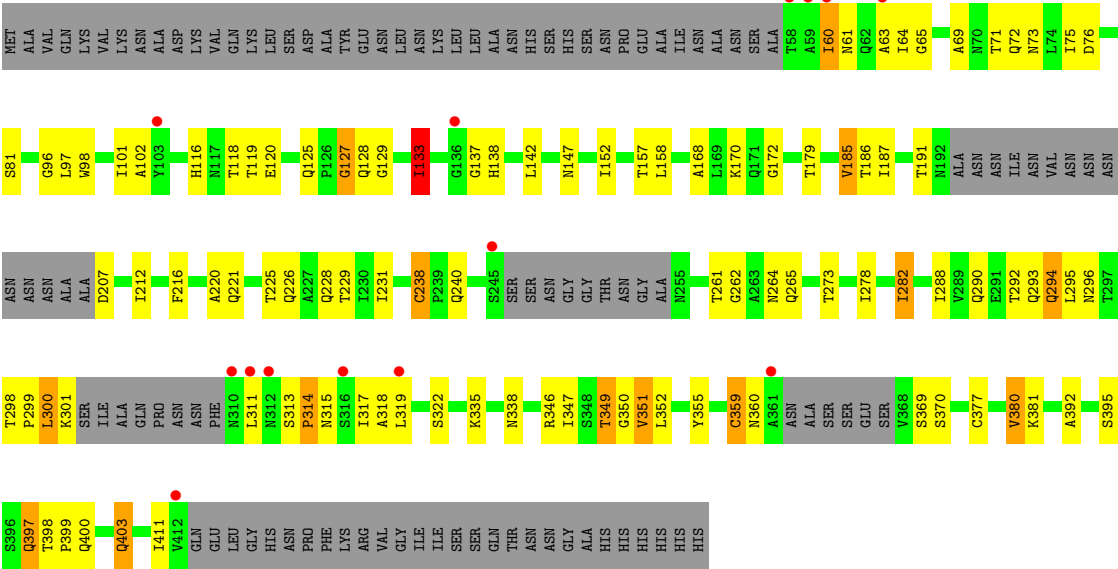
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		
4	C	4	Total	O	0	0
			4	4		



• Molecule 2: HopQ



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.82Å 169.67Å 198.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.05 – 2.59 99.05 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.3 (99.05-2.59) 98.3 (99.05-2.59)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.218 , 0.274 0.222 , 0.270	Depositor DCC
R_{free} test set	2071 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 85.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	B	0.84	1/866 (0.1%)	1.02	2/1181 (0.2%)
1	D	0.85	1/874 (0.1%)	1.00	5/1192 (0.4%)
2	A	1.03	0/2406	1.31	20/3272 (0.6%)
2	C	1.02	1/2391 (0.0%)	1.19	17/3250 (0.5%)
All	All	0.98	3/6537 (0.0%)	1.19	44/8895 (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	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	GLN	N-CA	-8.17	1.36	1.46
1	B	43	ARG	CA-C	5.80	1.60	1.52
2	C	149	SER	CA-C	-5.10	1.46	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	128	GLN	N-CA-C	14.21	126.46	110.97
2	A	349	THR	N-CA-C	10.02	121.89	110.97
2	A	347	ILE	CB-CA-C	-8.47	100.92	112.02
2	C	303	ILE	N-CA-CB	7.92	124.97	111.50
2	A	349	THR	CB-CA-C	-7.82	98.92	110.96
2	A	355	TYR	N-CA-C	7.29	119.85	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	75	ILE	CB-CA-C	-7.25	102.53	112.24
2	A	128	GLN	CB-CA-C	-7.25	99.80	110.96
2	A	170	LYS	N-CA-C	-7.08	103.49	111.07
2	A	282	ILE	CB-CA-C	-6.88	102.90	111.70
2	C	58	THR	N-CA-C	-6.82	103.85	111.28
2	C	282	ILE	CB-CA-C	-6.44	103.73	111.97
2	C	117	ASN	N-CA-C	6.39	121.34	112.45
2	C	282	ILE	N-CA-CB	6.25	117.86	110.55
2	C	282	ILE	N-CA-C	-6.22	104.45	110.42
2	A	129	GLY	N-CA-C	-6.18	98.53	113.18
2	A	133	ILE	CB-CA-C	-6.09	102.39	110.98
2	C	302	SER	CB-CA-C	-6.08	99.49	112.63
1	D	53	GLN	N-CA-C	6.00	119.69	111.54
2	A	294	GLN	N-CA-C	-5.99	104.83	111.36
2	A	359	CYS	N-CA-C	5.97	116.30	107.88
1	D	58	GLY	CA-C-N	5.97	125.45	119.24
1	D	58	GLY	C-N-CA	5.97	125.45	119.24
2	A	380	VAL	N-CA-C	5.92	116.04	110.30
2	C	173	LEU	CA-C-N	-5.91	114.46	120.85
2	C	173	LEU	C-N-CA	-5.91	114.46	120.85
1	B	11	VAL	N-CA-C	5.88	117.12	107.24
2	C	113	LYS	N-CA-C	-5.82	101.50	108.25
2	A	127	GLY	N-CA-C	-5.80	103.72	112.60
2	A	238	CYS	CA-C-N	-5.80	114.28	120.03
2	A	238	CYS	C-N-CA	-5.80	114.28	120.03
2	C	109	GLY	N-CA-C	-5.64	105.33	112.54
2	C	75	ILE	N-CA-C	5.59	117.09	111.00
2	C	237	ASN	N-CA-C	5.51	120.13	113.41
1	D	24	LEU	CA-C-N	-5.44	113.04	119.84
1	D	24	LEU	C-N-CA	-5.44	113.04	119.84
2	A	228	GLN	N-CA-C	-5.26	105.54	111.28
1	B	16	GLU	N-CA-CB	-5.21	103.48	111.56
2	A	351	VAL	N-CA-C	5.20	116.55	110.62
2	C	258	SER	CB-CA-C	-5.19	100.08	110.42
2	A	81	SER	CA-C-N	5.18	124.80	119.05
2	A	81	SER	C-N-CA	5.18	124.80	119.05
2	C	217	ILE	CB-CA-C	5.16	117.20	110.96
2	C	127	GLY	N-CA-C	-5.02	104.92	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	25	PRO	Peptide

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	B	847	0	821	23	0
1	D	852	0	827	16	0
2	A	2378	0	2341	66	0
2	C	2367	0	2329	67	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
3	C	5	0	0	1	0
3	D	15	0	0	1	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
All	All	6490	0	6318	169	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 13.

All (169) 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)
2:C:261:THR:O	2:C:263:ALA:N	1.77	1.16
1:B:83:THR:HB	1:B:106:VAL:HG12	1.45	0.98
2:C:316:SER:HA	2:C:319:LEU:HD23	1.53	0.88
2:A:346:ARG:O	2:A:349:THR:HB	1.75	0.87
2:A:120:GLU:HG3	2:A:152:ILE:HG21	1.54	0.87
2:C:118:THR:O	2:C:119:THR:OG1	1.95	0.84
2:C:152:ILE:H	2:C:152:ILE:HD12	1.49	0.78
2:A:75:ILE:HD13	2:A:296:ASN:HB2	1.66	0.77
2:C:75:ILE:HG12	2:C:292:THR:CG2	2.15	0.76
1:B:26:GLN:HG2	1:B:27:GLN:HG2	1.69	0.73
2:C:75:ILE:HG12	2:C:292:THR:HG22	1.69	0.73
2:C:75:ILE:CG2	2:C:177:SER:HB3	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:ILE:HG22	2:C:177:SER:HB3	1.70	0.71
2:C:75:ILE:CD1	2:C:296:ASN:HB2	2.20	0.71
2:C:392:ALA:O	2:A:403:GLN:HG2	1.89	0.71
2:C:179:THR:O	2:C:217:ILE:HD11	1.91	0.70
2:C:97:LEU:HD22	2:C:278:ILE:HD12	1.72	0.70
1:B:26:GLN:N	1:B:26:GLN:OE1	2.25	0.69
2:A:298:THR:HG22	2:A:298:THR:O	1.93	0.69
1:D:41:GLY:HA3	2:C:114:PRO:O	1.93	0.68
1:B:80:GLN:O	1:B:83:THR:HG22	1.95	0.67
1:D:48:TYR:OH	1:D:53:GLN:HB3	1.96	0.66
2:A:349:THR:HG22	2:A:350:GLY:N	2.08	0.66
2:C:118:THR:HG22	2:C:119:THR:H	1.62	0.64
1:B:31:TYR:HE1	1:B:67:ILE:HD11	1.62	0.64
2:A:187:ILE:HD12	2:A:187:ILE:O	2.00	0.62
2:C:191:THR:O	2:C:207:ASP:HB2	1.99	0.61
2:C:231:ILE:HD11	2:C:278:ILE:HG22	1.82	0.61
2:A:60:ILE:O	2:A:63:ALA:N	2.33	0.61
2:C:124:ASN:HB3	2:C:163:GLN:HE22	1.64	0.61
2:A:152:ILE:HD12	2:A:152:ILE:H	1.65	0.61
2:C:75:ILE:CG1	2:C:292:THR:CG2	2.78	0.61
2:A:191:THR:O	2:A:207:ASP:HB3	2.02	0.60
2:A:319:LEU:HA	2:A:322:SER:HB3	1.83	0.60
2:C:231:ILE:CD1	2:C:278:ILE:HG22	2.32	0.59
2:C:119:THR:HG22	2:C:119:THR:O	2.03	0.59
2:A:290:GLN:O	2:A:293:GLN:HB2	2.02	0.59
2:C:75:ILE:HD13	2:C:296:ASN:HB2	1.84	0.59
2:A:120:GLU:HG3	2:A:152:ILE:CG2	2.28	0.59
2:C:295:LEU:HA	2:C:298:THR:HG22	1.85	0.58
1:B:31:TYR:CE1	1:B:67:ILE:HD11	2.38	0.58
2:C:125:GLN:HG3	2:C:126:PRO:HD2	1.84	0.58
2:A:71:THR:O	2:A:72:GLN:C	2.46	0.58
1:D:24:LEU:HD12	1:D:25:PRO:CD	2.34	0.58
1:D:106:VAL:O	1:D:106:VAL:HG22	2.04	0.57
2:A:231:ILE:CD1	2:A:282:ILE:HG13	2.34	0.57
2:C:316:SER:HA	2:C:319:LEU:CD2	2.31	0.56
1:B:7:MET:HE3	1:B:20:LEU:HD12	1.87	0.56
2:C:75:ILE:CG1	2:C:292:THR:HG22	2.33	0.56
2:C:147:ASN:O	2:C:240:GLN:NE2	2.38	0.56
2:A:60:ILE:HG22	2:A:61:ASN:N	2.20	0.55
2:A:138:HIS:ND1	3:A:501:SO4:O2	2.32	0.55
2:A:392:ALA:O	2:A:395:SER:OG	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:395:SER:O	2:A:398:THR:HG22	2.07	0.54
1:B:7:MET:CE	1:B:20:LEU:HD12	2.37	0.54
2:A:75:ILE:HG22	2:A:76:ASP:OD1	2.07	0.54
2:A:319:LEU:HA	2:A:322:SER:CB	2.38	0.54
2:C:120:GLU:HG3	2:C:190:ALA:O	2.08	0.53
1:B:40:ASP:O	1:B:41:GLY:C	2.52	0.52
2:C:240:GLN:HG3	2:C:264:ASN:HB3	1.91	0.52
2:C:69:ALA:O	2:C:73:ASN:ND2	2.43	0.52
2:C:261:THR:O	2:C:261:THR:HG22	2.09	0.52
2:A:101:ILE:HD11	2:A:352:LEU:HD11	1.92	0.52
2:A:185:VAL:CG1	2:A:216:PHE:CD2	2.93	0.51
1:D:19:LEU:HD13	1:D:33:TRP:CZ3	2.45	0.51
2:A:185:VAL:CG1	2:A:216:PHE:HD2	2.23	0.51
2:A:261:THR:HG22	2:A:262:GLY:N	2.26	0.51
2:C:101:ILE:HD12	2:C:271:PHE:CZ	2.46	0.50
1:B:32:SER:HB2	1:B:34:TYR:CE1	2.47	0.50
2:C:118:THR:HG22	2:C:119:THR:N	2.24	0.50
2:A:97:LEU:O	2:A:101:ILE:HG12	2.12	0.50
2:C:187:ILE:N	2:C:187:ILE:HD12	2.28	0.49
1:B:88:LEU:O	1:B:99:GLU:HA	2.12	0.49
1:D:35:LYS:HE3	1:D:85:PHE:O	2.13	0.49
1:B:12:ALA:HB3	1:B:15:LYS:HG3	1.94	0.48
2:C:298:THR:HG23	2:C:298:THR:O	2.13	0.48
2:A:127:GLY:CA	2:A:133:ILE:CD1	2.91	0.48
1:D:48:TYR:OH	1:D:53:GLN:CB	2.62	0.48
2:C:82:PRO:HD3	2:C:390:SER:HB3	1.95	0.48
2:C:392:ALA:O	2:C:395:SER:OG	2.32	0.48
1:D:64:ARG:HH22	1:D:82:ASP:CG	2.21	0.48
2:C:118:THR:C	2:C:119:THR:HG1	2.03	0.48
2:A:240:GLN:NE2	2:A:265:GLN:C	2.71	0.48
2:A:314:PRO:C	2:A:315:ASN:CG	2.82	0.48
2:A:359:CYS:SG	2:A:360:ASN:N	2.86	0.48
1:D:97:ASN:ND2	3:C:501:SO4:O1	2.45	0.48
2:A:98:TRP:O	2:A:102:ALA:HB2	2.13	0.48
2:C:103:TYR:CD1	2:C:103:TYR:C	2.92	0.48
2:C:219:ASP:C	2:C:219:ASP:OD1	2.56	0.47
2:A:261:THR:HG22	2:A:262:GLY:H	1.79	0.47
2:C:411:ILE:O	2:C:412:VAL:HG23	2.13	0.47
1:B:3:THR:HB	1:B:22:HIS:HB2	1.94	0.47
2:C:163:GLN:HA	2:C:163:GLN:OE1	2.15	0.47
2:A:152:ILE:HD12	2:A:152:ILE:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:294:GLN:O	2:C:298:THR:HG22	2.15	0.47
2:C:152:ILE:H	2:C:152:ILE:CD1	2.25	0.47
2:A:119:THR:O	2:A:119:THR:OG1	2.33	0.46
2:C:261:THR:C	2:C:263:ALA:N	2.65	0.46
2:C:289:VAL:HG12	2:C:293:GLN:NE2	2.31	0.46
2:A:226:GLN:O	2:A:229:THR:HB	2.15	0.46
1:D:83:THR:HB	1:D:106:VAL:CG1	2.46	0.46
1:B:83:THR:HB	1:B:106:VAL:CG1	2.31	0.45
2:C:94:THR:CG2	2:C:282:ILE:HD11	2.47	0.45
2:C:75:ILE:HG21	2:C:177:SER:HB3	1.97	0.45
2:A:75:ILE:HD11	2:A:292:THR:HB	1.98	0.45
2:A:298:THR:O	2:A:298:THR:CG2	2.63	0.45
2:A:186:THR:HA	2:A:212:ILE:O	2.16	0.45
2:C:325:LYS:O	2:C:329:SER:OG	2.34	0.45
2:A:185:VAL:HG13	2:A:216:PHE:CD2	2.51	0.45
2:A:296:ASN:O	2:A:299:PRO:HD3	2.15	0.45
2:C:75:ILE:HG22	2:C:75:ILE:O	2.14	0.45
2:A:314:PRO:O	2:A:315:ASN:CG	2.60	0.45
2:A:179:THR:CG2	2:A:179:THR:O	2.65	0.45
2:C:392:ALA:O	2:A:403:GLN:CG	2.62	0.45
2:A:311:LEU:HB2	2:A:314:PRO:HB3	1.99	0.45
1:B:35:LYS:HD2	3:B:201:SO4:O3	2.16	0.44
1:D:23:ASN:N	3:D:202:SO4:O3	2.49	0.44
1:D:24:LEU:HD12	1:D:25:PRO:HD3	1.99	0.44
2:A:288:ILE:O	2:A:292:THR:HG23	2.17	0.44
2:A:220:ALA:O	2:A:221:GLN:C	2.59	0.44
2:C:152:ILE:HD12	2:C:152:ILE:N	2.24	0.44
2:C:238:CYS:N	2:C:239:PRO:CD	2.80	0.44
2:A:179:THR:O	2:A:179:THR:HG22	2.17	0.44
2:A:313:SER:N	2:A:314:PRO:HD3	2.33	0.44
1:B:31:TYR:CE1	1:B:71:ALA:HA	2.53	0.44
2:C:233:THR:O	2:C:237:ASN:HB2	2.17	0.44
2:C:293:GLN:O	2:C:294:GLN:C	2.59	0.43
2:A:300:LEU:O	2:A:301:LYS:HB2	2.18	0.43
1:D:40:ASP:OD1	1:D:42:ASN:N	2.51	0.43
2:A:125:GLN:HB3	2:A:133:ILE:HG12	2.00	0.43
1:D:17:VAL:HG22	1:D:18:LEU:N	2.33	0.43
2:A:314:PRO:O	2:A:315:ASN:ND2	2.52	0.43
2:C:165:ILE:O	2:C:169:LEU:HG	2.19	0.43
2:A:69:ALA:O	2:A:73:ASN:ND2	2.48	0.43
2:A:398:THR:N	2:A:399:PRO:CD	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ASP:O	1:D:41:GLY:C	2.61	0.43
2:C:411:ILE:O	2:C:411:ILE:HG22	2.18	0.43
2:A:397:GLN:HA	2:A:400[A]:GLN:OE1	2.19	0.43
2:A:380:VAL:O	2:A:381:LYS:C	2.60	0.42
1:B:68:TYR:HB3	1:B:69:PRO:CD	2.49	0.42
2:C:256:THR:HG22	2:C:257:PRO:O	2.19	0.42
2:C:91:LEU:O	2:C:94:THR:OG1	2.37	0.42
2:A:147:ASN:HA	2:A:238:CYS:O	2.19	0.42
2:A:96:GLY:O	2:A:97:LEU:C	2.62	0.42
1:D:11:VAL:O	1:D:106:VAL:HA	2.19	0.42
2:A:231:ILE:CD1	2:A:282:ILE:CG1	2.98	0.42
2:A:318:ALA:O	2:A:319:LEU:C	2.63	0.42
2:A:116:HIS:HA	2:A:137:GLY:O	2.20	0.41
2:A:168:ALA:O	2:A:172:GLY:N	2.48	0.41
1:B:16:GLU:HG3	1:B:75:ILE:O	2.21	0.41
2:C:359:CYS:SG	2:C:360:ASN:N	2.93	0.41
2:C:400:GLN:OE1	2:C:400:GLN:N	2.53	0.41
2:C:369:SER:OG	2:C:370:SER:N	2.53	0.41
1:B:62:SER:OG	1:B:65:GLU:OE2	2.30	0.41
1:B:68:TYR:HB3	1:B:69:PRO:HD2	2.03	0.41
2:C:146:LYS:O	2:C:147:ASN:HB2	2.20	0.41
2:C:237:ASN:O	2:C:238:CYS:C	2.64	0.41
2:C:94:THR:HG21	2:C:227:ALA:HB1	2.02	0.41
2:A:64:ILE:O	2:A:65:GLY:C	2.64	0.41
2:A:313:SER:HA	2:A:317:ILE:HD11	2.02	0.41
1:B:65:GLU:HA	1:B:74:LEU:O	2.21	0.41
1:B:86:TYR:CE2	1:B:104:PHE:CE2	3.09	0.40
2:A:127:GLY:CA	2:A:133:ILE:HD12	2.51	0.40
2:C:280:ASP:O	2:C:284:ASN:ND2	2.54	0.40
2:A:240:GLN:HG3	2:A:264:ASN:HB3	2.03	0.40
2:A:335:LYS:O	2:A:338:ASN:HB2	2.21	0.40
2:C:81:SER:HA	2:C:82:PRO:HD2	1.98	0.40
1:B:4:THR:CG2	1:B:102:GLY:HA3	2.52	0.40
2:C:231:ILE:HD11	2:C:282:ILE:HD11	2.02	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	B	106/115 (92%)	99 (93%)	6 (6%)	1 (1%)	14	30
1	D	107/115 (93%)	97 (91%)	9 (8%)	1 (1%)	14	30
2	A	309/425 (73%)	273 (88%)	33 (11%)	3 (1%)	12	28
2	C	308/425 (72%)	285 (92%)	20 (6%)	3 (1%)	12	28
All	All	830/1080 (77%)	754 (91%)	68 (8%)	8 (1%)	12	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	57	ALA
2	C	119	THR
2	C	262	GLY
1	B	41	GLY
2	A	314	PRO
1	D	25	PRO
2	A	377	CYS
2	A	60	ILE

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	B	92/99 (93%)	85 (92%)	7 (8%)	12	27
1	D	93/99 (94%)	86 (92%)	7 (8%)	12	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	269/355 (76%)	251 (93%)	18 (7%)	15	33
2	C	268/355 (76%)	245 (91%)	23 (9%)	10	22
All	All	722/908 (80%)	667 (92%)	55 (8%)	12	27

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

Mol	Chain	Res	Type
1	B	19	LEU
1	B	32	SER
1	B	35	LYS
1	B	45	ILE
1	B	50	ILE
1	B	76	GLN
1	B	87	THR
1	D	26	GLN
1	D	27	GLN
1	D	32	SER
1	D	35	LYS
1	D	37	GLU
1	D	53	GLN
1	D	106	VAL
2	C	94	THR
2	C	111	THR
2	C	112	ASP
2	C	125	GLN
2	C	130	SER
2	C	134	THR
2	C	142	LEU
2	C	152	ILE
2	C	185	VAL
2	C	211	SER
2	C	217	ILE
2	C	256	THR
2	C	260	GLN
2	C	273	THR
2	C	276	SER
2	C	303	ILE
2	C	329	SER
2	C	346	ARG
2	C	351	VAL
2	C	372	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	397	GLN
2	C	410	THR
2	C	412	VAL
2	A	118	THR
2	A	133	ILE
2	A	142	LEU
2	A	157	THR
2	A	158	LEU
2	A	185	VAL
2	A	225	THR
2	A	273	THR
2	A	278	ILE
2	A	294	GLN
2	A	295	LEU
2	A	300	LEU
2	A	351	VAL
2	A	369	SER
2	A	370	SER
2	A	397	GLN
2	A	403	GLN
2	A	411	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	ASN
1	B	42	ASN
1	B	44	GLN
1	B	81	ASN
1	D	22	HIS
1	D	23	ASN
2	C	124	ASN
2	C	159	ASN
2	C	163	GLN
2	C	228	GLN
2	C	237	ASN
2	C	326	ASN
2	C	328	GLN
2	A	68	ASN
2	A	128	GLN
2	A	166	GLN
2	A	232	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	284	ASN
2	A	294	GLN
2	A	315	ASN
2	A	360	ASN
2	A	402	ASN

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](#)

8 ligands are modelled in this entry.

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	D	203	-	4,4,4	0.41	0	6,6,6	0.16	0
3	SO4	D	202	-	4,4,4	0.48	0	6,6,6	0.15	0
3	SO4	A	501	-	4,4,4	0.49	0	6,6,6	0.43	0
3	SO4	B	202	-	4,4,4	0.47	0	6,6,6	0.52	0
3	SO4	C	501	-	4,4,4	0.41	0	6,6,6	0.21	0
3	SO4	A	502	-	4,4,4	0.45	0	6,6,6	0.22	0
3	SO4	D	201	-	4,4,4	0.38	0	6,6,6	0.31	0
3	SO4	B	201	-	4,4,4	0.53	0	6,6,6	0.67	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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	SO4	1	0
3	A	501	SO4	1	0
3	C	501	SO4	1	0
3	B	201	SO4	1	0

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	108/115 (93%)	0.70	5 (4%) 37 32	71, 100, 133, 150	0
1	D	108/115 (93%)	0.35	2 (1%) 66 61	66, 101, 128, 144	1 (0%)
2	A	318/425 (74%)	0.30	14 (4%) 39 33	53, 87, 132, 197	1 (0%)
2	C	318/425 (74%)	0.32	15 (4%) 36 30	66, 86, 120, 154	0
All	All	852/1080 (78%)	0.37	36 (4%) 40 35	53, 90, 128, 197	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	361	ALA	6.0
2	A	311	LEU	4.6
2	A	60	ILE	4.6
1	B	16	GLU	4.5
2	C	303	ILE	4.3
2	C	412	VAL	4.0
2	A	319	LEU	3.6
2	A	58	THR	3.5
2	A	412	VAL	3.5
2	C	411	ILE	3.3
1	B	108	PRO	2.8
2	C	179	THR	2.8
1	B	106	VAL	2.7
2	A	245	SER	2.7
2	A	310	ASN	2.6
2	C	367	SER	2.5
2	C	217	ILE	2.5
2	C	317	ILE	2.5
2	C	297	THR	2.4
1	D	7	MET	2.4
2	A	312	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	316	SER	2.4
1	D	108	PRO	2.3
2	C	319	LEU	2.3
1	B	9	PHE	2.3
2	A	59	ALA	2.2
2	A	136	GLY	2.2
2	C	315	ASN	2.1
2	A	316	SER	2.1
1	B	104	PHE	2.1
2	A	63	ALA	2.1
2	A	103	TYR	2.1
2	C	302	SER	2.1
2	C	76	ASP	2.0
2	C	57	ALA	2.0
2	C	75	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	202	5/5	0.60	0.10	121,129,137,137	0
3	SO4	A	501	5/5	0.71	0.12	98,130,136,152	0
3	SO4	D	203	5/5	0.73	0.07	145,160,164,169	0
3	SO4	D	202	5/5	0.75	0.07	136,140,156,164	0
3	SO4	D	201	5/5	0.82	0.08	116,121,142,142	0
3	SO4	B	201	5/5	0.82	0.09	93,107,128,140	0
3	SO4	A	502	5/5	0.84	0.09	109,117,133,155	0
3	SO4	C	501	5/5	0.85	0.07	112,131,141,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.