



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FIG
Title : ROUTES TO CATALYSIS: STRUCTURE OF A CATALYTIC ANTIBODY
AND COMPARISON WITH ITS NATURAL COUNTERPART
Authors : Haynes, M.R.; Stura, E.A.; Hilvert, D.; Wilson, I.A.
Deposited on : 1994-01-07
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

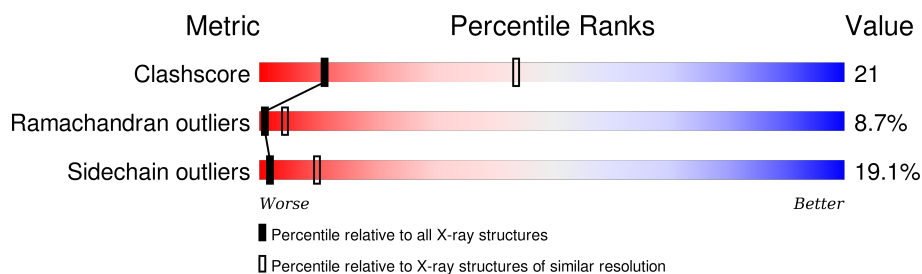
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	215	<div> <div style="width: 40%; background-color: green;"></div> <div style="width: 39%; background-color: yellow;"></div> <div style="width: 20%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>40% 39% 20% .</div>
2	H	216	<div> <div style="width: 38%; background-color: green;"></div> <div style="width: 43%; background-color: yellow;"></div> <div style="width: 15%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>38% 43% 15% .</div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3284 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.

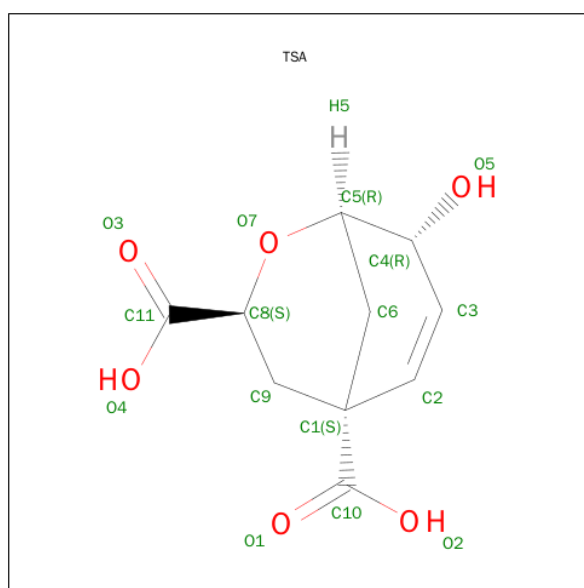
- Molecule 1 is a protein called IGG1-KAPPA 1F7 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1635	1014	272	341	8			

- Molecule 2 is a protein called IGG1-KAPPA 1F7 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1632	1033	272	321	6			

- Molecule 3 is 8-HYDROXY-2-OXA-BICYCLO[3.3.1]NON-6-ENE-3,5-DICARBOXYLIC ACID (three-letter code: TSA) (formula: C₁₀H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is water.

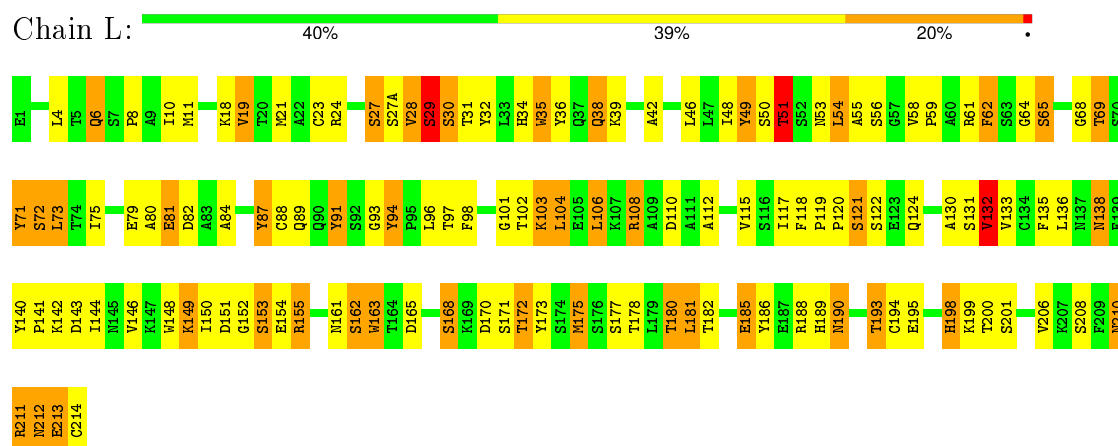
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		

3 Residue-property plots

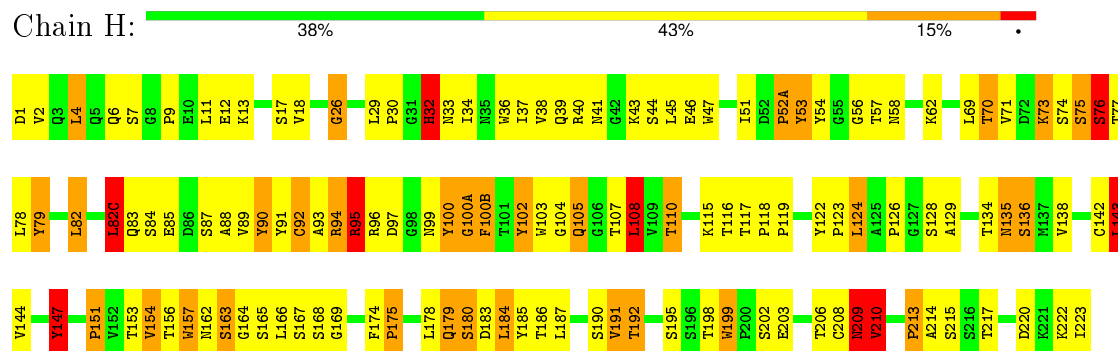
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: IGG1-KAPPA 1F7 FAB (LIGHT CHAIN)



• Molecule 2: IGG1-KAPPA 1F7 FAB (HEAVY CHAIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	37.10Å 63.30Å 178.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3284	wwPDB-VP
Average B, all atoms (Å ²)	3.0	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: TSA

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	L	0.94	0/1671	1.96	49/2269 (2.2%)
2	H	1.02	0/1676	2.07	76/2289 (3.3%)
All	All	0.98	0/3347	2.02	125/4558 (2.7%)

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	L	0	3
2	H	0	2
All	All	0	5

There are no bond length outliers.

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	79	TYR	CB-CG-CD2	-11.00	114.40	121.00
2	H	76	SER	N-CA-CB	-8.29	98.07	110.50
1	L	163	TRP	CD1-CG-CD2	8.21	112.87	106.30
2	H	199	TRP	CD1-CG-CD2	8.01	112.70	106.30
2	H	199	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	L	35	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	L	108	ARG	NE-CZ-NH1	7.19	123.89	120.30
2	H	105	GLN	N-CA-CB	-7.10	97.82	110.60
2	H	167	SER	N-CA-C	-7.09	91.85	111.00
2	H	47	TRP	CD1-CG-CD2	7.00	111.90	106.30
2	H	47	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	L	163	TRP	CE2-CD2-CG	-6.95	101.74	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	149	LYS	CA-CB-CG	6.95	128.68	113.40
1	L	81	GLU	CA-C-N	-6.93	101.95	117.20
1	L	96	LEU	CA-CB-CG	6.91	131.20	115.30
1	L	198	HIS	CA-CB-CG	6.90	125.34	113.60
1	L	175	MET	CA-CB-CG	6.80	124.86	113.30
2	H	217	THR	CA-C-N	-6.80	102.24	117.20
2	H	183	ASP	N-CA-C	-6.78	92.69	111.00
2	H	192	THR	N-CA-C	-6.76	92.75	111.00
2	H	157	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	L	211	ARG	NE-CZ-NH2	-6.69	116.96	120.30
2	H	76	SER	N-CA-C	6.65	128.96	111.00
2	H	157	TRP	CD1-CG-CD2	6.65	111.62	106.30
2	H	103	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	L	146	VAL	CG1-CB-CG2	-6.62	100.30	110.90
1	L	35	TRP	CD1-CG-CD2	6.61	111.59	106.30
2	H	129	ALA	N-CA-C	6.55	128.69	111.00
2	H	105	GLN	CA-CB-CG	6.54	127.79	113.40
2	H	151	PRO	CA-C-N	-6.52	102.85	117.20
1	L	54	LEU	CA-CB-CG	6.50	130.26	115.30
1	L	87	TYR	CA-CB-CG	6.50	125.75	113.40
2	H	100(A)	GLY	N-CA-C	-6.48	96.90	113.10
1	L	62	PHE	N-CA-C	6.43	128.36	111.00
1	L	180	THR	CA-CB-CG2	6.41	121.37	112.40
2	H	36	TRP	CD1-CG-CD2	6.39	111.41	106.30
2	H	103	TRP	CD1-CG-CD2	6.38	111.40	106.30
2	H	209	ASN	O-C-N	-6.35	112.54	122.70
2	H	210	VAL	CA-CB-CG2	-6.34	101.39	110.90
1	L	211	ARG	N-CA-C	6.33	128.08	111.00
2	H	210	VAL	CA-CB-CG1	6.32	120.38	110.90
2	H	36	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	L	73	LEU	N-CA-C	-6.23	94.18	111.00
1	L	108	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	L	91	TYR	CB-CG-CD2	-6.22	117.27	121.00
2	H	79	TYR	CB-CG-CD1	6.22	124.73	121.00
1	L	148	TRP	CE2-CD2-CG	-6.15	102.38	107.30
2	H	96	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	H	94	ARG	N-CA-C	6.06	127.37	111.00
2	H	124	LEU	CA-CB-CG	6.06	129.23	115.30
2	H	83	GLN	CA-CB-CG	6.04	126.68	113.40
2	H	208	CYS	CA-CB-SG	6.03	124.85	114.00
1	L	190	ASN	N-CA-C	5.97	127.11	111.00
1	L	181	LEU	CA-CB-CG	5.96	129.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	90	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	L	28	VAL	N-CA-C	-5.94	94.97	111.00
2	H	180	SER	CA-C-N	-5.94	104.14	117.20
2	H	58	ASN	N-CA-C	-5.91	95.03	111.00
1	L	29	SER	N-CA-C	5.91	126.96	111.00
2	H	151	PRO	N-CA-C	5.91	127.47	112.10
2	H	91	TYR	CB-CG-CD2	-5.90	117.46	121.00
2	H	103	TRP	CG-CD2-CE3	5.82	139.14	133.90
2	H	199	TRP	CB-CG-CD1	-5.81	119.45	127.00
1	L	103	LYS	CA-CB-CG	5.80	126.16	113.40
1	L	194	CYS	CA-CB-SG	5.76	124.36	114.00
1	L	138	ASN	N-CA-C	5.75	126.53	111.00
2	H	94	ARG	CA-CB-CG	5.73	126.00	113.40
2	H	147	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	L	140	TYR	CB-CG-CD1	-5.69	117.58	121.00
2	H	138	VAL	N-CA-C	5.69	126.35	111.00
1	L	146	VAL	CA-C-N	-5.68	104.70	117.20
2	H	136	SER	N-CA-C	5.67	126.30	111.00
1	L	132	VAL	N-CA-C	-5.65	95.75	111.00
2	H	135	ASN	CA-CB-CG	5.64	125.82	113.40
2	H	185	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	L	148	TRP	CD1-CG-CD2	5.60	110.78	106.30
2	H	53	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	H	13	LYS	CA-CB-CG	5.58	125.69	113.40
2	H	143	LEU	CA-CB-CG	5.57	128.10	115.30
1	L	181	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	L	50	SER	C-N-CA	5.55	135.58	121.70
2	H	217	THR	O-C-N	5.55	131.57	122.70
2	H	179	GLN	CA-CB-CG	5.53	125.57	113.40
2	H	13	LYS	N-CA-CB	-5.48	100.73	110.60
2	H	199	TRP	CA-C-N	5.48	132.45	117.10
1	L	108	ARG	CA-CB-CG	5.47	125.44	113.40
2	H	210	VAL	CG1-CB-CG2	-5.47	102.15	110.90
1	L	149	LYS	N-CA-C	-5.46	96.25	111.00
2	H	100(A)	GLY	CA-C-N	-5.45	105.21	117.20
1	L	62	PHE	O-C-N	-5.44	113.99	122.70
2	H	144	VAL	CG1-CB-CG2	-5.43	102.20	110.90
2	H	92	CYS	CA-CB-SG	5.43	123.77	114.00
2	H	102	TYR	CA-CB-CG	5.41	123.67	113.40
2	H	108	LEU	CA-CB-CG	5.40	127.72	115.30
1	L	71	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	L	180	THR	CA-CB-OG1	-5.39	97.67	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	222	LYS	O-C-N	5.39	131.32	122.70
2	H	26	GLY	CA-C-N	5.38	129.03	117.20
1	L	151	ASP	N-CA-C	-5.37	96.50	111.00
2	H	163	SER	N-CA-C	5.36	125.48	111.00
2	H	82(C)	LEU	CA-C-N	-5.35	105.42	117.20
2	H	54	TYR	CA-C-N	5.30	126.81	116.20
1	L	168	SER	N-CA-CB	-5.28	102.58	110.50
2	H	4	LEU	CA-CB-CG	5.27	127.42	115.30
2	H	47	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	L	214	CYS	N-CA-C	5.22	125.09	111.00
1	L	62	PHE	CA-C-N	5.21	128.66	117.20
2	H	95	ARG	CA-CB-CG	5.21	124.86	113.40
1	L	155	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	L	27(A)	SER	N-CA-C	-5.18	97.02	111.00
2	H	220	ASP	N-CA-C	-5.17	97.05	111.00
2	H	96	ARG	N-CA-C	-5.16	97.06	111.00
2	H	136	SER	N-CA-CB	-5.16	102.76	110.50
2	H	75	SER	CA-C-N	-5.14	105.89	117.20
2	H	70	THR	CA-CB-CG2	-5.12	105.23	112.40
2	H	29	LEU	CA-CB-CG	5.11	127.06	115.30
2	H	94	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	L	195	GLU	CA-CB-CG	5.09	124.61	113.40
2	H	209	ASN	CA-CB-CG	5.08	124.57	113.40
1	L	49	TYR	CA-C-N	5.06	128.33	117.20
2	H	73	LYS	CA-CB-CG	5.05	124.51	113.40
2	H	92	CYS	CA-C-N	5.03	128.25	117.20
2	H	115	LYS	CA-CB-CG	5.03	124.46	113.40
1	L	172	THR	N-CA-CB	-5.02	100.76	110.30
1	L	213	GLU	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	147	TYR	Sidechain
2	H	75	SER	Peptide
1	L	119	PRO	Peptide
1	L	186	TYR	Sidechain
1	L	58	VAL	Peptide

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	L	1635	0	1563	77	0
2	H	1632	0	1596	63	0
3	H	16	0	10	5	0
4	H	1	0	0	0	0
All	All	3284	0	3169	134	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 (134) 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:L:149:LYS:HA	1:L:153:SER:HA	1.54	0.87
1:L:150:ILE:HB	1:L:154:GLU:HB3	1.55	0.86
1:L:11:MET:SD	1:L:104:LEU:HG	2.18	0.84
1:L:19:VAL:HG12	1:L:75:ILE:HB	1.60	0.82
2:H:89:VAL:HG12	2:H:108:LEU:HG	1.64	0.80
2:H:118:PRO:HG3	2:H:215:SER:HB2	1.68	0.75
1:L:144:ILE:HD12	1:L:198:HIS:HB2	1.69	0.75
2:H:33:ASN:HB2	3:H:224:TSA:H61	1.68	0.74
1:L:185:GLU:HA	1:L:188:ARG:HH11	1.52	0.74
1:L:49:TYR:HE2	1:L:55:ALA:HB2	1.52	0.73
1:L:149:LYS:HB3	1:L:193:THR:HB	1.72	0.71
2:H:40:ARG:HB3	2:H:43:LYS:HB2	1.72	0.71
1:L:28:VAL:HG12	1:L:31:THR:HA	1.72	0.71
2:H:40:ARG:CB	2:H:43:LYS:HB2	2.21	0.70
2:H:94:ARG:HB3	2:H:102:TYR:HB2	1.73	0.70
1:L:162:SER:HB2	2:H:174:PHE:HB3	1.76	0.66
1:L:121:SER:HB3	1:L:124:GLN:HG3	1.79	0.65
2:H:156:THR:OG1	2:H:209:ASN:HB2	1.97	0.65
1:L:61:ARG:O	1:L:75:ILE:HA	1.97	0.64
1:L:8:PRO:O	1:L:102:THR:HG23	1.96	0.63
1:L:185:GLU:HA	1:L:188:ARG:NH1	2.13	0.63
2:H:124:LEU:HD21	2:H:143:LEU:HD13	1.79	0.63
1:L:181:LEU:HD21	1:L:185:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:27:SER:O	1:L:69:THR:HG23	1.99	0.62
2:H:122:TYR:HB2	2:H:143:LEU:CD2	2.30	0.62
2:H:12:GLU:HG3	2:H:18:VAL:HG22	1.81	0.62
1:L:115:VAL:HG12	1:L:136:LEU:HG	1.81	0.62
2:H:6:GLN:OE1	2:H:104:GLY:HA3	1.99	0.62
2:H:198:THR:O	2:H:203:GLU:HB2	2.01	0.60
1:L:6:GLN:HE22	1:L:101:GLY:HA2	1.66	0.60
1:L:31:THR:HG22	1:L:51:THR:HG21	1.85	0.58
1:L:91:TYR:HB3	1:L:93:GLY:H	1.68	0.58
2:H:122:TYR:HB2	2:H:143:LEU:HD23	1.85	0.57
1:L:149:LYS:HG3	1:L:152:GLY:O	2.04	0.57
1:L:118:PHE:HB3	2:H:124:LEU:HB3	1.85	0.57
1:L:135:PHE:CE2	2:H:190:SER:HB3	2.39	0.57
1:L:23:CYS:HB2	1:L:35:TRP:CZ2	2.39	0.57
1:L:121:SER:CB	1:L:124:GLN:HG3	2.35	0.56
1:L:188:ARG:HB2	1:L:188:ARG:HH11	1.68	0.56
2:H:52(A):PRO:HG3	2:H:78:LEU:HD11	1.86	0.56
2:H:33:ASN:HB2	3:H:224:TSA:C6	2.35	0.56
1:L:39:LYS:HZ2	1:L:81:GLU:HG2	1.71	0.55
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.89	0.55
2:H:142:CYS:HB2	2:H:157:TRP:CZ2	2.42	0.55
1:L:48:ILE:HD11	1:L:62:PHE:O	2.07	0.54
2:H:82:LEU:H	2:H:82:LEU:HD23	1.72	0.54
1:L:185:GLU:HA	1:L:188:ARG:HD3	1.88	0.54
1:L:120:PRO:HG3	1:L:130:ALA:HB1	1.89	0.54
1:L:141:PRO:HG2	1:L:199:LYS:HE3	1.89	0.54
2:H:95:ARG:HE	3:H:224:TSA:H4	1.73	0.53
1:L:135:PHE:CD2	2:H:190:SER:HB3	2.43	0.53
2:H:51:ILE:HG23	2:H:78:LEU:HD12	1.90	0.53
1:L:48:ILE:HD12	1:L:73:LEU:HG	1.90	0.53
2:H:71:VAL:HA	2:H:77:THR:O	2.09	0.52
2:H:153:THR:O	2:H:210:VAL:HA	2.09	0.52
1:L:65:SER:O	1:L:71:TYR:HA	2.09	0.52
1:L:155:ARG:HH11	1:L:155:ARG:HA	1.75	0.51
1:L:6:GLN:NE2	1:L:101:GLY:HA2	2.25	0.51
2:H:95:ARG:HB3	3:H:224:TSA:C11	2.39	0.51
1:L:80:ALA:HA	1:L:106:LEU:HG	1.93	0.51
1:L:121:SER:HB2	2:H:123:PRO:O	2.11	0.50
2:H:166:LEU:HD11	2:H:198:THR:HG21	1.91	0.50
1:L:4:LEU:HD13	1:L:23:CYS:SG	2.52	0.50
1:L:132:VAL:O	1:L:178:THR:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:64:GLY:O	1:L:65:SER:HB2	2.12	0.50
1:L:48:ILE:HA	1:L:53:ASN:O	2.11	0.50
2:H:9:PRO:HB3	2:H:108:LEU:HB3	1.94	0.49
2:H:2:VAL:HB	2:H:94:ARG:NH1	2.27	0.49
1:L:35:TRP:CE3	1:L:73:LEU:HD12	2.47	0.49
1:L:138:ASN:HA	1:L:172:THR:CG2	2.42	0.49
1:L:28:VAL:CG1	1:L:31:THR:HA	2.40	0.49
1:L:32:TYR:HB3	1:L:34:HIS:HE1	1.78	0.49
2:H:34:ILE:HG23	2:H:92:CYS:SG	2.53	0.49
2:H:41:ASN:O	2:H:43:LYS:HG3	2.13	0.48
2:H:166:LEU:HD11	2:H:198:THR:CG2	2.43	0.48
1:L:32:TYR:HD2	1:L:91:TYR:HE1	1.60	0.48
1:L:193:THR:HG21	1:L:206:VAL:HG13	1.94	0.48
1:L:163:TRP:HA	1:L:175:MET:HB3	1.96	0.48
2:H:157:TRP:CH2	2:H:223:ILE:HD11	2.49	0.48
1:L:120:PRO:CG	1:L:130:ALA:HB1	2.44	0.48
1:L:136:LEU:HD13	1:L:175:MET:SD	2.54	0.48
2:H:97:ASP:HB2	2:H:99:ASN:OD1	2.14	0.48
1:L:133:VAL:HA	1:L:177:SER:O	2.14	0.48
1:L:48:ILE:HG12	1:L:54:LEU:HD12	1.95	0.47
2:H:100:TYR:CD1	3:H:224:TSA:H2	2.49	0.47
1:L:89:GLN:HB2	1:L:98:PHE:CD1	2.50	0.47
1:L:34:HIS:O	1:L:88:CYS:HA	2.15	0.47
2:H:40:ARG:HB2	2:H:43:LYS:HB2	1.95	0.47
2:H:32:HIS:NE2	2:H:94:ARG:HG3	2.29	0.47
1:L:138:ASN:HA	1:L:172:THR:HG23	1.96	0.47
1:L:10:ILE:HD12	1:L:103:LYS:HE3	1.97	0.46
1:L:79:GLU:HG2	1:L:80:ALA:N	2.30	0.46
1:L:190:ASN:O	1:L:210:ASN:HA	2.16	0.46
1:L:32:TYR:CD2	1:L:91:TYR:HE1	2.34	0.46
1:L:23:CYS:HB3	1:L:71:TYR:HB2	1.98	0.46
2:H:90:TYR:HB2	2:H:107:THR:HB	1.98	0.46
2:H:168:SER:HB2	2:H:191:VAL:HG22	1.96	0.46
2:H:51:ILE:HG22	2:H:69:LEU:HD23	1.99	0.46
1:L:89:GLN:HB2	1:L:98:PHE:CE1	2.51	0.46
2:H:38:VAL:HG13	2:H:46:GLU:HG3	1.98	0.45
2:H:179:GLN:HG2	2:H:184:LEU:O	2.16	0.45
2:H:154:VAL:CG2	2:H:187:LEU:HD23	2.47	0.45
2:H:2:VAL:HG12	2:H:26:GLY:HA3	1.99	0.45
1:L:210:ASN:O	1:L:212:ASN:N	2.49	0.45
1:L:36:TYR:CE1	1:L:46:LEU:HG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:64:GLY:HA2	1:L:72:SER:O	2.17	0.44
1:L:188:ARG:HB2	1:L:188:ARG:NH1	2.31	0.44
2:H:147:TYR:O	2:H:184:LEU:HA	2.17	0.44
2:H:164:GLY:O	2:H:166:LEU:N	2.50	0.44
2:H:51:ILE:HA	2:H:56:GLY:O	2.18	0.44
2:H:142:CYS:HB2	2:H:157:TRP:CH2	2.53	0.44
2:H:39:GLN:O	2:H:88:ALA:HB1	2.17	0.44
2:H:82:LEU:HG	2:H:82(C):LEU:HD21	2.00	0.43
1:L:181:LEU:CD2	1:L:185:GLU:HG2	2.48	0.43
2:H:34:ILE:CG2	2:H:92:CYS:SG	3.07	0.43
1:L:29:SER:HB2	1:L:91:TYR:HD2	1.84	0.43
1:L:28:VAL:O	1:L:30:SER:N	2.50	0.43
2:H:32:HIS:CE1	2:H:94:ARG:HG3	2.54	0.43
1:L:131:SER:OG	2:H:143:LEU:HD11	2.19	0.42
1:L:121:SER:OG	1:L:124:GLN:HG3	2.19	0.42
2:H:40:ARG:HB3	2:H:43:LYS:HD2	2.00	0.42
2:H:11:LEU:HD23	2:H:110:THR:HB	2.02	0.42
1:L:28:VAL:O	1:L:31:THR:N	2.52	0.42
2:H:118:PRO:HA	2:H:119:PRO:HD2	1.85	0.42
1:L:142:LYS:HD3	1:L:173:TYR:CD1	2.55	0.42
2:H:37:ILE:HD11	2:H:100(B):PHE:CE2	2.54	0.41
1:L:32:TYR:HA	1:L:32:TYR:HD1	1.74	0.41
2:H:51:ILE:O	2:H:52(A):PRO:HD3	2.20	0.41
2:H:93:ALA:HB1	2:H:100(B):PHE:CB	2.51	0.41
2:H:99:ASN:O	2:H:100(A):GLY:N	2.53	0.41
2:H:44:SER:OG	2:H:45:LEU:N	2.54	0.41
2:H:69:LEU:HA	2:H:79:TYR:O	2.20	0.41
1:L:112:ALA:HB2	1:L:200:THR:HB	2.03	0.40
1:L:38:GLN:HG2	1:L:42:ALA:O	2.21	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	L	213/215 (99%)	170 (80%)	30 (14%)	13 (6%)	2	11
2	H	214/216 (99%)	159 (74%)	31 (14%)	24 (11%)	0	2
All	All	427/431 (99%)	329 (77%)	61 (14%)	37 (9%)	1	4

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	SER
1	L	211	ARG
2	H	74	SER
2	H	76	SER
2	H	84	SER
2	H	100	TYR
2	H	126	PRO
2	H	134	THR
2	H	136	SER
2	H	163	SER
2	H	165	SER
2	H	175	PRO
2	H	184	LEU
2	H	195	SER
1	L	51	THR
1	L	153	SER
2	H	30	PRO
2	H	53	TYR
2	H	73	LYS
2	H	180	SER
1	L	27	SER
1	L	30	SER
1	L	65	SER
1	L	94	TYR
1	L	121	SER
1	L	185	GLU
2	H	62	LYS
2	H	128	SER
2	H	214	ALA
1	L	84	ALA
2	H	32	HIS
2	H	87	SER
2	H	213	PRO
1	L	213	GLU
2	H	52(A)	PRO

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Mol	Chain	Res	Type
1	L	68	GLY
2	H	169	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	L	186/186 (100%)	149 (80%)	37 (20%)	1	8
2	H	185/185 (100%)	151 (82%)	34 (18%)	2	10
All	All	371/371 (100%)	300 (81%)	71 (19%)	2	10

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	18	LYS
1	L	19	VAL
1	L	21	MET
1	L	24	ARG
1	L	38	GLN
1	L	51	THR
1	L	56	SER
1	L	59	PRO
1	L	69	THR
1	L	72	SER
1	L	82	ASP
1	L	87	TYR
1	L	94	TYR
1	L	97	THR
1	L	104	LEU
1	L	106	LEU
1	L	108	ARG
1	L	110	ASP
1	L	117	ILE
1	L	122	SER

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Mol	Chain	Res	Type
1	L	132	VAL
1	L	143	ASP
1	L	161	ASN
1	L	162	SER
1	L	165	ASP
1	L	168	SER
1	L	170	ASP
1	L	171	SER
1	L	180	THR
1	L	182	THR
1	L	189	HIS
1	L	193	THR
1	L	201	SER
1	L	208	SER
1	L	210	ASN
1	L	212	ASN
2	H	1	ASP
2	H	4	LEU
2	H	7	SER
2	H	17	SER
2	H	32	HIS
2	H	57	THR
2	H	70	THR
2	H	76	SER
2	H	82	LEU
2	H	82(C)	LEU
2	H	85	GLU
2	H	95	ARG
2	H	100(B)	PHE
2	H	105	GLN
2	H	108	LEU
2	H	110	THR
2	H	116	THR
2	H	117	THR
2	H	135	ASN
2	H	143	LEU
2	H	151	PRO
2	H	154	VAL
2	H	162	ASN
2	H	175	PRO
2	H	178	LEU
2	H	186	THR

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Mol	Chain	Res	Type
2	H	191	VAL
2	H	192	THR
2	H	199	TRP
2	H	202	SER
2	H	206	THR
2	H	209	ASN
2	H	210	VAL
2	H	213	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	138	ASN
1	L	145	ASN
1	L	198	HIS
2	H	83	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	TSA	H	224	-	11,17,17	3.05	6 (54%)	7,26,26	2.17	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TSA	H	224	-	-	0/0/34/34	0/0/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	224	TSA	C6-C1	-4.70	1.47	1.56
3	H	224	TSA	C4-C3	-2.82	1.44	1.50
3	H	224	TSA	O7-C5	2.39	1.50	1.44
3	H	224	TSA	C1-C10	3.08	1.56	1.50
3	H	224	TSA	O7-C8	3.49	1.53	1.43
3	H	224	TSA	C9-C8	6.25	1.66	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	224	TSA	C5-O7-C8	5.00	122.40	112.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	224	TSA	5	0

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.