



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:39 AM UTC

PDB ID : 1EI6 / pdb_00001ei6
Title : CRYSTAL STRUCTURE OF PHOSPHONOACETATE HYDROLASE
COMPLEXED WITH PHOSPHONOFORMATE
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Deposited on : 2000-02-24
Resolution : 2.10 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

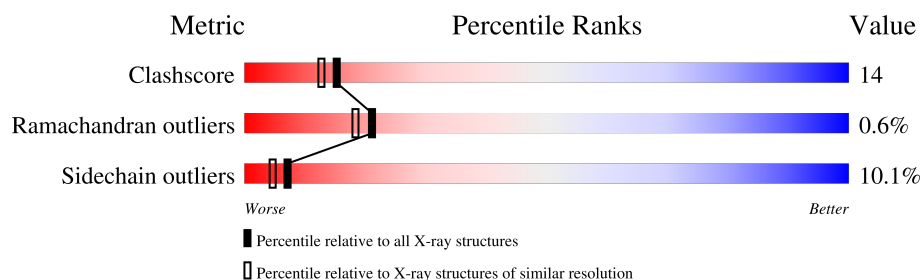
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	406	
1	B	406	
1	C	406	
1	D	406	

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
3	PPF	C	413	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12751 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 PHOSPHONOACETATE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3087	1953	535	586	13			
1	B	403	Total	C	N	O	S	0	0	0
			3068	1941	534	580	13			
1	C	401	Total	C	N	O	S	0	0	0
			3047	1928	529	577	13			
1	D	395	Total	C	N	O	S	0	0	0
			3011	1906	522	570	13			

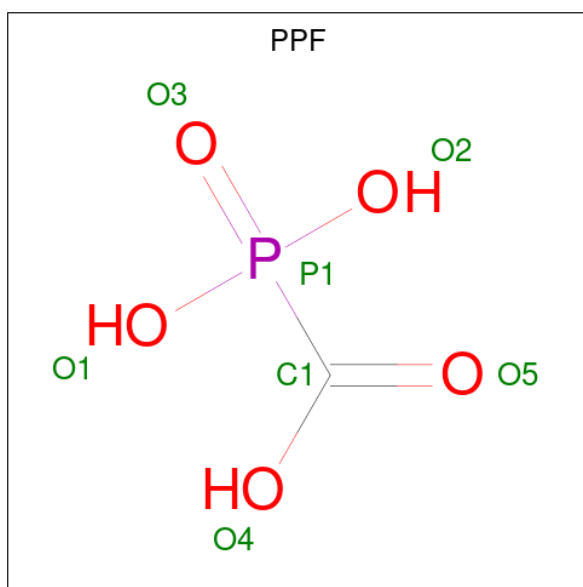
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASN	GLN	conflict	UNP Q51782
B	3	ASN	GLN	conflict	UNP Q51782
C	3	ASN	GLN	conflict	UNP Q51782
D	3	ASN	GLN	conflict	UNP Q51782

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

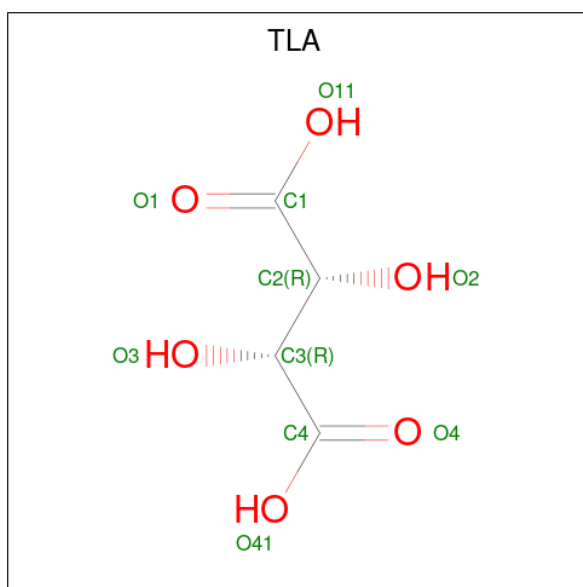
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is PHOSPHONOFORMIC ACID (CCD ID: PPF) (formula: CH₃O₅P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			7	1	5	1		
3	C	1	Total	C	O	P	0	0
			7	1	5	1		
3	D	1	Total	C	O	P	0	0
			7	1	5	1		

- Molecule 4 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O		
			10	4	6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total 137	O 137	0	0
5	B	137	Total 137	O 137	0	0
5	C	108	Total 108	O 108	0	0
5	D	117	Total 117	O 117	0	0

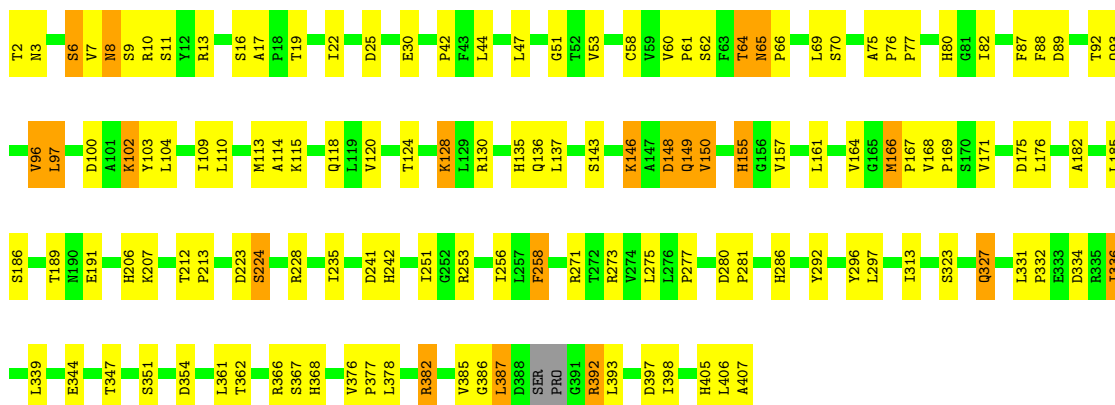
3 Residue-property plots

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.

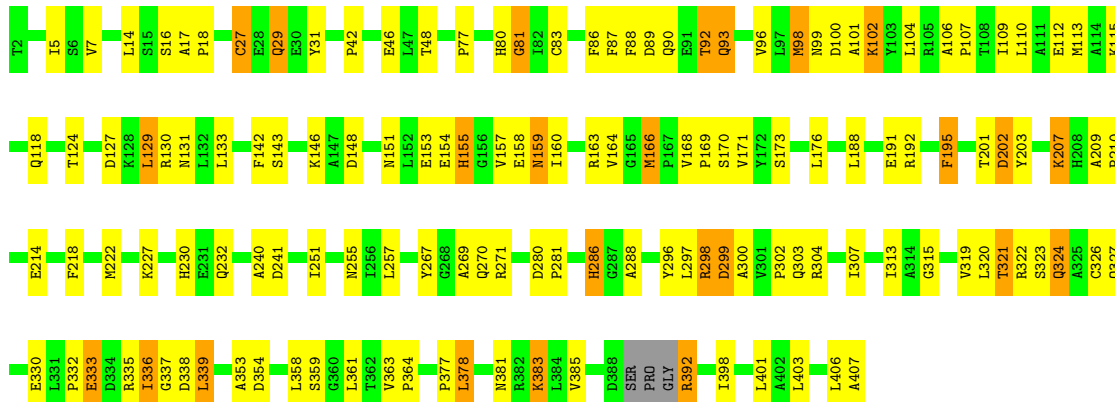
• Molecule 1: PHOSPHONOACETATE HYDROLASE

Chain A: 



• Molecule 1: PHOSPHONOACETATE HYDROLASE

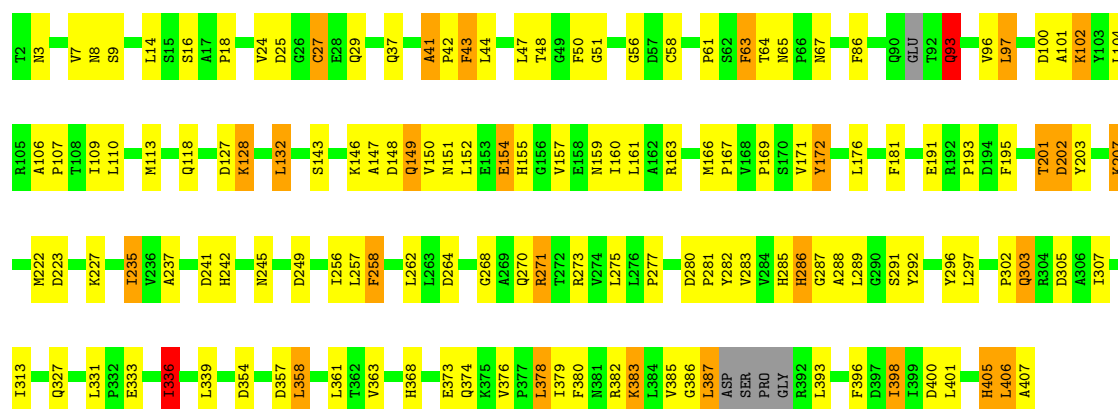
Chain B: 



• Molecule 1: PHOSPHONOACETATE HYDROLASE

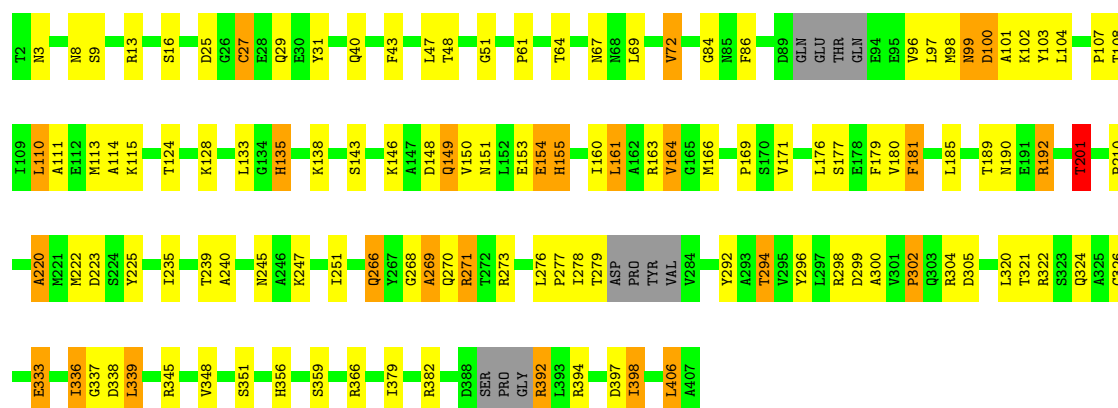
Chain C: 





• Molecule 1: PHOSPHONOACETATE HYDROLASE

Chain D: 67% 23% 6% •



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.50Å 129.54Å 133.38Å 90.00° 96.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	90.0 (20.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.192 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12751	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: PPF, ZN, TLA

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	1.22	7/3146 (0.2%)	1.49	25/4276 (0.6%)
1	B	1.19	0/3126	1.46	20/4250 (0.5%)
1	C	1.21	4/3104 (0.1%)	1.48	29/4218 (0.7%)
1	D	1.22	2/3066 (0.1%)	1.43	17/4163 (0.4%)
All	All	1.21	13/12442 (0.1%)	1.46	91/16907 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	135	HIS	ND1-CE1	10.20	1.42	1.32
1	D	135	HIS	CG-CD2	9.36	1.46	1.35
1	C	245	ASN	CA-CB	6.31	1.65	1.53
1	C	202	ASP	CG-OD2	6.00	1.36	1.25
1	A	405	HIS	CA-C	-6.00	1.45	1.52
1	A	368	HIS	ND1-CE1	5.26	1.37	1.32
1	A	182	ALA	N-CA	-5.21	1.40	1.46
1	C	398	ILE	CA-CB	-5.21	1.48	1.54
1	A	313	ILE	CA-CB	-5.19	1.47	1.54
1	A	19	THR	N-CA	-5.13	1.39	1.46
1	A	258	PHE	CA-C	-5.08	1.46	1.53
1	C	172	TYR	CA-C	-5.02	1.47	1.53
1	A	7	VAL	CA-C	-5.01	1.46	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	ASN	CA-CB-CG	8.71	121.31	112.60
1	C	398	ILE	N-CA-C	8.38	119.16	110.36
1	A	354	ASP	CA-CB-CG	8.28	120.88	112.60
1	A	135	HIS	CA-CB-CG	-8.23	105.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	405	HIS	CA-CB-CG	-7.96	105.84	113.80
1	A	64	THR	N-CA-C	7.78	119.40	111.07
1	A	405	HIS	CA-CB-CG	-7.20	106.61	113.80
1	A	256	ILE	N-CA-C	7.19	118.18	108.11
1	A	334	ASP	CA-C-N	-7.05	111.46	122.67
1	A	334	ASP	C-N-CA	-7.05	111.46	122.67
1	B	86	PHE	N-CA-CB	-7.03	98.42	111.13
1	C	249	ASP	CA-CB-CG	6.83	119.44	112.60
1	D	333	GLU	N-CA-CB	6.76	120.63	110.22
1	D	67	ASN	CA-CB-CG	-6.58	106.02	112.60
1	D	201	THR	N-CA-CB	6.54	122.93	111.55
1	B	333	GLU	N-CA-C	6.49	120.05	111.75
1	A	155	HIS	CA-CB-CG	-6.39	107.41	113.80
1	B	333	GLU	N-CA-CB	6.37	120.21	110.14
1	C	336	ILE	CB-CA-C	6.37	120.63	110.82
1	A	65	ASN	CA-CB-CG	6.32	118.92	112.60
1	C	27	CYS	N-CA-C	6.26	119.42	108.52
1	B	354	ASP	CB-CA-C	-6.21	100.28	110.85
1	C	379	ILE	N-CA-C	6.20	116.78	108.11
1	C	242	HIS	CA-CB-CG	-6.17	107.63	113.80
1	B	332	PRO	N-CA-CB	6.10	106.34	102.92
1	B	155	HIS	CA-CB-CG	-6.08	107.72	113.80
1	C	396	PHE	N-CA-CB	6.05	120.22	110.42
1	C	67	ASN	CA-CB-CG	-6.04	106.56	112.60
1	C	172	TYR	CA-CB-CG	-5.96	103.17	113.90
1	C	376	VAL	N-CA-C	5.94	115.58	108.45
1	B	166	MET	O-C-N	5.94	125.51	121.71
1	C	41	ALA	CA-C-N	5.92	125.79	119.28
1	C	41	ALA	C-N-CA	5.92	125.79	119.28
1	D	333	GLU	N-CA-C	5.90	118.50	111.71
1	C	106	ALA	N-CA-C	5.88	113.51	108.22
1	C	155	HIS	CA-CB-CG	-5.87	107.93	113.80
1	C	282	TYR	N-CA-C	5.85	119.73	112.59
1	C	289	LEU	N-CA-C	5.74	118.01	108.20
1	C	258	PHE	CA-CB-CG	-5.72	108.08	113.80
1	B	313	ILE	N-CA-C	5.70	116.37	108.84
1	C	398	ILE	N-CA-CB	5.70	116.84	110.51
1	B	86	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	29	GLN	N-CA-C	5.61	118.12	111.33
1	C	63	PHE	CA-CB-CG	5.60	119.40	113.80
1	D	181	PHE	CA-CB-CG	-5.59	108.21	113.80
1	D	64	THR	N-CA-C	5.57	117.04	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	ILE	CB-CA-C	-5.55	104.25	110.96
1	D	397	ASP	N-CA-C	-5.54	106.29	113.16
1	C	147	ALA	CA-C-N	5.50	129.79	120.88
1	C	147	ALA	C-N-CA	5.50	129.79	120.88
1	A	58	CYS	N-CA-C	-5.48	101.86	110.36
1	A	397	ASP	N-CA-C	-5.44	106.02	113.30
1	B	321	THR	N-CA-C	-5.44	103.21	110.55
1	A	387	LEU	CB-CA-C	5.43	119.84	110.77
1	C	256	ILE	N-CA-C	5.41	116.27	108.48
1	D	149	GLN	N-CA-C	5.40	119.39	112.26
1	B	302	PRO	N-CA-CB	5.40	107.62	103.30
1	B	195	PHE	CA-CB-CG	-5.40	108.40	113.80
1	B	98	MET	CB-CA-C	-5.37	104.12	112.07
1	D	398	ILE	N-CA-C	5.37	115.58	110.42
1	B	81	GLY	N-CA-C	5.37	122.19	115.21
1	B	353	ALA	CA-C-N	5.35	127.88	120.29
1	B	353	ALA	C-N-CA	5.35	127.88	120.29
1	D	379	ILE	N-CA-C	5.34	115.59	108.11
1	C	150	VAL	N-CA-CB	5.34	116.35	110.53
1	A	8	ASN	CA-CB-CG	-5.32	107.28	112.60
1	B	202	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	137	LEU	N-CA-C	5.25	117.79	109.24
1	B	286	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	22	ILE	N-CA-C	5.17	115.36	108.11
1	A	347	THR	N-CA-C	5.16	117.81	109.40
1	C	65	ASN	N-CA-C	5.16	119.77	112.75
1	A	327	GLN	N-CA-CB	-5.12	102.64	110.07
1	C	155	HIS	N-CA-C	5.11	119.56	113.23
1	D	27	CYS	N-CA-C	5.10	121.65	110.80
1	A	398	ILE	N-CA-C	5.08	115.29	110.42
1	B	377	PRO	CB-CA-C	-5.08	103.60	110.60
1	C	43	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	120	VAL	N-CA-CB	-5.07	105.05	111.64
1	D	133	LEU	N-CA-C	5.06	116.80	111.28
1	A	336	ILE	CA-CB-CG1	5.06	119.00	110.40
1	D	155	HIS	N-CA-C	5.06	120.08	113.30
1	A	332	PRO	N-CA-CB	5.05	106.61	103.23
1	D	220	ALA	N-CA-C	-5.05	105.78	111.28
1	D	29	GLN	N-CA-C	5.04	117.42	111.33
1	A	344	GLU	CA-C-N	5.03	127.33	120.54
1	A	344	GLU	C-N-CA	5.03	127.33	120.54
1	C	291	SER	N-CA-C	5.03	118.30	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	TYR	CA-CB-CG	-5.02	104.87	113.90
1	C	29	GLN	N-CA-C	5.01	118.86	112.34
1	A	387	LEU	N-CA-C	5.01	116.44	108.67

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	3087	0	3065	76	0
1	B	3068	0	3046	92	0
1	C	3047	0	3013	94	0
1	D	3011	0	2989	73	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	7	0	0	2	0
3	C	7	0	0	6	0
3	D	7	0	0	0	0
4	B	10	0	1	0	0
5	A	137	0	0	3	0
5	B	137	0	0	2	0
5	C	108	0	0	3	0
5	D	117	0	0	3	0
All	All	12751	0	12114	331	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 14.

All (331) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:VAL:HG13	1:A:407:ALA:HB2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:MET:HE2	1:D:179:PHE:HD1	1.37	0.89
1:A:77:PRO:HG2	1:A:331:LEU:HD23	1.57	0.85
1:B:7:VAL:HG22	1:B:112:GLU:HG3	1.58	0.84
1:B:154:GLU:HG2	1:B:155:HIS:CE1	2.12	0.84
1:D:192:ARG:HG2	1:D:192:ARG:HH11	1.43	0.83
1:B:321:THR:HA	1:B:339:LEU:HD12	1.64	0.80
1:C:64:THR:N	3:C:413:PPF:O5	2.16	0.79
1:C:97:LEU:HD21	1:C:281:PRO:HG2	1.66	0.78
1:D:161:LEU:HD12	1:D:166:MET:O	1.84	0.78
1:A:386:GLY:C	1:A:387:LEU:HD23	2.08	0.77
1:D:166:MET:HE2	1:D:179:PHE:CD1	2.19	0.77
1:C:148:ASP:HB3	1:C:149:GLN:HG2	1.68	0.76
1:A:25:ASP:HA	1:A:241:ASP:OD2	1.87	0.74
1:B:151:ASN:OD1	1:B:153:GLU:HG2	1.88	0.74
1:C:286:HIS:H	1:C:286:HIS:CD2	2.06	0.74
1:B:159:ASN:O	1:B:163:ARG:HG3	1.87	0.73
1:C:86:PHE:CD2	1:C:281:PRO:HD3	2.24	0.73
1:A:69:LEU:HD13	1:A:82:ILE:HG13	1.71	0.71
1:B:170:SER:O	1:B:173:SER:HB3	1.92	0.70
1:A:89:ASP:OD1	1:A:92:THR:HG23	1.90	0.70
1:B:113:MET:HE1	1:B:195:PHE:CG	2.27	0.70
1:B:148:ASP:HB3	1:B:168:VAL:HG21	1.72	0.69
1:C:331:LEU:HB3	1:C:336:ILE:CD1	2.22	0.69
1:B:326:CYS:SG	1:B:333:GLU:HB3	2.33	0.69
1:D:169:PRO:HG2	1:D:176:LEU:HD12	1.75	0.69
1:B:203:TYR:CZ	1:B:207:LYS:HD3	2.29	0.68
1:B:298:ARG:HD3	1:B:298:ARG:N	2.09	0.68
1:B:321:THR:OG1	1:B:324:GLN:HG3	1.95	0.67
1:D:201:THR:HG22	5:D:879:HOH:O	1.95	0.66
1:D:192:ARG:HG2	1:D:192:ARG:NH1	2.11	0.65
1:D:268:GLY:O	1:D:271:ARG:HB2	1.97	0.65
1:B:298:ARG:O	1:B:300:ALA:N	2.29	0.65
1:D:27:CYS:HB3	1:D:240:ALA:HB2	1.78	0.65
1:B:89:ASP:O	1:B:93:GLN:N	2.29	0.65
1:C:235:ILE:N	1:C:235:ILE:HD13	2.09	0.65
1:A:185:LEU:O	1:A:189:THR:HG23	1.97	0.65
1:A:377:PRO:O	1:A:378:LEU:HD22	1.97	0.65
1:C:385:VAL:HG13	1:C:407:ALA:HB2	1.78	0.65
1:B:81:GLY:O	1:B:335:ARG:NH1	2.29	0.64
1:A:77:PRO:HA	1:A:80:HIS:CE1	2.32	0.64
1:B:100:ASP:OD2	1:B:102:LYS:HD3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:VAL:HA	1:D:155:HIS:CE1	2.34	0.63
1:A:146:LYS:C	1:A:148:ASP:H	2.05	0.63
1:A:280:ASP:HB3	1:A:281:PRO:HD2	1.80	0.63
1:C:151:ASN:OD1	1:C:154:GLU:HB2	1.98	0.63
1:B:319:VAL:O	1:B:320:LEU:HD23	1.99	0.62
1:A:385:VAL:CG1	1:A:407:ALA:HB2	2.29	0.62
1:A:161:LEU:HD11	1:A:168:VAL:CG2	2.29	0.62
1:A:164:VAL:HG12	1:A:166:MET:HB2	1.79	0.62
1:C:166:MET:HB3	1:C:167:PRO:HD2	1.80	0.62
1:A:212:THR:HB	1:A:213:PRO:HD2	1.82	0.62
1:C:159:ASN:O	1:C:163:ARG:HG3	2.00	0.62
1:A:148:ASP:HB3	1:A:149:GLN:HG2	1.82	0.62
1:C:303:GLN:O	1:C:307:ILE:HG13	1.99	0.62
1:A:97:LEU:HD11	1:A:281:PRO:CD	2.30	0.61
1:C:113:MET:HE1	1:C:195:PHE:CG	2.35	0.61
1:A:387:LEU:HD23	1:A:387:LEU:N	2.14	0.61
1:B:27:CYS:HB3	1:B:240:ALA:HB2	1.83	0.61
1:C:50:PHE:C	1:C:383:LYS:HE3	2.26	0.60
1:A:128:LYS:HB3	5:A:545:HOH:O	2.00	0.60
1:B:322:ARG:HG3	1:B:336:ILE:HG22	1.83	0.60
1:B:359:SER:HB2	1:D:171:VAL:HG21	1.83	0.60
1:B:392:ARG:O	1:B:392:ARG:HG3	2.02	0.60
1:C:25:ASP:HA	1:C:241:ASP:OD2	2.01	0.60
1:C:172:TYR:HB3	1:C:203:TYR:CE2	2.37	0.60
1:C:101:ALA:O	1:C:104:LEU:HB2	2.02	0.60
1:C:331:LEU:HB3	1:C:336:ILE:HD12	1.82	0.60
1:A:6:SER:HA	1:A:10:ARG:O	2.01	0.60
1:A:150:VAL:HG22	1:A:155:HIS:CB	2.32	0.59
1:A:150:VAL:HG22	1:A:155:HIS:CG	2.37	0.59
1:C:64:THR:OG1	3:C:413:PPF:O3	2.21	0.59
1:A:224:SER:OG	1:A:228:ARG:NH2	2.27	0.58
1:D:13:ARG:HH11	1:D:13:ARG:HG2	1.68	0.58
1:D:150:VAL:HA	1:D:155:HIS:ND1	2.19	0.58
1:A:97:LEU:HD11	1:A:281:PRO:CG	2.33	0.58
1:A:224:SER:HG	1:A:228:ARG:HH21	1.47	0.58
1:B:88:PHE:HZ	1:B:93:GLN:NE2	2.00	0.58
1:C:146:LYS:C	1:C:148:ASP:H	2.12	0.58
1:B:267:TYR:O	1:B:271:ARG:HD3	2.03	0.57
1:C:191:GLU:OE2	1:C:191:GLU:N	2.27	0.57
1:A:75:ALA:HB1	1:A:76:PRO:HD2	1.85	0.57
1:B:100:ASP:OD2	1:B:102:LYS:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ALA:O	1:B:270:GLN:HB2	2.05	0.57
1:D:153:GLU:HG3	1:D:154:GLU:N	2.19	0.57
1:A:60:VAL:HG13	1:A:61:PRO:HA	1.87	0.57
1:D:151:ASN:OD1	1:D:154:GLU:HB2	2.05	0.56
1:A:77:PRO:HG2	1:A:331:LEU:CD2	2.33	0.56
1:B:151:ASN:OD1	1:B:154:GLU:HB3	2.05	0.56
1:C:169:PRO:HG2	1:C:176:LEU:HD12	1.86	0.56
1:C:285:HIS:CE1	1:C:287:GLY:HA3	2.41	0.56
1:B:214:GLU:OE2	1:B:214:GLU:N	2.29	0.56
1:C:283:VAL:O	1:C:288:ALA:HB2	2.06	0.56
1:C:61:PRO:HB2	1:C:63:PHE:CD2	2.41	0.56
1:B:171:VAL:HA	1:B:176:LEU:HD22	1.88	0.56
1:B:363:VAL:HB	1:B:364:PRO:HD2	1.87	0.56
1:B:99:ASN:OD1	1:B:99:ASN:N	2.33	0.55
1:D:351:SER:H	1:D:356:HIS:HE1	1.55	0.55
1:B:5:ILE:HD12	1:B:112:GLU:HB3	1.87	0.55
1:C:128:LYS:O	1:C:132:LEU:HD12	2.06	0.55
1:B:109:ILE:O	1:B:113:MET:HG3	2.05	0.55
1:D:110:LEU:HA	1:D:113:MET:HE2	1.88	0.55
1:A:17:ALA:HB3	1:A:235:ILE:CD1	2.37	0.55
1:C:368:HIS:HE1	3:C:413:PPF:O5	1.88	0.55
1:C:275:LEU:HD22	1:C:296:TYR:HE2	1.71	0.55
1:A:88:PHE:HB3	1:A:296:TYR:CZ	2.42	0.55
1:B:298:ARG:C	1:B:300:ALA:H	2.14	0.55
1:B:338:ASP:O	1:B:339:LEU:HD13	2.07	0.55
1:D:13:ARG:HG2	1:D:13:ARG:NH1	2.22	0.55
1:B:113:MET:HE1	1:B:195:PHE:CD1	2.42	0.54
1:B:296:TYR:CE1	1:B:337:GLY:HA2	2.43	0.54
1:C:25:ASP:HB2	5:C:696:HOH:O	2.07	0.54
1:C:181:PHE:CE2	1:C:222:MET:HG2	2.43	0.54
1:D:98:MET:HA	1:D:103:TYR:CD1	2.43	0.54
1:C:86:PHE:CG	1:C:281:PRO:HD3	2.43	0.53
1:A:171:VAL:HA	1:A:176:LEU:HD22	1.90	0.53
1:C:97:LEU:HD21	1:C:281:PRO:CG	2.37	0.53
1:B:42:PRO:O	1:B:46:GLU:HG2	2.08	0.53
1:C:47:LEU:HD23	1:C:47:LEU:C	2.34	0.53
1:C:100:ASP:OD2	1:C:102:LYS:HB3	2.08	0.53
1:C:25:ASP:OD1	1:C:202:ASP:HB3	2.07	0.53
1:D:84:GLY:O	1:D:98:MET:HE3	2.09	0.53
1:C:58:CYS:SG	1:C:374:GLN:HA	2.49	0.53
1:A:69:LEU:HD13	1:A:82:ILE:CG1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HG3	1:B:336:ILE:CG2	2.38	0.52
1:B:303:GLN:O	1:B:307:ILE:HG13	2.09	0.52
1:B:101:ALA:O	1:B:104:LEU:HB2	2.09	0.52
1:B:160:ILE:O	1:B:164:VAL:HG23	2.08	0.52
1:B:29:GLN:NE2	5:B:586:HOH:O	2.41	0.52
1:D:86:PHE:HB2	1:D:96:VAL:O	2.10	0.52
1:B:90:GLN:O	1:B:93:GLN:OE1	2.28	0.52
1:B:218:PHE:CD1	1:B:222:MET:HE2	2.45	0.52
1:D:338:ASP:O	1:D:339:LEU:HD12	2.10	0.52
1:A:113:MET:O	1:A:118:GLN:HB2	2.10	0.51
1:C:97:LEU:HD23	1:C:97:LEU:N	2.25	0.51
1:A:42:PRO:HD2	1:A:223:ASP:OD1	2.10	0.51
1:B:188:LEU:HD21	1:B:232:GLN:HB2	1.92	0.51
1:A:150:VAL:HA	1:A:155:HIS:ND1	2.25	0.51
1:A:69:LEU:CD1	1:A:82:ILE:HG13	2.39	0.51
1:D:247:LYS:HG3	1:D:348:VAL:CG1	2.40	0.51
1:C:285:HIS:HE1	1:C:287:GLY:HA3	1.76	0.51
1:C:201:THR:HG22	5:C:720:HOH:O	2.11	0.51
1:C:97:LEU:HD13	1:C:280:ASP:OD2	2.11	0.50
1:A:124:THR:O	1:A:143:SER:HA	2.11	0.50
1:B:87:PHE:CD2	1:B:98:MET:HG3	2.46	0.50
1:C:207:LYS:HG3	1:C:363:VAL:HG21	1.93	0.50
1:D:99:ASN:C	1:D:99:ASN:HD22	2.20	0.50
1:A:377:PRO:C	1:A:378:LEU:HD22	2.37	0.50
1:D:392:ARG:HD3	1:D:394:ARG:HD3	1.93	0.50
1:D:326:CYS:SG	1:D:333:GLU:HB3	2.52	0.50
1:A:64:THR:HB	3:A:410:PPF:C1	2.42	0.50
1:A:212:THR:HB	1:A:213:PRO:CD	2.42	0.50
1:D:47:LEU:C	1:D:47:LEU:HD23	2.37	0.50
1:D:47:LEU:O	1:D:51:GLY:N	2.41	0.50
1:B:280:ASP:HB2	1:B:281:PRO:HD2	1.94	0.49
1:B:378:LEU:HD23	1:B:398:ILE:HD12	1.92	0.49
1:B:209:ALA:HB1	1:B:210:PRO:HD2	1.93	0.49
1:B:148:ASP:HB3	1:B:168:VAL:CG2	2.40	0.49
1:C:14:LEU:HB3	1:C:118:GLN:NE2	2.27	0.49
1:B:14:LEU:HD13	1:B:118:GLN:HG3	1.94	0.49
1:B:83:CYS:SG	1:B:98:MET:HE1	2.53	0.49
1:C:358:LEU:N	1:C:358:LEU:HD13	2.27	0.49
1:C:44:LEU:HG	1:C:223:ASP:OD2	2.13	0.49
1:A:386:GLY:O	1:A:387:LEU:HD23	2.12	0.48
1:D:84:GLY:HA2	5:D:899:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ALA:HB3	1:A:235:ILE:HD11	1.96	0.48
1:B:207:LYS:HB3	1:B:207:LYS:HE2	1.52	0.48
1:C:64:THR:H	3:C:413:PPF:C1	2.24	0.48
1:A:53:VAL:HG11	1:D:251:ILE:HG12	1.95	0.48
1:B:129:LEU:HD23	1:B:129:LEU:HA	1.69	0.48
1:B:385:VAL:HG13	1:B:407:ALA:HB2	1.94	0.48
1:B:130:ARG:HD3	1:B:142:PHE:HA	1.96	0.48
1:B:319:VAL:C	1:B:320:LEU:HD23	2.38	0.48
1:D:296:TYR:CE1	1:D:337:GLY:HA2	2.49	0.48
1:A:47:LEU:O	1:A:51:GLY:N	2.37	0.48
1:B:106:ALA:HB1	1:B:107:PRO:HD2	1.96	0.48
1:B:157:VAL:HG22	1:B:158:GLU:H	1.78	0.48
1:D:302:PRO:HG2	1:D:305:ASP:OD2	2.13	0.47
1:B:169:PRO:HG2	1:B:176:LEU:HD12	1.96	0.47
1:A:87:PHE:CE2	1:A:96:VAL:HB	2.48	0.47
1:D:298:ARG:O	1:D:300:ALA:N	2.47	0.47
1:D:276:LEU:O	1:D:278:ILE:N	2.43	0.47
1:A:376:VAL:HB	1:A:377:PRO:HD2	1.95	0.47
1:C:172:TYR:CD1	1:C:172:TYR:N	2.79	0.47
1:B:113:MET:O	1:B:118:GLN:HB2	2.15	0.47
1:D:164:VAL:HG11	1:D:179:PHE:CE1	2.50	0.47
1:D:239:THR:HB	1:D:398:ILE:HD12	1.97	0.47
1:B:202:ASP:N	1:B:202:ASP:OD1	2.38	0.47
1:A:109:ILE:O	1:A:113:MET:HG3	2.14	0.47
1:B:171:VAL:HG21	1:D:359:SER:HB3	1.97	0.47
1:C:160:ILE:HG23	1:C:161:LEU:N	2.30	0.47
1:B:130:ARG:CD	1:B:142:PHE:HA	2.46	0.46
1:C:64:THR:HB	3:C:413:PPF:C1	2.45	0.46
1:A:64:THR:OG1	3:A:410:PPF:O4	2.22	0.46
1:B:87:PHE:CE2	1:B:96:VAL:CG1	2.98	0.46
1:B:88:PHE:HB3	1:B:296:TYR:CZ	2.50	0.46
1:C:285:HIS:ND1	1:C:287:GLY:N	2.57	0.46
1:D:181:PHE:HB3	1:D:225:TYR:CG	2.50	0.46
1:B:241:ASP:OD2	1:B:241:ASP:N	2.38	0.46
1:A:392:ARG:O	1:A:392:ARG:HG2	2.16	0.46
1:C:283:VAL:O	1:C:283:VAL:HG12	2.15	0.46
1:D:111:ALA:O	1:D:115:LYS:HG3	2.15	0.46
1:B:230:HIS:ND1	1:B:381:ASN:ND2	2.55	0.46
1:C:86:PHE:CE2	1:C:277:PRO:HA	2.51	0.46
1:A:146:LYS:C	1:A:148:ASP:N	2.74	0.46
1:C:109:ILE:O	1:C:113:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LEU:HD12	1:C:406:LEU:HA	1.76	0.46
1:D:72:VAL:HG23	1:D:108:THR:HG22	1.97	0.46
1:C:273:ARG:HD3	1:C:275:LEU:HD11	1.97	0.46
1:B:124:THR:O	1:B:143:SER:HA	2.16	0.46
1:B:385:VAL:HG13	1:B:407:ALA:HA	1.98	0.46
1:C:386:GLY:O	1:C:387:LEU:HD12	2.16	0.46
1:A:382:ARG:HG3	5:A:498:HOH:O	2.16	0.45
1:D:269:ALA:C	1:D:271:ARG:H	2.24	0.45
1:A:100:ASP:OD1	1:A:102:LYS:HB3	2.16	0.45
1:D:31:TYR:HA	1:D:210:PRO:HB3	1.98	0.45
1:A:327:GLN:HE21	1:A:327:GLN:HB2	1.65	0.45
1:B:298:ARG:C	1:B:300:ALA:N	2.73	0.45
1:C:18:PRO:HB3	1:C:193:PRO:O	2.17	0.45
1:D:181:PHE:CE2	1:D:222:MET:HG2	2.51	0.45
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.77	0.45
1:B:77:PRO:HA	1:B:80:HIS:CE1	2.51	0.45
1:A:114:ALA:HB3	5:A:442:HOH:O	2.15	0.45
1:C:271:ARG:HD2	5:C:779:HOH:O	2.16	0.45
1:A:258:PHE:HB3	1:A:351:SER:O	2.15	0.45
1:A:8:ASN:O	1:A:9:SER:HB2	2.17	0.45
1:D:294:THR:HG21	1:D:337:GLY:H	1.81	0.45
1:A:206:HIS:CE1	1:A:367:SER:HA	2.52	0.45
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.81	0.45
1:D:61:PRO:HB3	1:D:292:TYR:CG	2.52	0.45
1:C:401:LEU:HA	1:C:405:HIS:CD2	2.52	0.45
1:A:191:GLU:OE2	1:A:191:GLU:N	2.47	0.44
1:C:56:GLY:HA3	1:C:378:LEU:CD1	2.47	0.44
1:C:113:MET:HE1	1:C:195:PHE:CD1	2.51	0.44
1:C:51:GLY:O	1:C:383:LYS:HE2	2.17	0.44
1:D:61:PRO:HB3	1:D:292:TYR:CD2	2.52	0.44
1:C:235:ILE:CD1	1:C:382:ARG:NH2	2.80	0.44
1:B:188:LEU:HD21	1:B:232:GLN:CB	2.48	0.44
1:B:385:VAL:HG13	1:B:407:ALA:CB	2.48	0.44
1:A:60:VAL:HA	1:A:61:PRO:C	2.43	0.44
1:B:251:ILE:HD13	1:C:48:THR:HG22	1.99	0.44
1:C:368:HIS:CE1	3:C:413:PPF:O5	2.69	0.44
1:D:69:LEU:HD13	1:D:69:LEU:HA	1.69	0.44
1:A:206:HIS:O	1:A:366:ARG:HB2	2.18	0.44
1:B:129:LEU:HD22	1:B:133:LEU:HG	1.98	0.44
1:A:61:PRO:HB3	1:A:292:TYR:CG	2.53	0.44
1:C:258:PHE:O	1:C:262:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HA	1:C:50:PHE:CZ	2.53	0.43
1:C:61:PRO:O	1:C:63:PHE:N	2.51	0.43
1:C:358:LEU:O	1:C:361:LEU:HB2	2.18	0.43
1:A:110:LEU:HA	1:A:113:MET:CE	2.48	0.43
1:D:101:ALA:HB1	1:D:135:HIS:CG	2.53	0.43
1:B:191:GLU:OE2	1:B:191:GLU:N	2.48	0.43
1:C:8:ASN:OD1	1:C:107:PRO:HD2	2.18	0.43
1:D:113:MET:HE3	1:D:113:MET:HB2	1.76	0.43
1:A:275:LEU:O	1:A:277:PRO:HD3	2.18	0.43
1:A:251:ILE:HG13	1:A:253:ARG:HG3	2.01	0.43
1:D:321:THR:HG23	1:D:324:GLN:OE1	2.18	0.43
1:B:127:ASP:HA	1:B:143:SER:HB3	1.99	0.43
1:A:110:LEU:HA	1:A:113:MET:HE2	2.00	0.43
1:B:113:MET:HE1	1:B:195:PHE:CB	2.49	0.43
1:A:100:ASP:C	1:A:102:LYS:H	2.26	0.43
1:B:157:VAL:HG22	1:B:158:GLU:N	2.33	0.43
1:A:97:LEU:HD11	1:A:281:PRO:HD2	1.98	0.43
1:B:17:ALA:HB1	1:B:18:PRO:HD2	2.01	0.43
1:B:320:LEU:O	1:B:339:LEU:HA	2.19	0.43
1:C:43:PHE:HB3	1:C:223:ASP:OD1	2.19	0.43
1:D:104:LEU:HA	1:D:104:LEU:HD23	1.73	0.42
1:D:245:ASN:O	1:D:366:ARG:HA	2.19	0.42
1:C:161:LEU:HD23	1:C:161:LEU:HA	1.87	0.42
1:C:264:ASP:O	1:C:268:GLY:N	2.51	0.42
1:D:8:ASN:OD1	1:D:107:PRO:HD2	2.19	0.42
1:D:40:GLN:O	1:D:220:ALA:HA	2.19	0.42
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.86	0.42
1:B:164:VAL:HG12	1:B:166:MET:HB2	1.99	0.42
1:C:100:ASP:C	1:C:102:LYS:N	2.76	0.42
1:C:109:ILE:O	1:C:109:ILE:HG22	2.18	0.42
1:C:146:LYS:C	1:C:148:ASP:N	2.76	0.42
1:C:280:ASP:HB3	1:C:281:PRO:HD2	2.01	0.42
1:B:89:ASP:HB3	1:B:92:THR:OG1	2.19	0.42
1:C:257:LEU:HD23	1:C:257:LEU:HA	1.81	0.42
1:C:302:PRO:HG2	1:C:305:ASP:HB2	2.01	0.42
1:D:114:ALA:HB3	5:D:815:HOH:O	2.20	0.42
1:D:177:SER:O	1:D:180:VAL:HB	2.19	0.42
1:A:100:ASP:C	1:A:102:LYS:N	2.77	0.42
1:B:87:PHE:CD1	1:B:335:ARG:HG2	2.55	0.42
1:C:43:PHE:HB3	1:C:223:ASP:CG	2.44	0.42
1:D:100:ASP:C	1:D:102:LYS:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:LEU:HD12	1:D:406:LEU:HA	1.83	0.42
1:A:70:SER:HB3	1:A:75:ALA:O	2.20	0.42
1:C:41:ALA:N	1:C:42:PRO:HD3	2.35	0.42
1:C:380:PHE:CD1	1:C:380:PHE:N	2.87	0.42
1:D:101:ALA:O	1:D:104:LEU:HB2	2.19	0.42
1:D:247:LYS:HG3	1:D:348:VAL:HG13	2.01	0.42
1:C:237:ALA:HB1	1:C:398:ILE:HD11	2.02	0.41
1:D:86:PHE:HB3	1:D:97:LEU:HG	2.01	0.41
1:B:255:ASN:ND2	5:B:572:HOH:O	2.53	0.41
1:C:201:THR:HG23	1:C:203:TYR:H	1.85	0.41
1:D:43:PHE:HB3	1:D:223:ASP:OD2	2.19	0.41
1:D:96:VAL:C	1:D:97:LEU:HD12	2.46	0.41
1:A:62:SER:HB2	1:A:242:HIS:HB2	2.01	0.41
1:B:129:LEU:HD13	1:B:133:LEU:HD11	2.01	0.41
1:C:7:VAL:HG11	1:C:109:ILE:HA	2.02	0.41
1:D:124:THR:O	1:D:143:SER:HA	2.20	0.41
1:A:65:ASN:HB2	1:A:66:PRO:HD3	2.03	0.41
1:D:266:GLN:O	1:D:266:GLN:HG3	2.17	0.41
1:C:93:GLN:HE21	1:C:93:GLN:HB3	1.61	0.41
1:C:127:ASP:OD2	1:C:143:SER:OG	2.28	0.41
1:C:235:ILE:HD12	1:C:382:ARG:CZ	2.51	0.41
1:D:160:ILE:O	1:D:164:VAL:HB	2.20	0.41
1:D:163:ARG:HH21	1:D:190:ASN:HD22	1.68	0.41
1:D:322:ARG:HG3	1:D:336:ILE:HG22	2.03	0.41
1:C:24:VAL:HG12	1:C:27:CYS:HB2	2.01	0.41
1:C:86:PHE:HA	1:C:96:VAL:O	2.21	0.41
1:C:286:HIS:HB3	1:C:361:LEU:HG	2.03	0.41
1:D:148:ASP:HA	1:D:161:LEU:CD2	2.51	0.41
1:D:185:LEU:O	1:D:189:THR:HG23	2.21	0.41
1:B:31:TYR:HA	1:B:210:PRO:HB3	2.03	0.40
1:C:97:LEU:CD2	1:C:281:PRO:CG	2.98	0.40
1:C:368:HIS:HA	1:C:373:GLU:OE2	2.21	0.40
1:B:257:LEU:HD11	1:B:315:GLY:HA3	2.03	0.40
1:C:275:LEU:O	1:C:277:PRO:HD3	2.20	0.40
1:D:247:LYS:NZ	1:D:345:ARG:O	2.40	0.40
1:C:292:TYR:CD1	1:C:292:TYR:C	2.99	0.40
1:A:286:HIS:CG	1:A:361:LEU:HG	2.57	0.40
1:A:336:ILE:HD13	1:A:336:ILE:HG21	1.89	0.40
1:B:286:HIS:CE1	1:B:288:ALA:HA	2.57	0.40
1:B:383:LYS:HD2	1:B:383:LYS:HA	1.85	0.40
1:A:167:PRO:O	1:A:169:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ASP:HB3	1:D:201:THR:C	2.47	0.40
1:D:278:ILE:C	1:D:279:THR:HG23	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/406 (98%)	379 (95%)	21 (5%)	0	100	100
1	B	399/406 (98%)	381 (96%)	15 (4%)	3 (1%)	16	12
1	C	395/406 (97%)	373 (94%)	21 (5%)	1 (0%)	36	36
1	D	387/406 (95%)	366 (95%)	16 (4%)	5 (1%)	9	6
All	All	1581/1624 (97%)	1499 (95%)	73 (5%)	9 (1%)	21	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	ASP
1	D	299	ASP
1	D	269	ALA
1	D	277	PRO
1	B	330	GLU
1	C	93	GLN
1	D	270	GLN
1	B	27	CYS
1	D	302	PRO

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	A	330/333 (99%)	295 (89%)	35 (11%)	6	4
1	B	327/333 (98%)	295 (90%)	32 (10%)	7	5
1	C	323/333 (97%)	285 (88%)	38 (12%)	5	3
1	D	321/333 (96%)	294 (92%)	27 (8%)	10	7
All	All	1301/1332 (98%)	1169 (90%)	132 (10%)	7	5

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	ASN
1	A	6	SER
1	A	11	SER
1	A	13	ARG
1	A	16	SER
1	A	30	GLU
1	A	93	GLN
1	A	96	VAL
1	A	97	LEU
1	A	102	LYS
1	A	115	LYS
1	A	128	LYS
1	A	130	ARG
1	A	136	GLN
1	A	146	LYS
1	A	148	ASP
1	A	149	GLN
1	A	150	VAL
1	A	157	VAL
1	A	166	MET
1	A	175	ASP
1	A	186	SER
1	A	207	LYS

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Mol	Chain	Res	Type
1	A	224	SER
1	A	271	ARG
1	A	273	ARG
1	A	297	LEU
1	A	323	SER
1	A	339	LEU
1	A	362	THR
1	A	382	ARG
1	A	392	ARG
1	A	393	LEU
1	A	406	LEU
1	B	16	SER
1	B	48	THR
1	B	92	THR
1	B	93	GLN
1	B	102	LYS
1	B	110	LEU
1	B	115	LYS
1	B	129	LEU
1	B	131	ASN
1	B	146	LYS
1	B	159	ASN
1	B	192	ARG
1	B	201	THR
1	B	207	LYS
1	B	227	LYS
1	B	297	LEU
1	B	298	ARG
1	B	299	ASP
1	B	304	ARG
1	B	323	SER
1	B	324	GLN
1	B	327	GLN
1	B	336	ILE
1	B	339	LEU
1	B	358	LEU
1	B	361	LEU
1	B	378	LEU
1	B	383	LYS
1	B	392	ARG
1	B	401	LEU
1	B	403	LEU

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Mol	Chain	Res	Type
1	B	406	LEU
1	C	3	ASN
1	C	9	SER
1	C	16	SER
1	C	37	GLN
1	C	93	GLN
1	C	97	LEU
1	C	102	LYS
1	C	110	LEU
1	C	128	LYS
1	C	132	LEU
1	C	149	GLN
1	C	152	LEU
1	C	154	GLU
1	C	157	VAL
1	C	171	VAL
1	C	201	THR
1	C	207	LYS
1	C	227	LYS
1	C	235	ILE
1	C	270	GLN
1	C	271	ARG
1	C	286	HIS
1	C	297	LEU
1	C	303	GLN
1	C	313	ILE
1	C	327	GLN
1	C	333	GLU
1	C	336	ILE
1	C	339	LEU
1	C	354	ASP
1	C	357	ASP
1	C	358	LEU
1	C	378	LEU
1	C	383	LYS
1	C	387	LEU
1	C	393	LEU
1	C	400	ASP
1	C	406	LEU
1	D	9	SER
1	D	16	SER
1	D	48	THR

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Mol	Chain	Res	Type
1	D	72	VAL
1	D	99	ASN
1	D	100	ASP
1	D	110	LEU
1	D	128	LYS
1	D	138	LYS
1	D	146	LYS
1	D	149	GLN
1	D	154	GLU
1	D	161	LEU
1	D	164	VAL
1	D	192	ARG
1	D	201	THR
1	D	266	GLN
1	D	271	ARG
1	D	273	ARG
1	D	294	THR
1	D	304	ARG
1	D	320	LEU
1	D	336	ILE
1	D	339	LEU
1	D	382	ARG
1	D	392	ARG
1	D	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	68	ASN
1	A	93	GLN
1	A	266	GLN
1	A	327	GLN
1	B	29	GLN
1	B	33	ASN
1	B	149	GLN
1	B	266	GLN
1	C	33	ASN
1	C	40	GLN
1	C	65	ASN
1	C	93	GLN
1	C	149	GLN

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Mol	Chain	Res	Type
1	C	266	GLN
1	C	286	HIS
1	C	324	GLN
1	C	405	HIS
1	D	3	ASN
1	D	33	ASN
1	D	40	GLN
1	D	65	ASN
1	D	99	ASN
1	D	135	HIS
1	D	149	GLN
1	D	190	ASN
1	D	266	GLN
1	D	327	GLN
1	D	356	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PPF	D	412	2	4,6,6	1.71	2 (50%)	3,9,9	1.09	0
3	PPF	C	413	2	4,6,6	2.53	2 (50%)	3,9,9	1.18	0
4	TLA	B	411	2	9,9,9	2.07	3 (33%)	12,12,12	2.96	3 (25%)
3	PPF	A	410	2	4,6,6	2.30	1 (25%)	3,9,9	0.91	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
3	PPF	D	412	2	-	0/0/6/6	-
3	PPF	C	413	2	-	0/0/6/6	-
4	TLA	B	411	2	-	2/12/12/12	-
3	PPF	A	410	2	-	0/0/6/6	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	411	TLA	C3-C2	-4.56	1.38	1.53
3	A	410	PPF	O4-C1	-3.88	1.19	1.30
3	C	413	PPF	O4-C1	-3.86	1.19	1.30
4	B	411	TLA	O2-C2	-3.20	1.35	1.42
4	B	411	TLA	O3-C3	-2.28	1.37	1.42
3	D	412	PPF	P1-O2	-2.07	1.48	1.54
3	D	412	PPF	O4-C1	-2.06	1.24	1.30
3	C	413	PPF	P1-O2	-2.06	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	411	TLA	O2-C2-C3	7.93	126.31	110.17
4	B	411	TLA	C2-C3-C4	-5.24	98.20	109.82
4	B	411	TLA	O3-C3-C2	-2.87	104.33	110.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	411	TLA	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	411	TLA	O11-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	413	PPF	6	0
3	A	410	PPF	2	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.