



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:19 AM UTC

PDB ID : 1FIG / pdb_00001fig
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

<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)	:	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

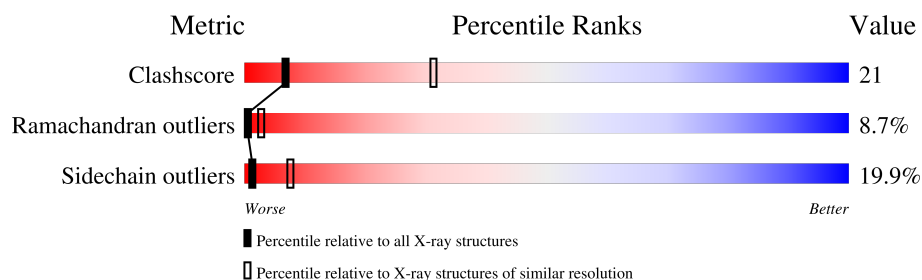
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 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	L	215	30% 41% 26% .
2	H	216	28% 46% 23% .

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.

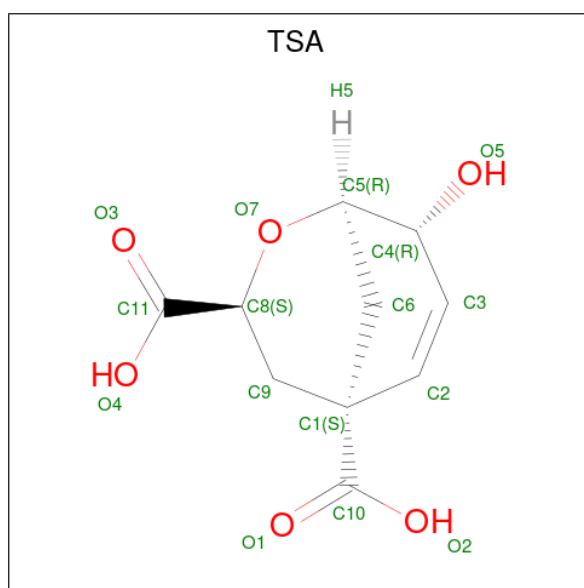
- Molecule 1 is a protein called IGG1-KAPPA 1F7 FAB (LIGHT CHAIN).

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 (CCD ID: TSA) (formula: C₁₀H₁₂O₆).



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

- Molecule 4 is water.

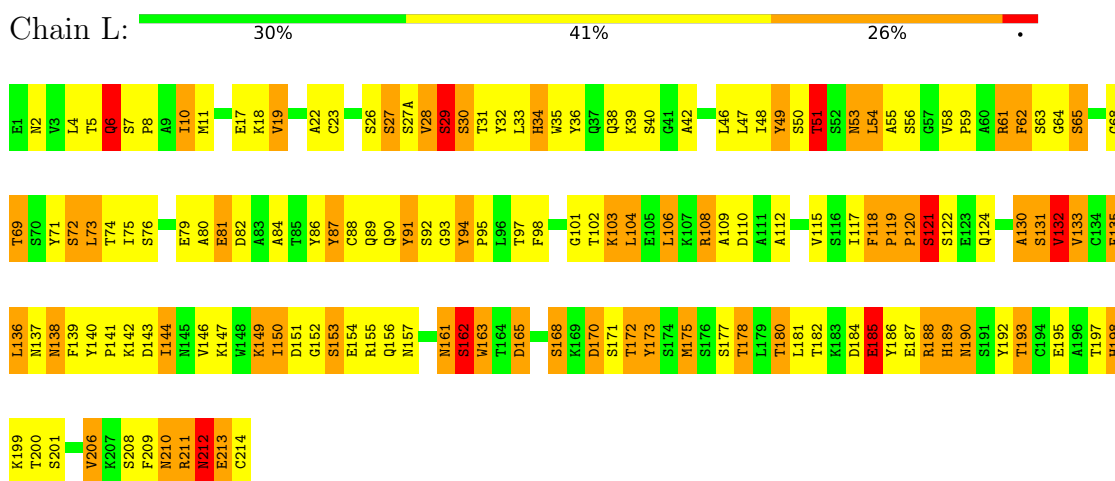
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		

3 Residue-property plots

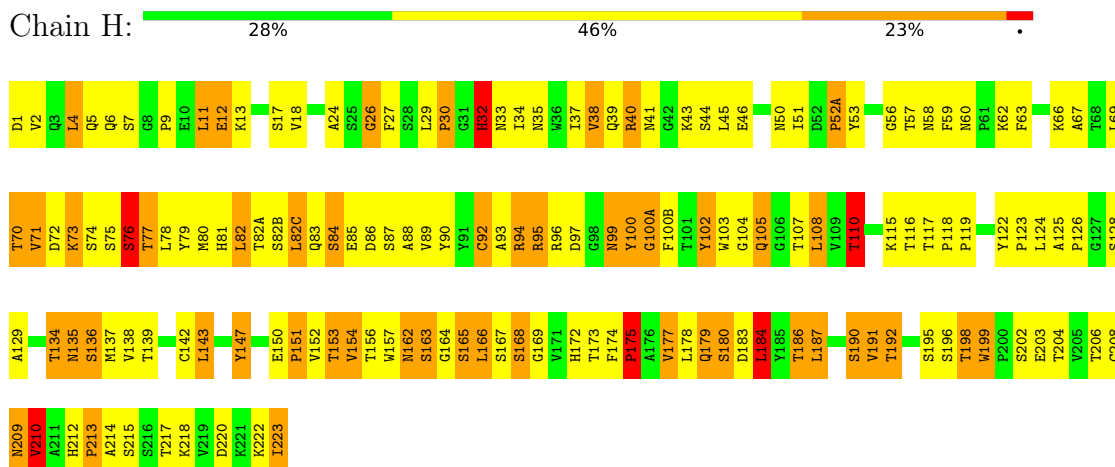
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 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 is therefore 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	1.19	7/1671 (0.4%)	2.42	106/2269 (4.7%)
2	H	1.29	11/1676 (0.7%)	2.48	119/2289 (5.2%)
All	All	1.24	18/3347 (0.5%)	2.45	225/4558 (4.9%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	32	HIS	CD2-NE2	-7.71	1.29	1.37
2	H	212	HIS	CD2-NE2	-7.70	1.29	1.37
2	H	204	THR	CA-CB	7.19	1.65	1.53
1	L	198	HIS	CD2-NE2	-7.04	1.30	1.37
2	H	172	HIS	CD2-NE2	-6.96	1.30	1.37
1	L	189	HIS	CD2-NE2	-6.47	1.30	1.37
1	L	34	HIS	CD2-NE2	-6.38	1.30	1.37
2	H	153	THR	CA-CB	6.37	1.63	1.53
2	H	81	HIS	CD2-NE2	-6.20	1.31	1.37
2	H	32	HIS	CG-ND1	-5.86	1.31	1.38
1	L	120	PRO	N-CA	-5.82	1.43	1.47
2	H	134	THR	CA-CB	5.81	1.63	1.53
2	H	71	VAL	CA-CB	5.76	1.61	1.54
1	L	144	ILE	CA-CB	5.65	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	172	HIS	CG-ND1	-5.49	1.32	1.38
1	L	146	VAL	CA-CB	5.24	1.60	1.54
1	L	189	HIS	CG-ND1	-5.14	1.32	1.38
2	H	138	VAL	CA-CB	5.13	1.60	1.54

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	62	PHE	N-CA-C	13.65	128.36	110.88
2	H	135	ASN	CA-CB-CG	13.22	125.82	112.60
2	H	138	VAL	N-CA-C	13.00	126.35	109.58
1	L	138	ASN	N-CA-C	12.40	126.53	111.02
2	H	209	ASN	CA-CB-CG	11.97	124.57	112.60
2	H	96	ARG	N-CA-C	-11.75	97.06	112.68
2	H	94	ARG	N-CA-C	11.70	127.37	109.23
1	L	2	ASN	CA-CB-CG	11.60	124.20	112.60
1	L	198	HIS	CA-CB-CG	11.54	125.34	113.80
2	H	99	ASN	CA-CB-CG	11.23	123.83	112.60
1	L	184	ASP	CA-CB-CG	11.20	123.80	112.60
1	L	53	ASN	CA-CB-CG	10.38	122.98	112.60
2	H	58	ASN	CA-CB-CG	10.06	122.66	112.60
2	H	72	ASP	CA-CB-CG	9.58	122.18	112.60
1	L	165	ASP	CA-CB-CG	9.51	122.11	112.60
2	H	86	ASP	CA-CB-CG	9.47	122.07	112.60
1	L	212	ASN	CA-CB-CG	9.28	121.88	112.60
2	H	209	ASN	O-C-N	-9.25	112.54	123.27
2	H	150	GLU	N-CA-C	-8.84	98.93	110.07
1	L	170	ASP	CA-CB-CG	8.72	121.32	112.60
2	H	58	ASN	N-CA-C	-8.72	95.03	109.24
2	H	76	SER	N-CA-C	8.52	128.96	110.80
2	H	58	ASN	OD1-CG-ND2	-8.51	114.09	122.60
2	H	183	ASP	N-CA-C	-8.50	92.69	110.80
2	H	192	THR	N-CA-C	-8.47	92.75	110.80
2	H	60	ASN	OD1-CG-ND2	-8.46	114.14	122.60
2	H	129	ALA	N-CA-C	8.40	128.69	110.80
1	L	138	ASN	OD1-CG-ND2	-8.28	114.32	122.60
1	L	82	ASP	N-CA-C	-8.18	100.27	113.19
1	L	132	VAL	N-CA-C	-8.16	95.75	108.23
1	L	211	ARG	N-CA-C	8.11	128.08	110.80
2	H	209	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	L	180	THR	CA-CB-OG1	-7.95	97.67	109.60
1	L	22	ALA	N-CA-C	7.91	121.31	108.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	209	PHE	CA-C-O	7.81	129.14	120.31
2	H	167	SER	N-CA-C	-7.70	91.85	107.41
1	L	61	ARG	N-CA-C	-7.68	102.97	112.88
1	L	139	PHE	CA-CB-CG	7.67	121.47	113.80
1	L	190	ASN	N-CA-C	7.66	127.11	110.80
1	L	73	LEU	N-CA-C	-7.65	94.18	107.49
2	H	217	THR	O-C-N	7.62	131.57	122.96
1	L	29	SER	N-CA-C	7.58	126.96	110.80
2	H	83	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	L	156	GLN	OE1-CD-NE2	-7.50	115.10	122.60
2	H	105	GLN	N-CA-CB	-7.50	97.82	110.49
1	L	27(A)	SER	N-CA-C	-7.48	97.02	109.07
2	H	95	ARG	N-CA-C	7.43	120.77	108.96
2	H	50	ASN	CA-CB-CG	7.42	120.02	112.60
2	H	27	PHE	CA-CB-CG	7.38	121.18	113.80
1	L	50	SER	CA-C-N	7.35	135.58	121.54
1	L	50	SER	C-N-CA	7.35	135.58	121.54
2	H	76	SER	N-CA-CB	-7.35	98.07	110.49
1	L	135	PHE	CA-CB-CG	7.34	121.14	113.80
2	H	67	ALA	CA-C-O	7.33	127.49	120.09
2	H	66	LYS	N-CA-C	-7.31	104.31	112.57
2	H	208	CYS	N-CA-C	-7.30	97.96	109.50
1	L	149	LYS	CA-CB-CG	7.29	128.68	114.10
2	H	136	SER	N-CA-C	7.28	126.30	110.80
2	H	162	ASN	OD1-CG-ND2	-7.26	115.34	122.60
2	H	178	LEU	N-CA-C	-7.03	97.77	108.67
2	H	179	GLN	OE1-CD-NE2	-7.01	115.59	122.60
2	H	220	ASP	N-CA-C	-6.97	97.05	108.41
2	H	198	THR	N-CA-C	-6.95	103.72	111.71
1	L	151	ASP	N-CA-C	-6.93	96.50	107.93
1	L	28	VAL	N-CA-C	-6.91	94.97	109.34
2	H	163	SER	N-CA-C	6.89	125.48	110.80
2	H	190	SER	N-CA-C	6.88	119.86	109.41
2	H	100(A)	GLY	N-CA-C	-6.87	96.90	113.18
2	H	105	GLN	CA-CB-CG	6.85	127.79	114.10
1	L	47	LEU	O-C-N	6.83	129.62	121.76
1	L	34	HIS	CB-CG-CD2	-6.82	122.33	131.20
2	H	13	LYS	N-CA-CB	-6.78	100.73	109.55
1	L	130	ALA	N-CA-C	6.75	119.40	108.34
2	H	212	HIS	CB-CG-CD2	-6.74	122.44	131.20
2	H	222	LYS	O-C-N	6.74	131.32	123.30
1	L	40	SER	N-CA-C	6.69	120.47	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	47	LEU	N-CA-C	-6.66	100.90	111.02
2	H	162	ASN	CB-CG-ND2	6.65	126.37	116.40
2	H	12	GLU	CB-CG-CD	6.63	123.88	112.60
2	H	204	THR	CB-CA-C	6.63	120.73	109.72
1	L	33	LEU	N-CA-C	6.60	119.70	109.07
1	L	87	TYR	CA-CB-CG	6.58	125.75	113.90
2	H	135	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	L	189	HIS	N-CA-C	6.52	122.04	113.30
2	H	168	SER	CA-CB-OG	6.52	124.14	111.10
2	H	92	CYS	N-CA-C	-6.51	99.21	109.50
1	L	63	SER	N-CA-C	6.51	120.11	109.76
2	H	162	ASN	CA-CB-CG	6.51	119.11	112.60
1	L	137	ASN	CA-C-N	6.40	132.51	122.78
1	L	137	ASN	C-N-CA	6.40	132.51	122.78
1	L	206	VAL	N-CA-CB	-6.39	100.68	111.23
1	L	180	THR	CA-CB-CG2	6.39	121.37	110.50
2	H	151	PRO	CA-C-N	6.39	132.12	122.92
2	H	151	PRO	C-N-CA	6.39	132.12	122.92
2	H	139	THR	CA-C-N	6.35	132.13	122.93
2	H	139	THR	C-N-CA	6.35	132.13	122.93
1	L	161	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	L	10	ILE	N-CA-C	-6.33	99.43	109.17
2	H	83	GLN	CA-CB-CG	6.29	126.68	114.10
1	L	172	THR	N-CA-CB	-6.26	100.76	110.46
1	L	146	VAL	CA-C-O	6.18	127.14	120.53
2	H	196	SER	N-CA-C	-6.17	104.97	113.18
2	H	24	ALA	N-CA-C	-6.16	99.97	109.76
1	L	151	ASP	CA-CB-CG	6.13	118.73	112.60
2	H	179	GLN	CG-CD-NE2	6.11	125.57	116.40
2	H	70	THR	N-CA-C	6.11	119.19	108.75
1	L	81	GLU	CA-C-O	6.06	130.29	121.86
2	H	72	ASP	N-CA-C	-6.06	100.31	109.95
2	H	165	SER	N-CA-C	6.06	123.70	110.80
2	H	177	VAL	N-CA-C	-6.05	99.86	109.17
1	L	136	LEU	N-CA-C	-6.04	98.67	108.52
2	H	184	LEU	N-CA-C	6.03	123.65	110.80
1	L	103	LYS	CA-CB-CG	6.03	126.16	114.10
2	H	199	TRP	CA-C-O	-6.01	113.14	120.05
2	H	99	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	L	92	SER	CA-CB-OG	5.98	123.06	111.10
2	H	94	ARG	CA-CB-CG	5.95	126.00	114.10
2	H	59	PHE	N-CA-C	5.92	118.86	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	151	PRO	N-CA-C	5.91	127.47	112.10
1	L	26	SER	CA-C-N	5.90	132.82	121.54
1	L	26	SER	C-N-CA	5.90	132.82	121.54
1	L	90	GLN	N-CA-C	5.90	123.38	110.80
2	H	210	VAL	CA-CB-CG1	5.87	120.38	110.40
1	L	6	GLN	OE1-CD-NE2	-5.87	116.73	122.60
1	L	157	ASN	CA-CB-CG	5.81	118.41	112.60
1	L	62	PHE	O-C-N	-5.80	113.99	121.83
2	H	13	LYS	CA-CB-CG	5.79	125.69	114.10
2	H	212	HIS	CB-CG-ND1	5.79	131.39	122.70
1	L	86	TYR	CA-C-O	5.78	126.57	120.33
2	H	152	VAL	N-CA-C	-5.75	100.40	108.80
2	H	4	LEU	N-CA-C	-5.75	97.97	108.02
2	H	60	ASN	CA-CB-CG	5.74	118.34	112.60
2	H	179	GLN	CA-CB-CG	5.73	125.57	114.10
2	H	35	ASN	CA-CB-CG	5.72	118.32	112.60
1	L	178	THR	CA-CB-OG1	-5.72	101.02	109.60
1	L	198	HIS	CB-CG-ND1	5.72	131.27	122.70
1	L	149	LYS	N-CA-C	-5.69	96.25	107.69
1	L	140	TYR	CA-C-O	-5.69	113.89	120.03
1	L	108	ARG	CA-CB-CG	5.67	125.44	114.10
1	L	119	PRO	N-CA-C	5.67	117.61	110.70
2	H	199	TRP	O-C-N	-5.66	114.40	121.70
1	L	91	TYR	CB-CA-C	-5.65	103.51	111.65
1	L	170	ASP	N-CA-C	-5.65	100.03	109.24
2	H	180	SER	CA-C-O	5.65	128.59	120.51
2	H	86	ASP	N-CA-C	-5.61	106.39	113.18
1	L	163	TRP	CE2-CD2-CE3	5.60	124.40	118.80
2	H	179	GLN	N-CA-C	5.59	120.10	113.28
1	L	198	HIS	CB-CG-CD2	-5.59	123.94	131.20
2	H	29	LEU	CA-C-N	5.57	126.80	119.84
2	H	29	LEU	C-N-CA	5.57	126.80	119.84
1	L	162	SER	O-C-N	-5.57	115.89	123.24
1	L	157	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	L	173	TYR	N-CA-C	-5.55	100.86	109.24
1	L	17	GLU	CA-C-O	-5.53	115.07	121.15
1	L	118	PHE	CA-C-N	5.52	126.07	120.38
1	L	118	PHE	C-N-CA	5.52	126.07	120.38
2	H	84	SER	N-CA-C	5.52	122.56	110.80
1	L	76	SER	N-CA-C	5.52	117.29	111.28
1	L	150	ILE	CA-C-N	5.50	130.50	121.58
1	L	150	ILE	C-N-CA	5.50	130.50	121.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	150	GLU	CA-C-O	-5.49	115.58	120.19
1	L	121	SER	N-CA-C	5.49	122.49	110.80
2	H	30	PRO	N-CA-C	5.48	123.77	112.47
2	H	77	THR	N-CA-C	5.46	119.13	109.96
2	H	100(A)	GLY	CA-C-N	-5.45	105.21	117.20
2	H	102	TYR	CA-CB-CG	5.43	123.67	113.90
2	H	173	THR	N-CA-C	-5.43	100.33	109.07
1	L	7	SER	O-C-N	-5.42	115.47	121.66
1	L	49	TYR	N-CA-C	5.41	122.31	110.80
1	L	133	VAL	CB-CA-C	5.39	119.01	110.81
2	H	60	ASN	CB-CG-ND2	5.39	124.48	116.40
1	L	175	MET	CA-CB-CG	5.38	124.86	114.10
2	H	95	ARG	CA-CB-CG	5.38	124.86	114.10
2	H	63	PHE	CA-C-O	5.36	127.58	121.58
1	L	197	THR	CA-C-O	-5.35	114.58	120.36
2	H	186	THR	O-C-N	-5.34	116.75	123.27
1	L	187	GLU	CB-CG-CD	5.32	121.64	112.60
2	H	210	VAL	CA-CB-CG2	-5.30	101.39	110.40
1	L	131	SER	CA-C-O	5.29	126.56	120.84
2	H	92	CYS	O-C-N	-5.28	116.74	123.24
2	H	137	MET	CA-C-N	5.27	128.24	120.91
2	H	137	MET	C-N-CA	5.27	128.24	120.91
1	L	195	GLU	CA-CB-CG	5.25	124.61	114.10
1	L	54	LEU	N-CA-C	-5.25	102.42	110.14
2	H	162	ASN	CA-C-N	5.25	131.56	121.54
2	H	162	ASN	C-N-CA	5.25	131.56	121.54
2	H	103	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	L	189	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	L	62	PHE	N-CA-CB	-5.23	103.77	111.51
2	H	110	THR	O-C-N	-5.22	116.44	123.23
2	H	92	CYS	CA-C-O	-5.22	115.00	121.11
2	H	83	GLN	CG-CD-NE2	5.21	124.22	116.40
2	H	73	LYS	CA-CB-CG	5.21	124.51	114.10
2	H	99	ASN	CA-C-N	5.19	131.45	121.54
2	H	99	ASN	C-N-CA	5.19	131.45	121.54
1	L	138	ASN	CB-CG-ND2	5.18	124.18	116.40
2	H	115	LYS	CA-CB-CG	5.18	124.46	114.10
1	L	109	ALA	CA-C-O	-5.17	115.46	121.15
2	H	59	PHE	CA-CB-CG	5.16	118.96	113.80
2	H	81	HIS	CA-CB-CG	5.16	118.96	113.80
1	L	213	GLU	CA-CB-CG	5.15	124.41	114.10
1	L	161	ASN	CB-CG-ND2	5.15	124.13	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	58	ASN	O-C-N	-5.14	117.46	123.27
1	L	74	THR	CA-C-O	-5.14	115.08	120.58
1	L	168	SER	N-CA-CB	-5.14	102.58	110.44
1	L	133	VAL	N-CA-CB	-5.13	101.72	111.21
1	L	5	THR	N-CA-C	-5.12	100.10	108.76
2	H	40	ARG	CA-CB-CG	5.12	124.34	114.10
1	L	197	THR	O-C-N	-5.11	117.22	123.30
1	L	2	ASN	N-CA-C	-5.09	98.99	107.80
1	L	147	LYS	CA-CB-CG	5.08	124.25	114.10
1	L	34	HIS	CB-CG-ND1	5.07	130.31	122.70
2	H	81	HIS	CB-CG-CD2	-5.07	124.61	131.20
2	H	212	HIS	CA-C-N	5.06	126.16	119.84
2	H	212	HIS	C-N-CA	5.06	126.16	119.84
2	H	175	PRO	N-CA-C	5.05	122.88	112.47
2	H	5	GLN	CB-CG-CD	5.05	121.19	112.60
1	L	121	SER	CA-CB-OG	5.04	121.19	111.10
1	L	188	ARG	CA-CB-CG	5.04	124.19	114.10
1	L	214	CYS	N-CA-C	5.03	125.09	111.00
1	L	49	TYR	O-C-N	-5.02	115.91	122.59
2	H	199	TRP	CE2-CD2-CG	-5.02	101.17	107.20
2	H	125	ALA	N-CA-C	-5.02	102.87	110.50
1	L	192	TYR	N-CA-C	5.00	117.13	109.07
2	H	26	GLY	O-C-N	-5.00	116.20	122.70

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	78	0
2	H	1632	0	1596	66	0
3	H	16	0	10	5	0
4	H	1	0	0	0	0
All	All	3284	0	3169	138	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 (138) 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
1:L:144:ILE:HD12	1:L:198:HIS:HB2	1.69	0.75
2:H:118:PRO:HG3	2:H:215:SER:HB2	1.68	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
1:L:27:SER:O	1:L:69:THR:HG23	1.99	0.62
2:H:12:GLU:HG3	2:H:18:VAL:HG22	1.81	0.62
2:H:122:TYR:HB2	2:H:143:LEU:CD2	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:L:188:ARG:HB2	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
2:H:156:THR:HG1	2:H:209:ASN:HB2	1.74	0.52
1:L:65:SER:O	1:L:71:TYR:HA	2.09	0.52
1:L:155:ARG:HA	1:L:155:ARG:HH11	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
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
1:L:35:TRP:CE3	1:L:73:LEU:HD12	2.47	0.49
2:H:2:VAL:HB	2:H:94:ARG:NH1	2.27	0.49
1:L:138:ASN:HA	1:L:172:THR:CG2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:32:TYR:HD2	1:L:91:TYR:HE1	1.60	0.48
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: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:133:VAL:HA	1:L:177:SER:O	2.14	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: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
1:L:138:ASN:HA	1:L:172:THR:HG23	1.96	0.47
2:H:32:HIS:NE2	2:H:94:ARG:HG3	2.29	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:23:CYS:HB3	1:L:71:TYR:HB2	1.98	0.46
1:L:32:TYR:CD2	1:L:91:TYR:HE1	2.34	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
1:L:89:GLN:HB2	1:L:98:PHE:CE1	2.51	0.46
2:H:51:ILE:HG22	2:H:69:LEU:HD23	1.99	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
1:L:210:ASN:O	1:L:212:ASN:N	2.49	0.45
2:H:2:VAL:HG12	2:H:26:GLY:HA3	1.99	0.45
1:L:36:TYR:CE1	1:L:46:LEU:HG	2.52	0.44
2:H:80:MET:HE3	2:H:82:LEU:HD22	1.99	0.44
1:L:64:GLY:HA2	1:L:72:SER:O	2.17	0.44
1:L:188:ARG:NH1	1:L:188:ARG:HB2	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:39:GLN:O	2:H:88:ALA:HB1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:32:HIS:HE2	2:H:94:ARG:HG3	1.83	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:91:TYR:C	1:L:93:GLY:H	2.27	0.42
1:L:121:SER:OG	1:L:124:GLN:HG3	2.19	0.42
2:H:11:LEU:HD23	2:H:110:THR:HB	2.02	0.42
2:H:40:ARG:HB3	2:H:43:LYS:HD2	2.00	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:HD1	1:L:32:TYR:HA	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:38:GLN:HG2	1:L:42:ALA:O	2.21	0.40
1:L:112:ALA:HB2	1:L:200:THR:HB	2.03	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%)	1	7
2	H	214/216 (99%)	159 (74%)	31 (14%)	24 (11%)	0	1
All	All	427/431 (99%)	329 (77%)	61 (14%)	37 (9%)	0	3

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

Continued on next page...

Continued from previous page...

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%)	151 (81%)	35 (19%)	1	9
2	H	185/185 (100%)	146 (79%)	39 (21%)	1	6
All	All	371/371 (100%)	297 (80%)	74 (20%)	1	7

All (74) 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	51	THR
1	L	56	SER
1	L	59	PRO
1	L	69	THR
1	L	72	SER
1	L	87	TYR
1	L	94	TYR
1	L	95	PRO
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
1	L	132	VAL
1	L	143	ASP
1	L	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	185	GLU
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	11	LEU
2	H	17	SER
2	H	32	HIS
2	H	38	VAL
2	H	57	THR
2	H	70	THR
2	H	76	SER
2	H	82	LEU
2	H	82(A)	THR
2	H	82(B)	SER
2	H	82(C)	LEU
2	H	85	GLU
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	166	LEU
2	H	175	PRO
2	H	177	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	186	THR
2	H	187	LEU
2	H	191	VAL
2	H	192	THR
2	H	199	TRP
2	H	202	SER
2	H	206	THR
2	H	210	VAL
2	H	213	PRO
2	H	218	LYS
2	H	223	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	137	ASN
1	L	138	ASN
1	L	145	ASN
1	L	198	HIS
2	H	5	GLN
2	H	58	ASN
2	H	81	HIS
2	H	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-	16,17,17	3.03	7 (43%)	16,26,26	2.38	4 (25%)

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	-	-	1/10/34/34	1/3/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	224	TSA	C9-C8	7.21	1.66	1.52
3	H	224	TSA	O7-C8	5.16	1.53	1.43
3	H	224	TSA	C6-C1	-4.87	1.47	1.55
3	H	224	TSA	C8-C11	3.68	1.56	1.52
3	H	224	TSA	C4-C3	-2.57	1.44	1.50
3	H	224	TSA	O7-C5	2.44	1.50	1.44
3	H	224	TSA	O4-C11	-2.10	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	224	TSA	O7-C8-C11	7.11	121.15	107.72
3	H	224	TSA	O4-C11-C8	3.00	120.51	112.71
3	H	224	TSA	C5-C4-C3	2.39	114.47	108.83
3	H	224	TSA	O2-C10-O1	-2.14	117.02	123.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	224	TSA	O3-C11-C8-O7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	224	TSA	C1-C2-C3-C4-C5-C8-C9-O7

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 [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.