



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:01 AM UTC

PDB ID : 1EKJ / pdb_00001ekj
Title : THE X-RAY CRYSTALLOGRAPHIC STRUCTURE OF BETA CARBONIC ANHYDRASE FROM THE C3 DICOT PISUM SATIVUM
Authors : Kimber, M.S.; Pai, E.F.
Deposited on : 2000-03-08
Resolution : 1.93 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

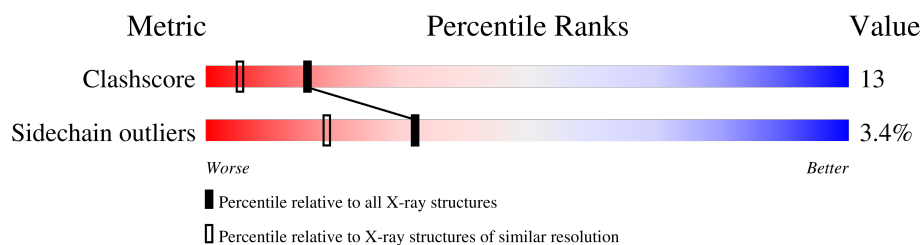
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1494 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)

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	A	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	
1	F	221	
1	G	221	
1	H	221	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	3001	-	-	X	-
2	ACT	C	3007	-	-	X	-
2	ACT	E	3005	-	-	X	-
2	ACT	F	3008	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14070 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 BETA-CARBONIC ANHYDRASE.

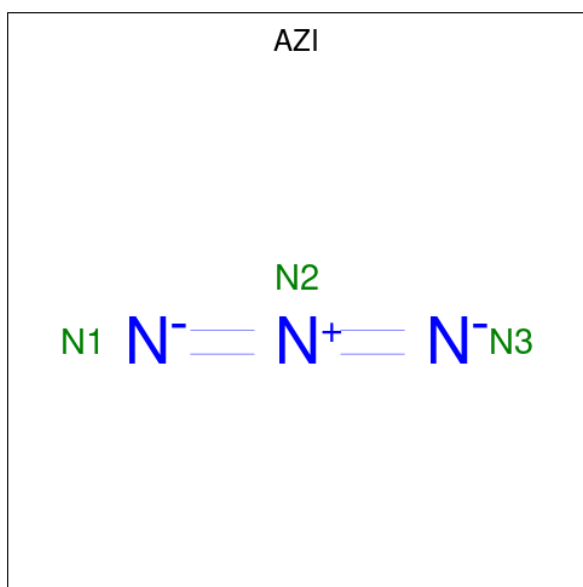
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1618	1051	264	297	6			
1	B	213	Total	C	N	O	S	0	0	0
			1640	1065	268	301	6			
1	C	217	Total	C	N	O	S	0	1	0
			1672	1083	273	309	7			
1	D	211	Total	C	N	O	S	0	1	0
			1630	1057	266	300	7			
1	E	212	Total	C	N	O	S	0	0	0
			1633	1060	267	300	6			
1	F	214	Total	C	N	O	S	0	0	0
			1648	1071	269	302	6			
1	G	220	Total	C	N	O	S	0	1	0
			1691	1093	276	315	7			
1	H	211	Total	C	N	O	S	0	1	0
			1630	1057	266	300	7			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0
3	D	1	Total N 3 3	0	0
3	E	1	Total N 3 3	0	0
3	H	1	Total N 3 3	0	0

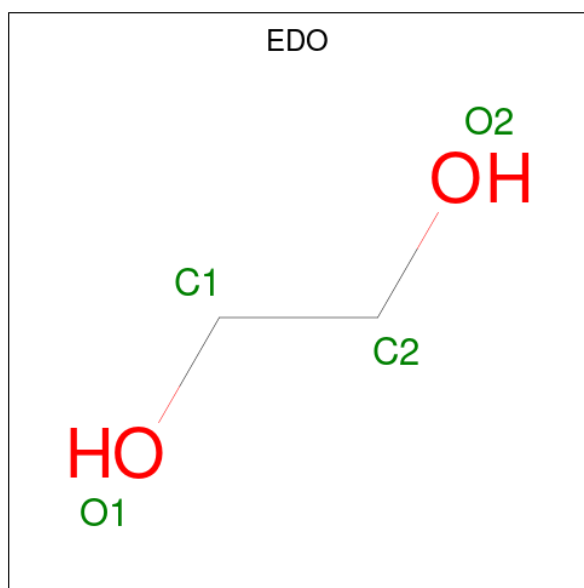
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0

Continued on next page...

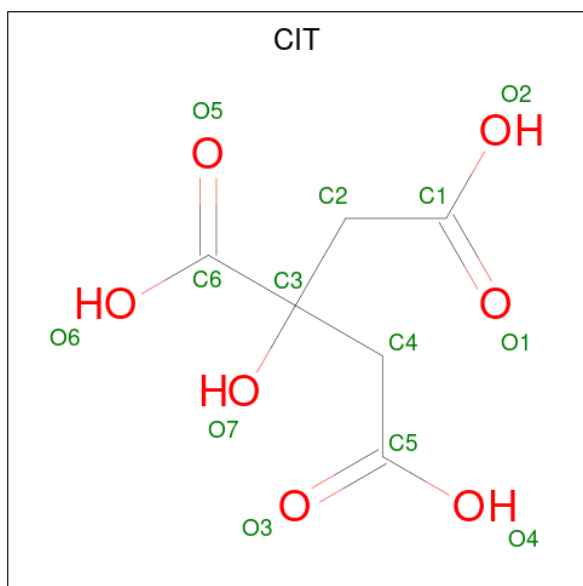
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cu	0	0
			1	1		
7	C	1	Total	Cu	0	0
			1	1		
7	E	1	Total	Cu	0	0
			1	1		
7	G	1	Total	Cu	0	0
			1	1		

- Molecule 8 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	50	Total	O	0	0
			50	50		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	43	Total 43	O 43	0	0
9	C	138	Total 138	O 138	0	0
9	D	131	Total 131	O 131	0	0
9	E	71	Total 71	O 71	0	0
9	F	84	Total 84	O 84	0	0
9	G	150	Total 150	O 150	0	0
9	H	144	Total 144	O 144	0	0

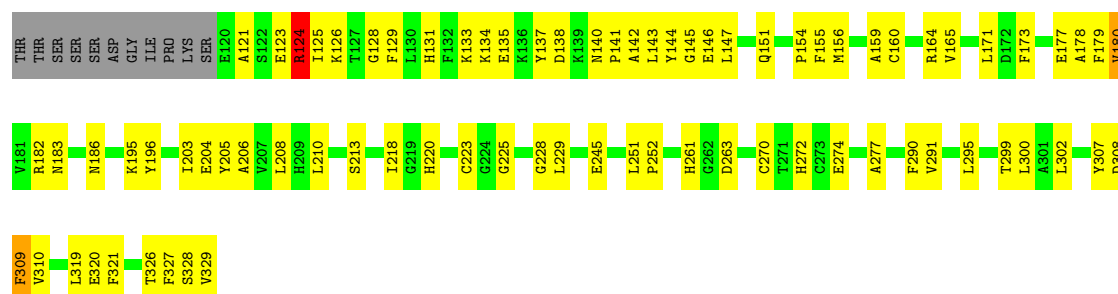
3 Residue-property plots

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.

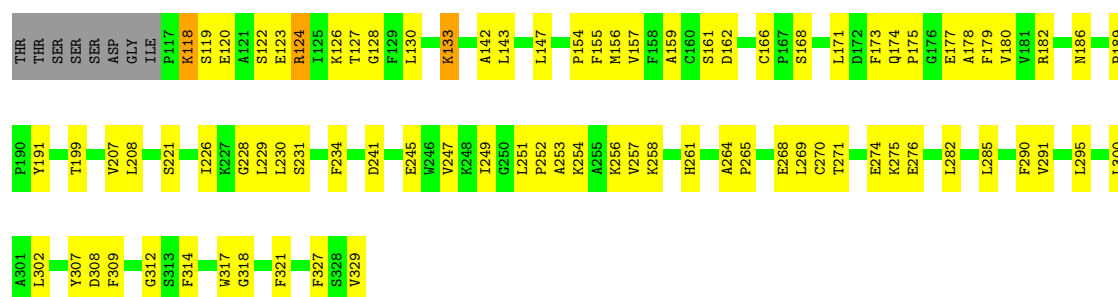
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain A: 



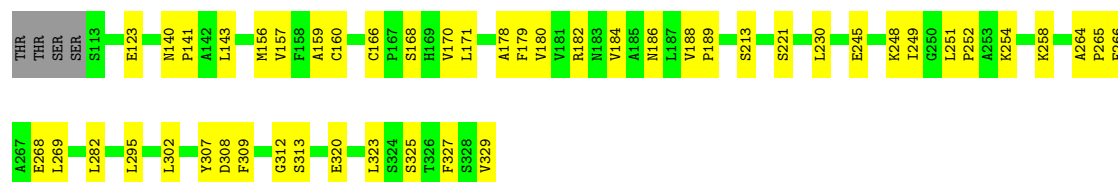
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain B: 



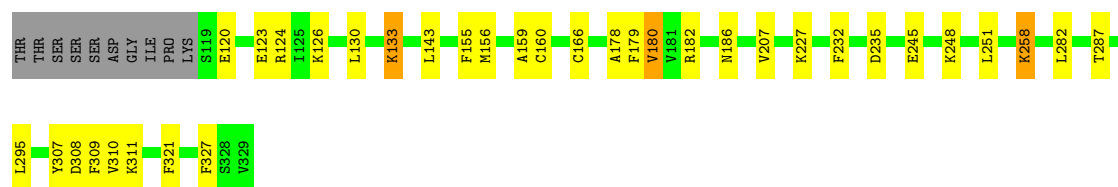
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain C: 



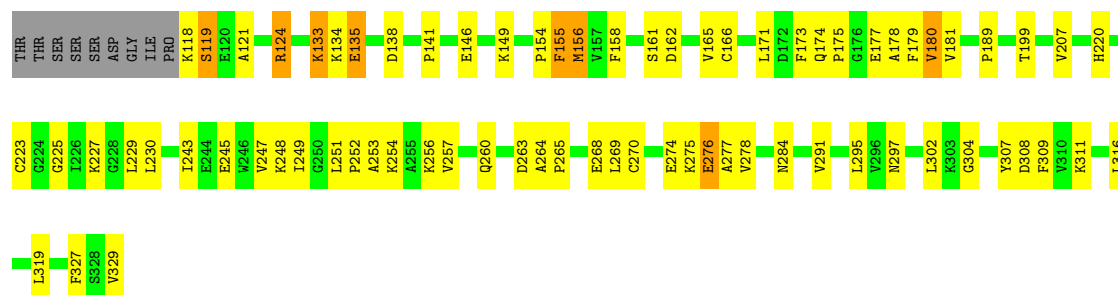
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain D:  80% 14% 5%



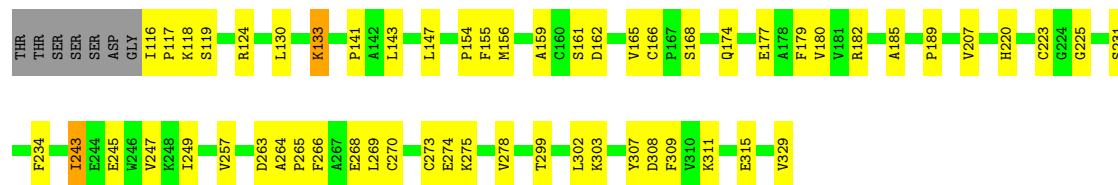
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain E:  62% 30% 2%



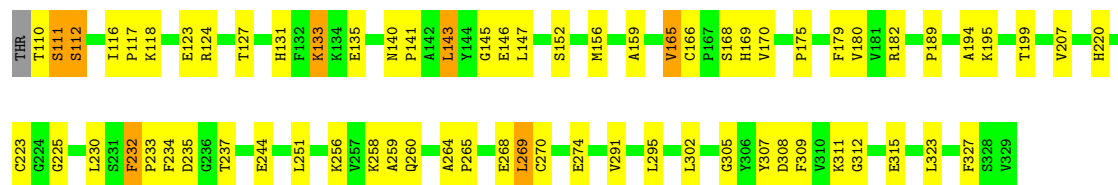
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain F:  71% 25% 2%



• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain G:  69% 28% 1%



• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain H:  74% 18% 5%



F232	E244	E245	K248	L251	P252	A253	K254	A255	K256	V257	K258	L269	E276	Y307	D308	F309	E320	F327	S328	V329
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	136.91Å 143.32Å 202.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.93	Depositor
% Data completeness (in resolution range)	87.5 (40.00-1.93)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.229 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14070	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: AZI, CL, CIT, ZN, EDO, CU, ACT

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	0.52	0/1662	1.00	10/2250 (0.4%)
1	B	0.46	0/1685	0.99	7/2280 (0.3%)
1	C	0.69	1/1717 (0.1%)	1.09	10/2325 (0.4%)
1	D	0.85	0/1674	1.16	14/2267 (0.6%)
1	E	0.53	0/1677	1.02	9/2269 (0.4%)
1	F	0.57	0/1693	1.01	6/2292 (0.3%)
1	G	0.75	0/1736	1.13	11/2351 (0.5%)
1	H	0.86	0/1674	1.11	5/2267 (0.2%)
All	All	0.67	1/13518 (0.0%)	1.07	72/18301 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	156	MET	SD-CE	5.26	1.92	1.79

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	112	SER	N-CA-C	10.22	124.67	110.06
1	F	207	VAL	N-CA-C	8.25	118.28	110.53
1	H	180	VAL	N-CA-C	8.05	120.08	108.48
1	A	180	VAL	N-CA-C	8.00	119.37	108.17
1	E	180	VAL	N-CA-C	7.98	120.10	108.53
1	F	179	PHE	N-CA-C	-7.32	97.32	108.96
1	G	180	VAL	N-CA-C	7.29	118.97	108.48
1	G	156	MET	N-CA-C	-7.20	97.16	108.90
1	H	156	MET	N-CA-C	-7.01	97.47	108.90
1	G	179	PHE	N-CA-C	-6.77	98.20	108.96
1	B	291	VAL	N-CA-C	-6.70	104.32	110.82
1	F	180	VAL	N-CA-C	6.53	118.00	108.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	180	VAL	N-CA-C	6.46	117.89	108.53
1	A	156	MET	N-CA-C	-6.42	97.91	108.76
1	D	207	VAL	N-CA-C	6.40	116.54	110.53
1	D	156	MET	N-CA-C	-6.39	98.48	108.90
1	B	156	MET	N-CA-C	-6.37	97.42	108.69
1	H	179	PHE	N-CA-C	-6.34	98.87	108.96
1	B	207	VAL	N-CA-C	6.32	116.47	110.53
1	A	299	THR	N-CA-C	-6.30	104.86	113.30
1	A	291	VAL	N-CA-C	-6.29	104.15	111.00
1	C	170	VAL	N-CA-C	6.16	117.64	110.62
1	C	179	PHE	N-CA-C	-6.15	99.18	108.96
1	D	155	PHE	N-CA-C	6.14	119.55	109.72
1	G	291	VAL	N-CA-C	-6.12	105.76	111.45
1	F	243	ILE	N-CA-C	6.12	116.78	110.36
1	G	232	PHE	CA-C-N	6.08	127.44	119.84
1	G	232	PHE	C-N-CA	6.08	127.44	119.84
1	C	180	VAL	N-CA-C	5.99	117.21	108.53
1	A	218	ILE	N-CA-C	5.93	116.15	107.37
1	G	207	VAL	N-CA-C	5.89	116.06	110.53
1	A	124	ARG	N-CA-C	-5.87	104.22	111.33
1	D	287	THR	N-CA-C	-5.83	106.17	113.28
1	E	156	MET	N-CA-C	-5.82	99.42	108.90
1	H	232	PHE	CA-C-N	5.77	125.31	119.19
1	H	232	PHE	C-N-CA	5.77	125.31	119.19
1	C	156	MET	N-CA-C	-5.75	99.52	108.90
1	G	170	VAL	N-CA-C	5.75	117.18	110.62
1	F	299	THR	N-CA-C	-5.70	105.66	113.30
1	D	310	VAL	N-CA-C	-5.68	106.17	111.45
1	B	178	ALA	N-CA-C	5.65	118.32	108.76
1	D	179	PHE	N-CA-C	-5.60	100.68	109.25
1	A	178	ALA	N-CA-C	5.59	118.58	109.24
1	D	282	LEU	N-CA-C	-5.59	105.19	111.28
1	E	179	PHE	N-CA-C	-5.57	100.04	108.67
1	B	179	PHE	N-CA-C	-5.53	100.78	109.25
1	B	180	VAL	N-CA-C	5.49	117.30	108.85
1	E	297	ASN	N-CA-C	-5.45	106.47	113.02
1	E	178	ALA	N-CA-C	5.44	118.32	108.69
1	E	277	ALA	N-CA-C	-5.43	105.44	111.36
1	D	178	ALA	N-CA-C	5.42	117.27	108.26
1	F	156	MET	N-CA-C	-5.41	99.47	108.34
1	C	248	LYS	N-CA-C	-5.39	105.96	112.54
1	G	165	VAL	N-CA-C	5.31	120.39	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	TYR	N-CA-C	5.26	116.75	110.44
1	E	155	PHE	N-CA-C	5.23	118.26	109.95
1	G	145	GLY	N-CA-C	-5.21	106.10	112.77
1	A	277	ALA	N-CA-C	-5.20	105.69	111.36
1	B	157	VAL	N-CA-C	5.18	116.18	108.46
1	C	178	ALA	N-CA-C	5.15	116.79	108.34
1	C	282	LEU	N-CA-C	-5.15	105.75	111.36
1	D	251	LEU	CA-C-N	-5.12	113.65	119.28
1	D	251	LEU	C-N-CA	-5.12	113.65	119.28
1	D	232	PHE	CA-C-N	5.12	124.43	118.85
1	D	232	PHE	C-N-CA	5.12	124.43	118.85
1	D	248	LYS	N-CA-C	-5.10	106.16	112.38
1	E	207	VAL	N-CA-C	5.10	115.32	110.42
1	A	145	GLY	N-CA-C	-5.07	106.60	113.24
1	C	188	VAL	CA-C-N	-5.06	115.17	120.38
1	C	188	VAL	C-N-CA	-5.06	115.17	120.38
1	C	157	VAL	N-CA-C	5.06	115.76	108.48
1	E	119	SER	N-CA-C	5.05	117.17	111.11

There are no chirality outliers.

There are no planarity outliers.

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	A	1618	0	1593	60	0
1	B	1640	0	1619	66	0
1	C	1672	0	1646	32	0
1	D	1630	0	1603	16	0
1	E	1633	0	1611	55	0
1	F	1648	0	1629	40	0
1	G	1691	0	1664	53	0
1	H	1630	0	1604	47	0
2	A	8	0	6	3	0
2	C	8	0	6	2	0
2	E	4	0	3	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	4	0	3	2	0
2	G	8	0	6	2	0
2	H	4	0	3	0	0
3	A	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	H	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	4	0	6	0	0
6	D	4	0	6	0	0
6	E	4	0	6	1	0
6	H	4	0	6	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	D	13	0	4	1	0
9	A	50	0	0	0	0
9	B	43	0	0	4	0
9	C	138	0	0	3	0
9	D	131	0	0	1	0
9	E	71	0	0	2	0
9	F	84	0	0	4	0
9	G	150	0	0	12	0
9	H	144	0	0	4	0
All	All	14070	0	13024	349	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 (349) 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:G:111:SER:HA	1:G:117:PRO:HA	1.29	1.10
1:H:134:LYS:HG3	1:H:135:GLU:H	1.23	1.03
1:F:166:CYS:HB2	9:F:1130:HOH:O	1.63	0.99
1:G:110:THR:O	1:G:111:SER:HB2	1.60	0.99
1:H:146:GLU:O	1:H:149:LYS:HG2	1.66	0.94
1:E:166:CYS:HB2	9:E:1168:HOH:O	1.72	0.89
1:E:225:GLY:H	2:E:3005:ACT:H1	1.40	0.85
1:A:225:GLY:H	2:A:3001:ACT:H1	1.40	0.85
1:G:166[A]:CYS:SG	9:G:1185:HOH:O	2.35	0.84
1:B:142:ALA:HB3	9:B:1175:HOH:O	1.80	0.82
1:E:265:PRO:HD2	1:E:268:GLU:OE2	1.79	0.82
1:A:225:GLY:N	2:A:3001:ACT:H1	1.96	0.80
1:F:264:ALA:HB3	1:F:269:LEU:HD11	1.62	0.80
1:H:124:ARG:C	1:H:124:ARG:HD3	2.08	0.79
1:G:308:ASP:OD1	1:G:311:LYS:HD3	1.84	0.77
1:H:124:ARG:HD3	1:H:124:ARG:O	1.83	0.77
1:F:270:CYS:O	1:F:274:GLU:HG3	1.86	0.76
1:A:138:ASP:O	1:A:141:PRO:HD3	1.85	0.76
1:B:154:PRO:HG2	1:B:155:PHE:CD1	2.22	0.75
1:G:111:SER:HA	1:G:117:PRO:CA	2.12	0.74
1:E:295:LEU:HD21	1:E:302:LEU:HD13	1.69	0.74
1:C:166[B]:CYS:SG	9:C:1064:HOH:O	2.46	0.73
1:D:308:ASP:OD2	1:D:311:LYS:HD3	1.89	0.72
1:E:189:PRO:HB3	1:E:249:ILE:HD13	1.72	0.72
1:A:205:TYR:CE2	2:A:3003:ACT:H3	2.25	0.71
1:E:118:LYS:N	1:F:303:LYS:HZ1	1.87	0.71
1:B:166:CYS:HB2	9:B:1221:HOH:O	1.90	0.70
1:A:319:LEU:HD12	1:A:320:GLU:N	2.05	0.70
1:B:329:VAL:HG11	1:D:130:LEU:HD21	1.74	0.70
1:D:124:ARG:HD3	1:D:124:ARG:C	2.17	0.69
1:E:308:ASP:OD2	1:E:311:LYS:HD3	1.93	0.69
1:B:120:GLU:CD	1:B:120:GLU:H	2.00	0.69
1:B:230:LEU:HD13	1:B:269:LEU:HD12	1.74	0.68
1:A:160:CYS:HB2	1:A:186:ASN:HD22	1.58	0.68
1:B:221:SER:HB3	1:B:308:ASP:HA	1.76	0.68
1:C:312:GLY:O	1:D:133:LYS:HE2	1.94	0.68
1:C:295:LEU:HD21	1:C:302:LEU:HD13	1.75	0.67
1:D:124:ARG:HD3	1:D:124:ARG:O	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:SER:HB3	9:G:1924:HOH:O	1.94	0.67
1:A:124:ARG:NH2	1:A:128:GLY:HA3	2.10	0.67
1:B:230:LEU:HA	1:B:254:LYS:HE3	1.76	0.66
1:B:270:CYS:O	1:B:274:GLU:HG3	1.96	0.66
1:B:182:ARG:HD2	9:B:1085:HOH:O	1.95	0.65
1:B:174:GLN:O	1:B:177:GLU:HB2	1.96	0.65
1:D:258:LYS:HE3	9:D:1386:HOH:O	1.97	0.64
1:E:118:LYS:HB3	1:E:121:ALA:HB3	1.79	0.64
1:B:282:LEU:HD23	1:B:285:LEU:HD12	1.78	0.64
1:G:140:ASN:HB2	9:G:1413:HOH:O	1.97	0.64
1:F:308:ASP:OD2	1:F:311:LYS:HD3	1.98	0.64
1:E:307:TYR:CZ	1:E:309:PHE:HB3	2.32	0.64
1:H:134:LYS:HG3	1:H:135:GLU:N	2.04	0.64
1:B:118:LYS:C	1:B:118:LYS:HD2	2.22	0.64
1:A:121:ALA:O	1:A:125:ILE:HG13	1.99	0.63
1:E:245:GLU:O	1:E:248:LYS:HG2	1.98	0.63
1:A:203:ILE:HG22	1:A:290:PHE:HE1	1.63	0.63
1:H:166[B]:CYS:SG	9:H:1094:HOH:O	2.35	0.63
1:A:307:TYR:CZ	1:A:309:PHE:HB3	2.33	0.63
1:C:307:TYR:CZ	1:C:309:PHE:HB3	2.35	0.62
1:H:146:GLU:O	1:H:149:LYS:CG	2.46	0.62
1:A:164:ARG:HG2	1:B:147:LEU:HD22	1.82	0.61
1:A:295:LEU:HD21	1:A:302:LEU:HD13	1.81	0.61
1:C:189:PRO:HB3	1:C:249:ILE:CD1	2.31	0.61
1:F:116:ILE:N	1:F:117:PRO:HD2	2.16	0.61
1:E:154:PRO:HG2	1:E:155:PHE:CD1	2.36	0.61
1:F:225:GLY:H	2:F:3008:ACT:H1	1.66	0.61
1:H:146:GLU:OE1	1:H:149:LYS:HG3	2.01	0.60
1:G:124:ARG:NE	1:H:177:GLU:OE2	2.34	0.60
1:E:134:LYS:HG3	1:E:135:GLU:N	2.17	0.60
1:E:146:GLU:HA	1:E:149:LYS:HD3	1.83	0.59
1:A:140:ASN:HB3	1:A:143:LEU:CB	2.32	0.59
1:G:189:PRO:HD2	1:G:199:THR:HG21	1.83	0.59
1:G:110:THR:O	1:G:111:SER:CB	2.45	0.59
1:B:307:TYR:CE2	1:B:309:PHE:HB3	2.38	0.58
1:C:254:LYS:HE2	1:C:258:LYS:HE3	1.84	0.58
1:G:166[B]:CYS:SG	9:G:1185:HOH:O	2.52	0.58
1:C:168:SER:OG	1:D:166[A]:CYS:SG	2.58	0.58
1:G:312:GLY:O	1:H:133:LYS:HE3	2.03	0.58
1:G:168:SER:OG	1:H:166[A]:CYS:SG	2.49	0.58
1:G:307:TYR:CE2	1:G:309:PHE:HB3	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:ALA:HB3	1:F:269:LEU:CD1	2.31	0.58
1:B:118:LYS:HD3	1:B:123:GLU:HB2	1.86	0.57
1:B:230:LEU:HD23	1:B:254:LYS:HG3	1.85	0.57
1:E:189:PRO:HB3	1:E:249:ILE:CD1	2.34	0.57
1:F:133:LYS:O	1:F:133:LYS:HD3	2.03	0.57
1:C:189:PRO:HB3	1:C:249:ILE:HD13	1.85	0.57
1:E:124:ARG:HD2	1:E:124:ARG:O	2.04	0.57
1:A:171:LEU:HD12	1:A:173:PHE:HE1	1.69	0.57
1:A:124:ARG:HH21	1:A:128:GLY:HA3	1.69	0.57
1:B:171:LEU:HD12	1:B:173:PHE:HE1	1.70	0.57
1:C:327:PHE:CD1	1:C:329:VAL:HG22	2.40	0.57
1:C:329:VAL:HG23	1:C:329:VAL:O	2.05	0.57
1:B:295:LEU:HD21	1:B:302:LEU:HD13	1.85	0.57
1:A:142:ALA:O	1:A:146:GLU:HG2	2.04	0.56
1:B:154:PRO:HG2	1:B:155:PHE:HD1	1.66	0.56
1:H:131:HIS:ND1	1:H:131:HIS:C	2.63	0.56
1:H:245:GLU:O	1:H:248:LYS:HG2	2.06	0.56
1:E:189:PRO:HD2	1:E:199:THR:HG21	1.87	0.56
1:A:144:TYR:CD2	1:A:147:LEU:HD12	2.41	0.56
1:B:265:PRO:HD2	1:B:268:GLU:OE2	2.04	0.56
1:B:123:GLU:O	1:B:127:THR:HG23	2.06	0.56
1:G:110:THR:N	9:G:1117:HOH:O	2.39	0.56
1:A:154:PRO:HG2	1:A:155:PHE:CD1	2.41	0.55
1:H:174:GLN:HG2	1:H:177:GLU:OE1	2.06	0.55
1:H:168:SER:O	1:H:172:ASP:N	2.38	0.55
1:E:174:GLN:HB3	1:E:175:PRO:HD2	1.87	0.55
1:E:134:LYS:HG3	1:E:135:GLU:H	1.72	0.55
1:H:160:CYS:HB2	1:H:186:ASN:HD22	1.71	0.55
1:E:124:ARG:HD2	1:E:124:ARG:C	2.33	0.54
1:A:134:LYS:HD3	1:A:135:GLU:OE1	2.07	0.54
1:A:270:CYS:O	1:A:274:GLU:HG3	2.08	0.54
1:B:307:TYR:CZ	1:B:309:PHE:HB3	2.41	0.54
1:A:327:PHE:CD1	1:A:327:PHE:C	2.86	0.54
1:H:168:SER:HA	1:H:173:PHE:HB2	1.89	0.54
1:A:138:ASP:C	1:A:140:ASN:H	2.16	0.54
9:F:1748:HOH:O	2:G:3009:ACT:H1	2.06	0.54
1:A:329:VAL:HG12	1:A:329:VAL:O	2.07	0.54
1:E:270:CYS:O	1:E:274:GLU:HG3	2.07	0.54
1:H:146:GLU:OE1	1:H:146:GLU:HA	2.08	0.54
1:C:265:PRO:HD2	1:C:268:GLU:OE1	2.08	0.53
1:G:146:GLU:HG2	9:G:1678:HOH:O	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:CE2	1:B:312:GLY:HA3	2.44	0.53
1:F:265:PRO:HG2	1:F:268:GLU:HB2	1.91	0.53
1:H:146:GLU:C	1:H:149:LYS:HG2	2.33	0.53
1:A:295:LEU:HD13	1:A:321:PHE:HB3	1.91	0.53
1:E:264:ALA:HB3	1:E:269:LEU:CD2	2.38	0.53
1:E:275:LYS:O	1:E:278:VAL:HB	2.08	0.53
1:B:329:VAL:OXT	1:C:313:SER:HB2	2.08	0.53
1:B:257:VAL:HG13	1:B:258:LYS:N	2.24	0.53
1:A:129:PHE:CE1	1:B:314:PHE:HB2	2.43	0.53
1:C:123:GLU:HG3	9:C:1385:HOH:O	2.08	0.53
1:F:141:PRO:HA	9:F:1736:HOH:O	2.09	0.53
1:E:133:LYS:O	1:E:133:LYS:HD3	2.09	0.52
1:A:251:LEU:N	1:A:252:PRO:HD2	2.24	0.52
1:B:189:PRO:HB3	1:B:249:ILE:HD13	1.90	0.52
1:D:327:PHE:CD1	1:D:327:PHE:C	2.87	0.52
1:C:166[A]:CYS:HB2	9:C:1064:HOH:O	2.08	0.52
1:C:251:LEU:N	1:C:252:PRO:HD2	2.25	0.52
1:A:171:LEU:HB2	1:A:173:PHE:CE1	2.45	0.52
1:G:123:GLU:O	1:G:127:THR:HG23	2.10	0.52
1:G:308:ASP:CG	1:G:311:LYS:HD3	2.34	0.52
1:E:165:VAL:HG23	1:E:165:VAL:O	2.09	0.52
1:E:251:LEU:N	1:E:252:PRO:HD2	2.24	0.52
1:E:229:LEU:HD13	1:E:247:VAL:O	2.10	0.52
1:G:264:ALA:HB3	1:G:269:LEU:HD13	1.92	0.52
1:A:220:HIS:CE1	1:A:223:CYS:HA	2.45	0.51
1:B:226:ILE:O	1:B:229:LEU:HB3	2.10	0.51
1:B:251:LEU:N	1:B:252:PRO:HD2	2.25	0.51
1:H:132:PHE:HE1	1:H:136:LYS:HD2	1.75	0.51
1:A:319:LEU:HD12	1:A:320:GLU:H	1.75	0.51
1:G:233:PRO:HG2	1:G:235:ASP:OD1	2.11	0.51
1:C:230:LEU:HA	1:C:254:LYS:HE3	1.93	0.51
1:E:133:LYS:HD3	1:E:133:LYS:C	2.35	0.50
1:E:329:VAL:HG12	1:E:329:VAL:O	2.11	0.50
1:H:256:LYS:HE3	1:H:276:GLU:OE2	2.12	0.50
1:F:225:GLY:N	2:F:3008:ACT:H1	2.25	0.50
1:G:131:HIS:NE2	1:G:135:GLU:HG3	2.26	0.50
1:B:208:LEU:HD21	1:B:290:PHE:HB2	1.93	0.50
1:B:329:VAL:HG12	1:B:329:VAL:O	2.11	0.50
1:C:230:LEU:HD23	1:C:254:LYS:HG3	1.94	0.50
1:D:227:LYS:HD3	8:D:3101:CIT:H42	1.92	0.50
1:F:329:VAL:HG22	1:H:126:LYS:NZ	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:VAL:HG12	1:H:269:LEU:HD22	1.92	0.50
1:F:143:LEU:HD12	1:F:147:LEU:HD13	1.93	0.50
1:H:254:LYS:HE3	1:H:258:LYS:HE3	1.94	0.50
1:H:232:PHE:CD1	1:H:244:GLU:HG2	2.46	0.49
1:F:265:PRO:O	1:F:268:GLU:N	2.40	0.49
1:H:258:LYS:NZ	9:H:1166:HOH:O	2.42	0.49
1:A:134:LYS:HG3	1:A:135:GLU:H	1.76	0.49
1:F:234:PHE:HZ	1:F:247:VAL:HG23	1.77	0.49
1:D:123:GLU:OE2	1:D:126:LYS:HD2	2.12	0.49
1:F:119:SER:HB2	9:F:1259:HOH:O	2.12	0.49
1:B:261:HIS:HB3	1:B:264:ALA:HB2	1.95	0.49
1:G:270:CYS:O	1:G:274:GLU:HG3	2.12	0.49
1:A:140:ASN:HB3	1:A:143:LEU:HB3	1.94	0.49
1:E:154:PRO:HG2	1:E:155:PHE:HD1	1.77	0.49
1:C:221:SER:HB3	1:C:308:ASP:HA	1.94	0.49
1:A:160:CYS:N	1:A:186:ASN:HB3	2.28	0.49
1:E:220:HIS:CE1	1:E:223:CYS:HA	2.48	0.48
1:A:140:ASN:HB3	1:A:143:LEU:HB2	1.95	0.48
1:B:318:GLY:O	1:C:323:LEU:HA	2.13	0.48
1:G:237:THR:HA	9:G:1759:HOH:O	2.12	0.48
1:B:189:PRO:HD2	1:B:199:THR:HG21	1.96	0.48
1:C:307:TYR:CE2	1:C:309:PHE:HB3	2.48	0.48
1:G:307:TYR:CZ	1:G:309:PHE:HB3	2.47	0.48
1:C:159:ALA:O	1:C:182:ARG:HA	2.13	0.48
1:B:300:LEU:HB2	9:B:1706:HOH:O	2.14	0.48
1:E:161:SER:O	1:E:162:ASP:C	2.57	0.48
1:E:274:GLU:O	1:E:278:VAL:HG23	2.13	0.48
1:F:308:ASP:CG	1:F:311:LYS:HD3	2.38	0.48
1:B:228:GLY:HA2	1:B:231:SER:OG	2.14	0.48
1:H:307:TYR:CZ	1:H:309:PHE:HB3	2.48	0.48
1:E:134:LYS:CD	1:E:135:GLU:OE1	2.62	0.47
1:G:111:SER:OG	1:G:117:PRO:HB3	2.14	0.47
1:G:230:LEU:HD12	1:G:270:CYS:SG	2.54	0.47
1:A:151:GLN:HG3	1:A:210:LEU:HD22	1.96	0.47
1:C:160:CYS:HB2	1:C:186:ASN:HD22	1.79	0.47
1:E:256:LYS:HD3	1:E:276:GLU:HG2	1.97	0.47
1:B:317:TRP:CB	1:C:325:SER:HA	2.45	0.47
1:B:126:LYS:O	1:B:130:LEU:HG	2.15	0.47
1:B:159:ALA:C	1:B:186:ASN:HB3	2.39	0.47
1:E:256:LYS:HD3	1:E:276:GLU:CG	2.45	0.47
1:H:132:PHE:CE1	1:H:136:LYS:HD2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:ASN:OD1	6:E:3304:EDO:H11	2.15	0.47
1:E:307:TYR:CE2	1:E:309:PHE:HB3	2.49	0.47
1:A:131:HIS:O	1:A:135:GLU:HG2	2.15	0.46
1:B:234:PHE:HZ	1:B:247:VAL:HG23	1.80	0.46
1:G:256:LYS:HE2	1:G:260:GLN:OE1	2.15	0.46
1:B:321:PHE:C	1:B:321:PHE:CD2	2.93	0.46
1:F:133:LYS:HD3	1:F:133:LYS:C	2.40	0.46
1:B:154:PRO:HD2	1:B:177:GLU:O	2.15	0.46
1:C:160:CYS:SG	2:C:3007:ACT:H2	2.55	0.46
1:C:140:ASN:N	1:C:141:PRO:CD	2.78	0.46
1:A:228:GLY:O	1:A:229:LEU:C	2.58	0.46
1:B:253:ALA:O	1:B:257:VAL:HG12	2.16	0.46
1:E:230:LEU:HD23	1:E:254:LYS:HG3	1.97	0.46
1:H:131:HIS:ND1	1:H:131:HIS:O	2.49	0.46
1:B:317:TRP:HA	1:C:325:SER:HA	1.97	0.46
1:B:133:LYS:O	1:B:133:LYS:HD3	2.15	0.45
1:E:291:VAL:O	1:E:295:LEU:HG	2.16	0.45
1:A:131:HIS:CE1	1:A:135:GLU:HG3	2.51	0.45
1:B:264:ALA:HB1	1:B:268:GLU:OE2	2.16	0.45
1:E:327:PHE:CD1	1:E:327:PHE:C	2.94	0.45
1:F:257:VAL:HG11	1:F:273:CYS:HA	1.97	0.45
1:B:161:SER:O	1:B:162:ASP:C	2.59	0.45
1:B:119:SER:HB3	1:B:122:SER:OG	2.17	0.45
1:F:189:PRO:HB3	1:F:249:ILE:CD1	2.47	0.45
1:H:165:VAL:O	1:H:166[A]:CYS:C	2.59	0.45
1:A:159:ALA:C	1:A:186:ASN:HB3	2.42	0.45
1:A:261:HIS:CD2	1:A:272:HIS:NE2	2.85	0.45
1:C:264:ALA:HB1	1:C:265:PRO:HD2	1.98	0.45
1:F:269:LEU:CD1	1:F:269:LEU:N	2.78	0.45
1:A:307:TYR:CE2	1:A:309:PHE:HB3	2.51	0.45
1:B:189:PRO:HB3	1:B:249:ILE:CD1	2.46	0.45
1:G:116:ILE:CD1	9:G:1278:HOH:O	2.65	0.45
1:F:174:GLN:O	1:F:177:GLU:HB2	2.17	0.45
1:G:159:ALA:O	1:G:182:ARG:HA	2.17	0.45
1:G:295:LEU:HD21	1:G:302:LEU:HG	1.98	0.45
1:G:311:LYS:N	1:G:311:LYS:CD	2.80	0.45
1:D:160:CYS:HB2	1:D:186:ASN:HD22	1.82	0.45
1:G:124:ARG:HH21	1:H:177:GLU:CD	2.24	0.45
1:G:259:ALA:HB2	9:G:1596:HOH:O	2.15	0.45
1:H:174:GLN:O	1:H:177:GLU:HB2	2.17	0.45
1:E:227:LYS:HE2	9:E:1688:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:LYS:HE3	1:E:260:GLN:OE1	2.16	0.44
1:F:116:ILE:N	1:F:117:PRO:CD	2.80	0.44
1:G:225:GLY:H	2:G:3002:ACT:H1	1.81	0.44
1:B:327:PHE:CD1	1:B:327:PHE:C	2.95	0.44
1:A:195:LYS:HE2	1:A:195:LYS:HB3	1.72	0.44
1:A:180:VAL:HG12	1:A:182:ARG:HG3	2.00	0.44
1:E:276:GLU:OE1	1:E:276:GLU:HA	2.18	0.44
1:G:143:LEU:HD11	1:G:175:PRO:HG2	1.99	0.44
1:H:327:PHE:CD1	1:H:327:PHE:C	2.95	0.44
1:A:154:PRO:HG2	1:A:155:PHE:HD1	1.81	0.44
1:B:174:GLN:HB3	1:B:175:PRO:HD2	1.99	0.44
1:F:265:PRO:O	1:F:266:PHE:C	2.60	0.44
1:G:327:PHE:CD1	1:G:327:PHE:C	2.96	0.44
1:E:156:MET:HE2	1:E:158:PHE:CE1	2.53	0.44
1:B:282:LEU:HA	1:B:285:LEU:HD12	2.00	0.43
1:G:165:VAL:O	1:G:166[B]:CYS:C	2.61	0.43
1:D:180:VAL:HG12	1:D:182:ARG:HG3	2.00	0.43
1:E:243:ILE:O	1:E:247:VAL:HG22	2.18	0.43
1:G:195:LYS:HG2	1:H:194:ALA:O	2.18	0.43
1:B:124:ARG:NH2	1:B:128:GLY:HA3	2.34	0.43
1:B:143:LEU:HD21	1:B:175:PRO:HG2	1.99	0.43
1:B:256:LYS:HD3	1:B:276:GLU:CD	2.44	0.43
1:H:144:TYR:HA	1:H:147:LEU:HD12	2.00	0.43
1:B:271:THR:O	1:B:275:LYS:HG3	2.19	0.43
1:C:327:PHE:CD1	1:C:327:PHE:C	2.96	0.43
1:B:269:LEU:C	1:B:269:LEU:HD13	2.43	0.43
1:A:213:SER:O	1:A:300:LEU:HA	2.19	0.43
1:B:191:TYR:C	1:B:191:TYR:CD2	2.96	0.43
1:D:307:TYR:CZ	1:D:309:PHE:HB3	2.53	0.43
1:E:134:LYS:HD2	1:E:135:GLU:OE1	2.18	0.43
1:G:147:LEU:HD23	1:G:147:LEU:HA	1.80	0.43
1:B:124:ARG:O	1:B:124:ARG:NE	2.47	0.43
1:B:168:SER:HA	1:B:173:PHE:HB2	2.01	0.43
1:B:251:LEU:O	1:B:252:PRO:C	2.60	0.43
1:F:130:LEU:HA	1:F:130:LEU:HD23	1.83	0.43
1:G:232:PHE:CG	1:G:244:GLU:HG2	2.53	0.43
1:B:120:GLU:CD	1:B:120:GLU:N	2.73	0.43
1:D:159:ALA:O	1:D:182:ARG:HA	2.18	0.43
1:A:183:ASN:OD1	1:A:183:ASN:C	2.62	0.42
1:A:179:PHE:CD2	1:A:206:ALA:HB2	2.54	0.42
1:A:177:GLU:OE2	1:B:124:ARG:HD2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:GLY:O	1:E:316:LEU:HD12	2.19	0.42
1:G:258:LYS:HE3	9:G:1389:HOH:O	2.19	0.42
1:H:134:LYS:HG3	1:H:135:GLU:HG2	2.01	0.42
1:A:126:LYS:HG3	1:C:329:VAL:HG21	2.01	0.42
1:C:266:PHE:O	1:C:269:LEU:HB2	2.19	0.42
1:E:171:LEU:HB2	1:E:173:PHE:CD1	2.53	0.42
1:D:295:LEU:HD13	1:D:321:PHE:HB3	2.02	0.42
1:E:174:GLN:O	1:E:177:GLU:HB2	2.19	0.42
1:F:159:ALA:O	1:F:182:ARG:HA	2.20	0.42
1:F:185:ALA:HB2	1:F:225:GLY:HA3	2.00	0.42
1:G:133:LYS:HD3	1:G:133:LYS:C	2.43	0.42
1:G:141:PRO:HA	9:G:1490:HOH:O	2.19	0.42
1:H:166[A]:CYS:SG	9:H:1932:HOH:O	2.62	0.42
1:F:165:VAL:HG23	1:F:165:VAL:O	2.19	0.42
1:G:233:PRO:O	1:G:234:PHE:C	2.62	0.42
1:G:305:GLY:HA2	1:G:315:GLU:O	2.19	0.42
1:A:124:ARG:HH21	1:A:128:GLY:CA	2.32	0.41
1:E:319:LEU:C	1:E:319:LEU:HD23	2.44	0.41
1:F:269:LEU:N	1:F:269:LEU:HD12	2.35	0.41
1:F:275:LYS:O	1:F:278:VAL:HB	2.20	0.41
1:F:307:TYR:CZ	1:F:309:PHE:HB3	2.55	0.41
1:G:194:ALA:O	1:H:195:LYS:HG2	2.19	0.41
1:H:251:LEU:N	1:H:252:PRO:HD2	2.35	0.41
1:A:326:THR:O	1:A:327:PHE:HB3	2.20	0.41
1:A:123:GLU:O	1:A:124:ARG:C	2.63	0.41
1:A:165:VAL:HG23	1:A:165:VAL:O	2.19	0.41
1:A:171:LEU:HB2	1:A:173:PHE:CD1	2.55	0.41
1:E:253:ALA:O	1:E:257:VAL:HG22	2.20	0.41
1:F:143:LEU:HD12	1:F:143:LEU:C	2.46	0.41
1:E:138:ASP:O	1:E:141:PRO:HD3	2.21	0.41
1:F:161:SER:O	1:F:162:ASP:C	2.63	0.41
1:A:204:GLU:HG3	1:A:208:LEU:HD12	2.02	0.41
1:A:295:LEU:HD23	1:A:300:LEU:O	2.21	0.41
1:G:265:PRO:HD2	1:G:268:GLU:CD	2.45	0.41
1:H:307:TYR:CE2	1:H:309:PHE:HB3	2.56	0.41
1:B:124:ARG:HE	1:B:124:ARG:C	2.29	0.41
1:E:225:GLY:N	2:E:3005:ACT:H1	2.22	0.41
1:F:124:ARG:HD2	1:F:124:ARG:O	2.21	0.41
1:F:220:HIS:CE1	1:F:223:CYS:HA	2.55	0.41
1:H:134:LYS:O	1:H:135:GLU:C	2.63	0.41
1:A:137:TYR:HA	1:A:144:TYR:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:VAL:HG13	2:C:3007:ACT:H1	2.03	0.41
1:E:180:VAL:HG12	1:E:181:VAL:N	2.35	0.41
1:G:166[B]:CYS:SG	1:G:169:HIS:HD2	2.44	0.41
1:E:173:PHE:HD2	1:E:177:GLU:HB3	1.85	0.41
1:G:116:ILE:HD12	9:G:1278:HOH:O	2.20	0.41
1:F:154:PRO:HG2	1:F:155:PHE:CD1	2.57	0.40
1:A:129:PHE:CZ	1:B:314:PHE:HB2	2.56	0.40
1:F:166:CYS:SG	1:F:168:SER:HB2	2.62	0.40
1:F:189:PRO:HB3	1:F:249:ILE:HD13	2.03	0.40
1:G:220:HIS:CE1	1:G:223:CYS:HA	2.55	0.40
1:G:265:PRO:O	1:G:268:GLU:HB2	2.22	0.40
1:H:140:ASN:N	1:H:141:PRO:CD	2.84	0.40
1:H:232:PHE:CG	1:H:244:GLU:HG2	2.56	0.40
1:A:138:ASP:C	1:A:140:ASN:N	2.79	0.40
1:A:308:ASP:OD1	1:A:310:VAL:HB	2.21	0.40
1:H:146:GLU:HA	1:H:149:LYS:HG2	2.03	0.40
1:C:171:LEU:HD23	1:C:171:LEU:HA	1.83	0.40
1:D:235:ASP:C	1:D:235:ASP:OD1	2.64	0.40
1:G:251:LEU:HA	1:G:251:LEU:HD23	1.89	0.40
1:H:320:GLU:HG3	9:H:1907:HOH:O	2.22	0.40
1:F:243:ILE:O	1:F:247:VAL:HG22	2.21	0.40
1:G:133:LYS:HD3	1:G:133:LYS:O	2.21	0.40
1:H:146:GLU:OE1	1:H:149:LYS:NZ	2.50	0.40
1:H:189:PRO:HB2	1:H:196:TYR:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	170/180 (94%)	164 (96%)	6 (4%)	32	18
1	B	173/180 (96%)	168 (97%)	5 (3%)	37	24
1	C	177/180 (98%)	173 (98%)	4 (2%)	44	33
1	D	172/180 (96%)	167 (97%)	5 (3%)	37	24
1	E	172/180 (96%)	166 (96%)	6 (4%)	32	18
1	F	174/180 (97%)	167 (96%)	7 (4%)	28	14
1	G	180/180 (100%)	173 (96%)	7 (4%)	28	15
1	H	172/180 (96%)	165 (96%)	7 (4%)	27	14
All	All	1390/1440 (96%)	1343 (97%)	47 (3%)	32	19

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ARG
1	A	133	LYS
1	A	245	GLU
1	A	263	ASP
1	A	309	PHE
1	A	328	SER
1	B	118	LYS
1	B	124	ARG
1	B	133	LYS
1	B	241	ASP
1	B	245	GLU
1	C	143	LEU
1	C	213	SER
1	C	245	GLU
1	C	320	GLU
1	D	120	GLU
1	D	133	LYS
1	D	143	LEU
1	D	245	GLU
1	D	258	LYS
1	E	119	SER
1	E	124	ARG
1	E	133	LYS
1	E	135	GLU
1	E	263	ASP
1	E	276	GLU
1	F	118	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	133	LYS
1	F	231	SER
1	F	245	GLU
1	F	263	ASP
1	F	302	LEU
1	F	315	GLU
1	G	111	SER
1	G	118	LYS
1	G	133	LYS
1	G	143	LEU
1	G	152	SER
1	G	269	LEU
1	G	323	LEU
1	H	123	GLU
1	H	126	LYS
1	H	131	HIS
1	H	133	LYS
1	H	140	ASN
1	H	174	GLN
1	H	320	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	186	ASN
1	B	186	ASN
1	B	214	ASN
1	B	260	GLN
1	C	131	HIS
1	C	169	HIS
1	C	186	ASN
1	C	214	ASN
1	C	260	GLN
1	D	186	ASN
1	D	261	HIS
1	F	209	HIS
1	G	169	HIS
1	G	193	GLN
1	H	186	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 ⓘ

Of 38 ligands modelled in this entry, 20 are monoatomic - leaving 18 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	$\# Z > 2$
2	ACT	C	3007	-	3,3,3	0.63	0	3,3,3	0.92	0
2	ACT	F	3008	-	3,3,3	0.55	0	3,3,3	0.88	0
2	ACT	A	3003	4	3,3,3	0.54	0	3,3,3	0.79	0
3	AZI	A	3203	-	2,2,2	0.75	0	0,1,1	-	-
3	AZI	E	3204	-	2,2,2	0.70	0	0,1,1	-	-
2	ACT	C	3004	-	3,3,3	0.67	0	3,3,3	0.64	0
3	AZI	H	3201	-	2,2,2	1.29	0	0,1,1	-	-
6	EDO	E	3304	-	3,3,3	0.69	0	2,2,2	0.46	0
3	AZI	D	3202	-	2,2,2	0.76	0	0,1,1	-	-
6	EDO	H	3301	-	3,3,3	1.22	0	2,2,2	0.55	0
6	EDO	D	3302	-	3,3,3	0.76	0	2,2,2	1.00	0
2	ACT	E	3005	4	3,3,3	0.52	0	3,3,3	0.85	0
2	ACT	G	3009	-	3,3,3	0.68	0	3,3,3	0.84	0
6	EDO	A	3303	-	3,3,3	0.73	0	2,2,2	0.44	0
2	ACT	A	3001	4	3,3,3	0.59	0	3,3,3	0.92	0
8	CIT	D	3101	-	12,12,12	2.02	1 (8%)	17,17,17	1.13	1 (5%)
2	ACT	G	3002	4	3,3,3	0.77	0	3,3,3	0.96	0
2	ACT	H	3006	4	3,3,3	0.94	0	3,3,3	1.01	0

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
6	EDO	H	3301	-	-	0/1/1/1	-
6	EDO	E	3304	-	-	0/1/1/1	-
6	EDO	D	3302	-	-	0/1/1/1	-
8	CIT	D	3101	-	-	10/16/16/16	-
6	EDO	A	3303	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	3101	CIT	O7-C3	-5.78	1.32	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	3101	CIT	O6-C6-C3	3.49	119.84	113.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	3101	CIT	C1-C2-C3-O7
8	D	3101	CIT	C1-C2-C3-C4
8	D	3101	CIT	C1-C2-C3-C6
8	D	3101	CIT	O7-C3-C4-C5
8	D	3101	CIT	C6-C3-C4-C5
8	D	3101	CIT	O7-C3-C6-O5
8	D	3101	CIT	O7-C3-C6-O6
8	D	3101	CIT	C4-C3-C6-O5
8	D	3101	CIT	C4-C3-C6-O6
8	D	3101	CIT	C2-C3-C4-C5

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3007	ACT	2	0
2	F	3008	ACT	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3003	ACT	1	0
6	E	3304	EDO	1	0
2	E	3005	ACT	2	0
2	G	3009	ACT	1	0
2	A	3001	ACT	2	0
8	D	3101	CIT	1	0
2	G	3002	ACT	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

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.