



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:03 PM UTC

PDB ID : 5KS8 / pdb_00005ks8
Title : Crystal structure of two-subunit pyruvate carboxylase from *Methylobacillus flagellatus*
Authors : Choi, P.H.; Tong, L.
Deposited on : 2016-07-07
Resolution : 3.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

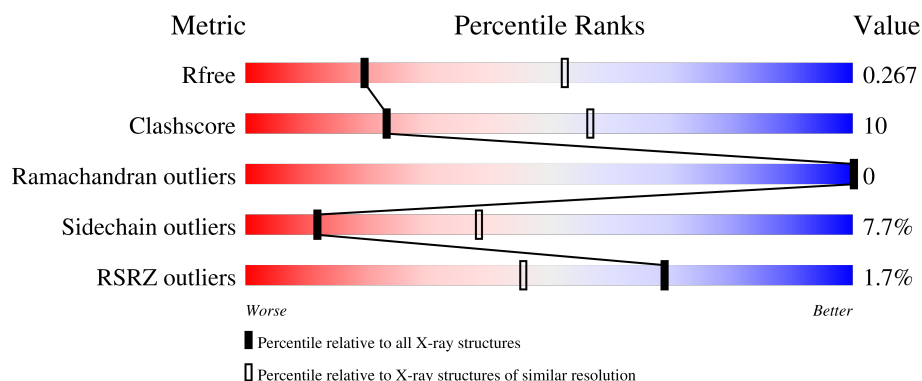
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	405	
1	B	405	
2	C	617	
2	D	617	
2	E	617	

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Mol	Chain	Length	Quality of chain
2	F	617	% 63% 14% 22%

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
4	PYR	D	2001	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21684 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 Pyruvate carboxylase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3139	1985	557	582	15			
1	B	404	Total	C	N	O	S	0	0	0
			3149	1992	558	583	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	GLY	-	linker	UNP Q1H158
A	132	SER	-	linker	UNP Q1H158
A	200	SER	-	linker	UNP Q1H158
A	201	GLY	-	linker	UNP Q1H158
B	131	GLY	-	linker	UNP Q1H158
B	132	SER	-	linker	UNP Q1H158
B	200	SER	-	linker	UNP Q1H158
B	201	GLY	-	linker	UNP Q1H158

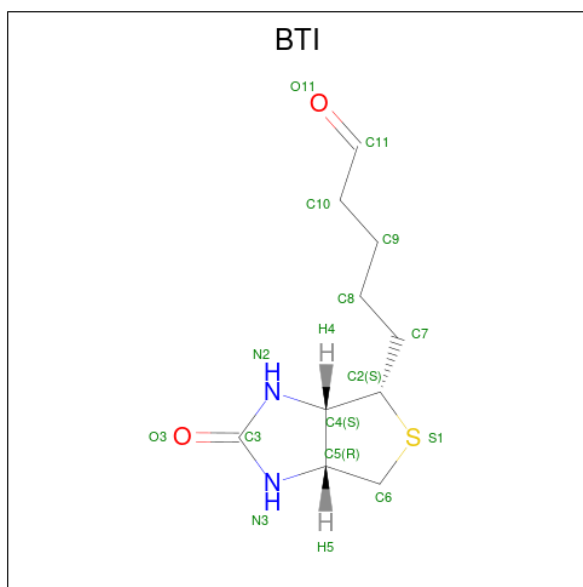
- Molecule 2 is a protein called Pyruvate carboxylase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	603	Total	C	N	O	S	0	0	0
			4554	2862	787	885	20			
2	D	580	Total	C	N	O	S	0	0	0
			4410	2777	760	853	20			
2	E	430	Total	C	N	O	S	0	0	0
			2871	1768	514	581	8			
2	F	482	Total	C	N	O	S	0	0	0
			3531	2211	606	698	16			

There are 12 discrepancies between the modelled and reference sequences:

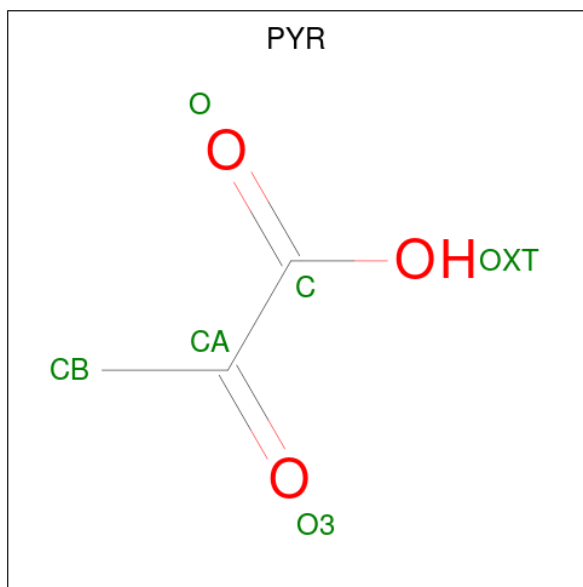
Chain	Residue	Modelled	Actual	Comment	Reference
C	419	ALA	LYS	conflict	UNP Q1H157
C	421	ALA	GLU	conflict	UNP Q1H157
C	422	ALA	GLU	conflict	UNP Q1H157
D	419	ALA	LYS	conflict	UNP Q1H157
D	421	ALA	GLU	conflict	UNP Q1H157
D	422	ALA	GLU	conflict	UNP Q1H157
E	419	ALA	LYS	conflict	UNP Q1H157
E	421	ALA	GLU	conflict	UNP Q1H157
E	422	ALA	GLU	conflict	UNP Q1H157
F	419	ALA	LYS	conflict	UNP Q1H157
F	421	ALA	GLU	conflict	UNP Q1H157
F	422	ALA	GLU	conflict	UNP Q1H157

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

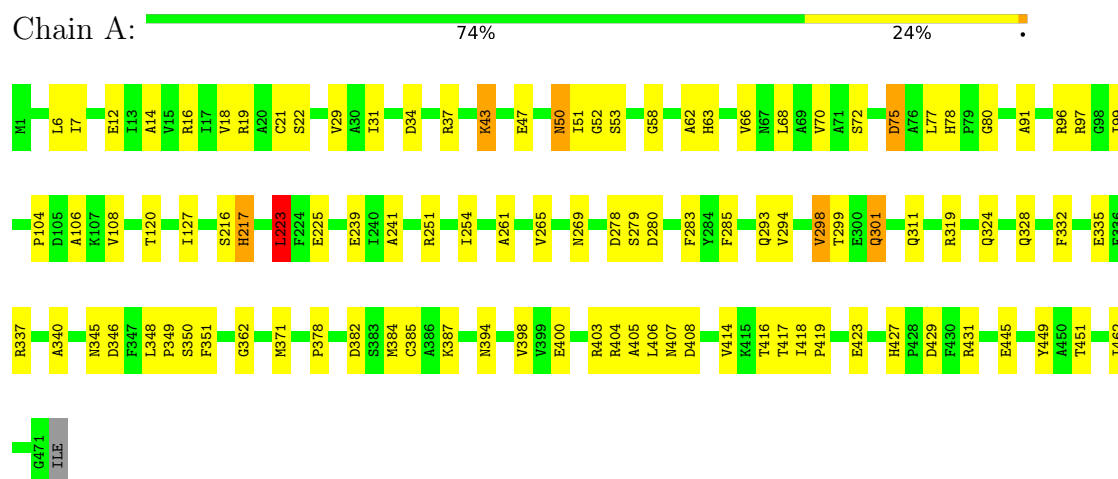
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	F	1	Total	Mn	0	0
			1	1		

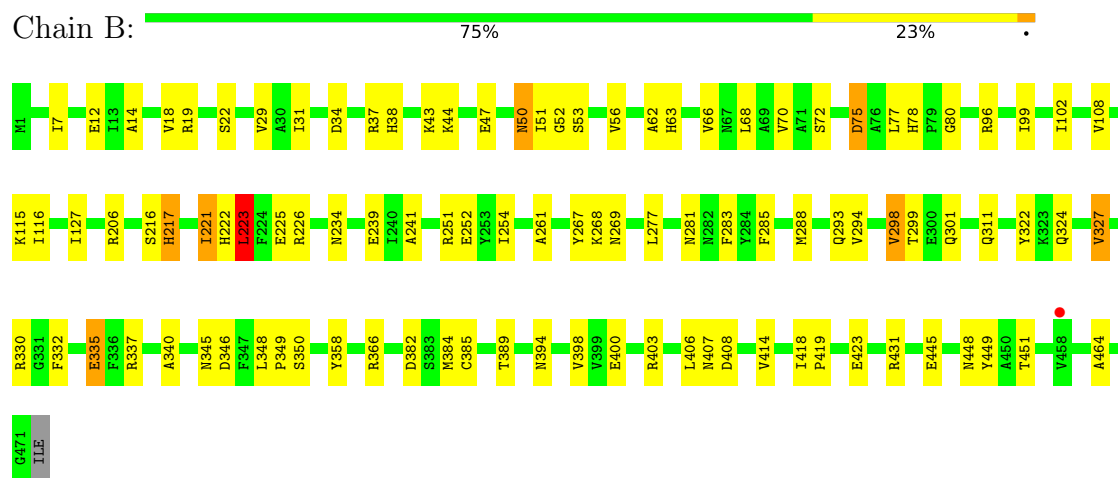
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyruvate carboxylase subunit alpha

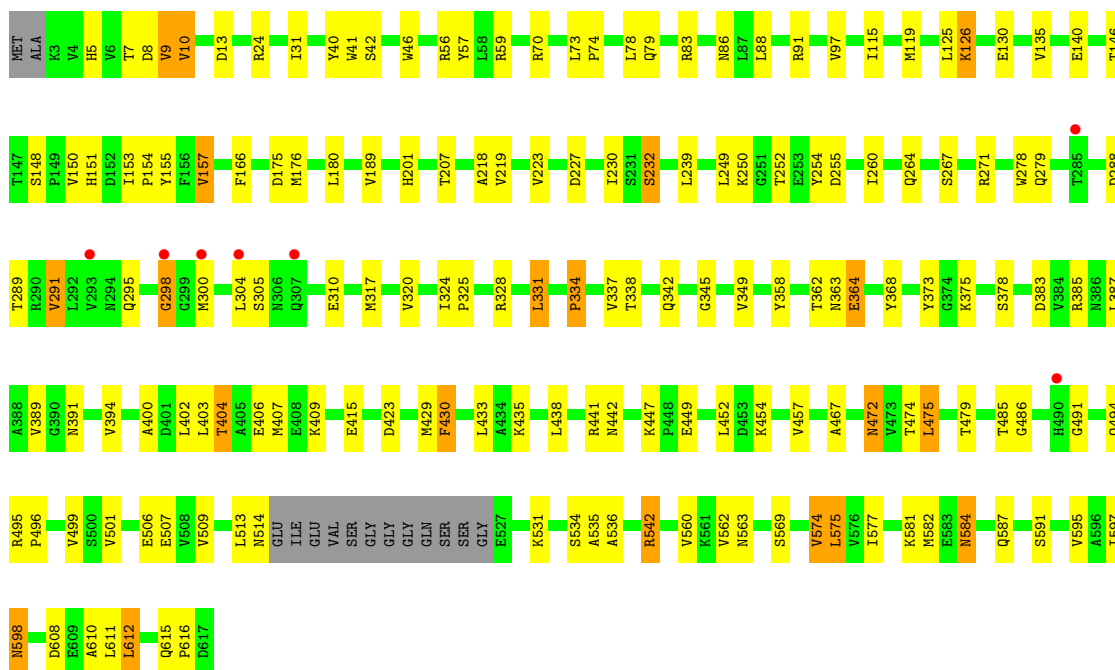


• Molecule 1: Pyruvate carboxylase subunit alpha

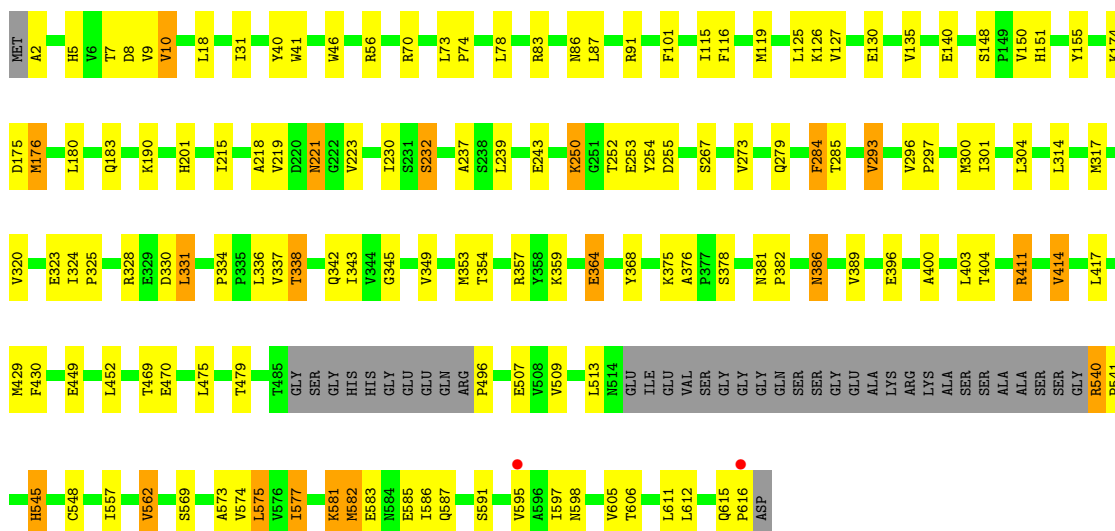


• Molecule 2: Pyruvate carboxylase subunit beta

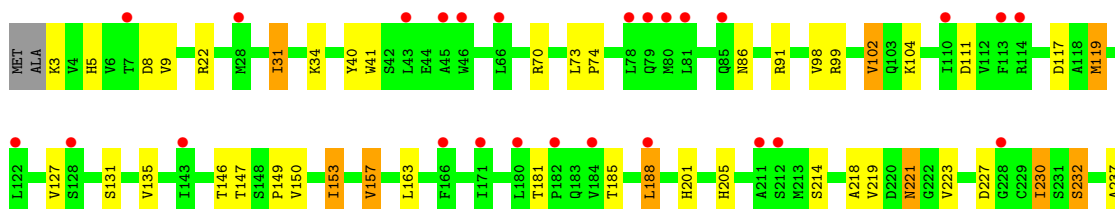




- Molecule 2: Pyruvate carboxylase subunit beta



- Molecule 2: Pyruvate carboxylase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	285.76 Å 285.76 Å 274.87 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.44 – 3.01 47.44 – 3.01	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.44-3.01) 95.6 (47.44-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.225 , 0.272 0.224 , 0.267	Depositor DCC
R_{free} test set	4072 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21684	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BTI, MN, PYR

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	0.74	0/3203	0.99	6/4340 (0.1%)
1	B	0.81	0/3214	1.03	7/4353 (0.2%)
2	C	0.74	0/4629	1.01	10/6287 (0.2%)
2	D	0.77	0/4484	0.99	8/6093 (0.1%)
2	E	0.65	0/2910	0.96	5/3989 (0.1%)
2	F	0.62	0/3586	0.88	1/4884 (0.0%)
All	All	0.73	0/22026	0.98	37/29946 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	LEU	N-CA-C	-9.11	97.78	110.35
1	B	223	LEU	N-CA-C	-8.64	98.42	110.35
2	C	291	VAL	CB-CA-C	-8.41	99.78	112.05
2	C	9	VAL	CB-CA-C	-7.39	102.63	112.46
1	B	63	HIS	N-CA-C	6.92	118.83	111.28
2	D	301	ILE	N-CA-C	6.49	119.20	111.09
2	C	475	LEU	N-CA-C	6.45	118.96	108.76
1	A	394	ASN	N-CA-C	6.44	117.93	108.14
2	F	10	VAL	CB-CA-C	-6.41	103.76	111.97
1	B	394	ASN	N-CA-C	6.34	117.78	108.14
2	D	10	VAL	CB-CA-C	-6.30	103.90	111.97
1	B	56	VAL	N-CA-C	6.18	117.13	111.81
2	C	10	VAL	CB-CA-C	-6.15	104.10	111.97
2	E	264	GLN	N-CA-CB	6.06	119.03	110.12
2	C	334	PRO	O-C-N	6.00	123.97	121.15
2	E	153	ILE	CB-CA-C	-5.98	108.02	113.70
1	B	384	MET	N-CA-C	5.95	118.14	108.63
1	A	378	PRO	O-C-N	5.94	123.94	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	298	GLY	N-CA-C	-5.88	104.48	111.36
2	E	363	ASN	N-CA-C	5.79	117.59	111.28
2	D	296	VAL	CB-CA-C	-5.69	104.74	110.89
1	B	108	VAL	CB-CA-C	-5.59	104.51	112.22
2	C	9	VAL	N-CA-CB	-5.45	105.08	112.22
1	B	448	ASN	CB-CA-C	-5.45	103.23	112.00
1	A	371	MET	N-CA-C	5.41	117.31	110.33
2	D	284	PHE	N-CA-C	5.36	118.62	112.57
2	C	271	ARG	CG-CD-NE	5.33	123.73	112.00
2	E	331	LEU	N-CA-C	5.32	119.48	112.25
2	E	31	ILE	CB-CA-C	5.32	119.16	111.88
2	D	127	VAL	CB-CA-C	-5.31	105.17	111.97
2	C	435	LYS	N-CA-CB	5.30	117.64	109.91
2	D	273	VAL	CB-CA-C	-5.29	105.11	111.88
1	A	63	HIS	N-CA-C	5.25	117.00	111.28
2	C	467	ALA	N-CA-C	5.14	115.51	109.60
1	A	384	MET	N-CA-C	5.12	116.83	108.63
2	D	293	VAL	N-CA-C	5.09	116.40	112.12
2	D	386	ASN	CB-CA-C	-5.01	102.48	110.79

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	3139	0	3117	68	0
1	B	3149	0	3128	63	0
2	C	4554	0	4540	118	0
2	D	4410	0	4410	103	0
2	E	2871	0	2421	61	1
2	F	3531	0	3343	63	1
3	C	15	0	15	1	0
4	C	6	0	0	0	0
4	D	6	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
5	F	1	0	0	0	0
All	All	21684	0	20974	440	1

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 10.

All (440) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:548:CYS:SG	2:F:610:ALA:HB1	1.86	1.15
2:F:548:CYS:SG	2:F:610:ALA:CB	2.49	1.00
2:E:119:MET:HE1	2:E:340:THR:HG21	1.43	0.97
2:E:22:ARG:HG3	2:E:280:PHE:CE1	2.08	0.88
2:D:2:ALA:O	2:D:254:TYR:HA	1.72	0.88
2:F:474:THR:HG22	2:F:479:THR:HG23	1.54	0.87
2:E:22:ARG:HG3	2:E:280:PHE:CD1	2.12	0.85
1:B:37:ARG:NH2	2:C:507:GLU:OE1	2.09	0.84
2:D:9:VAL:HG21	2:D:239:LEU:HD12	1.59	0.84
2:D:545:HIS:HB2	2:D:548:CYS:SG	2.16	0.84
2:D:9:VAL:HG21	2:D:239:LEU:CD1	2.11	0.81
2:C:260:ILE:O	2:C:264:GLN:HG3	1.82	0.80
2:E:9:VAL:HG21	2:E:239:LEU:HD12	1.64	0.79
2:D:116:PHE:CE1	2:D:337:VAL:HG11	2.19	0.78
2:C:475:LEU:HD13	2:D:507:GLU:O	1.84	0.77
1:A:22:SER:O	1:B:403:ARG:NH2	2.17	0.77
1:A:400:GLU:OE2	1:A:403:ARG:NH1	2.19	0.76
2:E:119:MET:CE	2:E:340:THR:HG21	2.14	0.76
2:C:9:VAL:HG11	2:C:13:ASP:HB3	1.67	0.75
2:D:582:MET:SD	2:D:583:GLU:N	2.60	0.74
1:A:265:VAL:HG12	1:A:265:VAL:O	1.87	0.73
2:F:548:CYS:HG	2:F:610:ALA:HB1	1.53	0.73
2:C:126:LYS:HG3	2:C:166:PHE:CE2	2.25	0.72
2:E:119:MET:HE1	2:E:340:THR:CG2	2.19	0.71
2:D:331:LEU:HB3	2:D:368:TYR:CE1	2.25	0.71
2:C:423:ASP:CG	2:C:441:ARG:HH22	1.98	0.71
1:B:222:HIS:CD2	1:B:324:GLN:HE22	2.11	0.68
1:A:403:ARG:NH2	1:B:22:SER:O	2.27	0.68
1:A:269:ASN:OD1	1:A:311:GLN:HG2	1.95	0.67
2:C:278:TRP:CZ2	2:C:454:LYS:HA	2.30	0.66
2:C:9:VAL:HG21	2:C:239:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:189:VAL:HG11	2:C:223:VAL:HG23	1.78	0.66
2:D:304:LEU:HD23	2:D:317:MET:HE1	1.77	0.66
2:C:150:VAL:HG21	2:C:378:SER:HB2	1.78	0.65
2:F:55:VAL:HG12	2:F:433:LEU:HD21	1.78	0.65
1:A:349:PRO:HB3	1:A:351:PHE:CE2	2.31	0.65
2:E:346:THR:O	2:E:349:VAL:HG22	1.96	0.65
2:C:9:VAL:HG12	2:C:9:VAL:O	1.96	0.65
2:C:331:LEU:HB3	2:C:368:TYR:CE1	2.32	0.65
2:D:330:ASP:OD2	2:D:357:ARG:NH2	2.29	0.65
1:A:68:LEU:O	1:A:72:SER:OG	2.07	0.65
2:D:148:SER:OG	2:D:151:HIS:ND1	2.30	0.65
2:E:119:MET:HE2	2:E:334:PRO:CB	2.26	0.64
2:C:542:ARG:NH1	2:C:608:ASP:OD1	2.31	0.64
1:B:269:ASN:OD1	1:B:311:GLN:HG2	1.96	0.64
2:C:597:ILE:HG22	2:C:612:LEU:HD22	1.80	0.64
1:A:223:LEU:N	1:A:223:LEU:HD23	2.13	0.63
1:B:223:LEU:HD23	1:B:223:LEU:N	2.11	0.63
2:C:9:VAL:CG1	2:C:13:ASP:HB3	2.28	0.63
2:D:174:LYS:HG2	2:D:176:MET:HG3	1.80	0.63
2:C:400:ALA:HA	2:C:403:LEU:HD12	1.80	0.62
2:D:116:PHE:CE1	2:D:337:VAL:CG1	2.82	0.62
2:F:543:PRO:HB3	2:F:548:CYS:SG	2.38	0.62
2:C:300:MET:CE	2:C:324:ILE:HD13	2.30	0.62
2:D:126:LYS:O	2:D:130:GLU:HG3	2.00	0.62
2:F:548:CYS:SG	2:F:610:ALA:HB2	2.40	0.62
2:C:148:SER:OG	2:C:151:HIS:ND1	2.30	0.62
1:A:241:ALA:HB3	1:A:298:VAL:HG13	1.82	0.61
2:C:126:LYS:O	2:C:130:GLU:HG3	2.00	0.61
2:E:205:HIS:HA	2:E:239:LEU:HD23	1.80	0.61
2:F:400:ALA:HA	2:F:403:LEU:HD12	1.82	0.61
2:C:9:VAL:CG1	2:C:13:ASP:CB	2.78	0.61
2:D:540:ARG:HG3	2:D:541:PRO:HD2	1.82	0.61
2:C:300:MET:HE2	2:C:324:ILE:HD13	1.82	0.61
2:C:582:MET:SD	2:D:364:GLU:HG3	2.40	0.61
2:C:305:SER:HB3	2:C:317:MET:CE	2.30	0.60
2:E:496:PRO:HB3	2:E:509:VAL:HG22	1.83	0.60
1:B:78:HIS:HD2	1:B:80:GLY:H	1.48	0.60
2:C:304:LEU:HD11	2:C:320:VAL:HG11	1.81	0.60
2:D:70:ARG:CZ	2:D:78:LEU:CD1	2.79	0.60
2:C:496:PRO:HB3	2:C:509:VAL:HG22	1.84	0.60
2:F:148:SER:OG	2:F:151:HIS:ND1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLU:OE1	1:A:431:ARG:NH2	2.35	0.60
2:D:496:PRO:HB3	2:D:509:VAL:HG22	1.83	0.60
2:C:362:THR:HG22	2:C:364:GLU:H	1.65	0.60
2:D:215:ILE:O	2:D:219:VAL:HG23	2.01	0.60
2:D:176:MET:SD	2:D:337:VAL:HG22	2.42	0.59
1:B:241:ALA:HB3	1:B:298:VAL:HG13	1.84	0.59
2:C:9:VAL:HG11	2:C:13:ASP:CB	2.32	0.59
2:E:150:VAL:HG21	2:E:378:SER:HB2	1.84	0.59
1:B:239:GLU:OE1	1:B:335:GLU:OE1	2.21	0.59
2:C:581:LYS:HE2	2:D:56:ARG:CD	2.33	0.59
2:E:153:ILE:CB	2:E:188:LEU:HD22	2.33	0.58
2:D:400:ALA:HA	2:D:403:LEU:HD12	1.84	0.58
2:E:102:VAL:HG21	2:E:131:SER:HB3	1.84	0.58
2:F:38:VAL:HG21	2:F:40:TYR:CD2	2.39	0.58
2:C:475:LEU:CD1	2:D:507:GLU:O	2.51	0.58
1:B:68:LEU:O	1:B:72:SER:OG	2.09	0.58
1:A:265:VAL:O	1:A:265:VAL:CG1	2.51	0.58
1:B:221:ILE:CD1	1:B:322:TYR:O	2.51	0.58
1:B:34:ASP:OD1	1:B:37:ARG:NH1	2.36	0.57
2:C:320:VAL:O	2:C:324:ILE:HG13	2.04	0.57
2:C:581:LYS:HE2	2:D:56:ARG:NE	2.19	0.57
2:D:150:VAL:HG21	2:D:378:SER:HB2	1.87	0.57
1:B:66:VAL:O	1:B:70:VAL:HG23	2.04	0.57
2:E:22:ARG:CG	2:E:280:PHE:CD1	2.87	0.57
1:A:6:LEU:HD22	1:A:77:LEU:HD12	1.86	0.57
2:C:404:THR:O	2:C:406:GLU:HG3	2.04	0.57
2:D:320:VAL:O	2:D:324:ILE:HG13	2.04	0.57
2:C:70:ARG:CZ	2:C:78:LEU:CD1	2.82	0.57
2:C:491:GLY:O	2:C:495:ARG:N	2.38	0.57
2:F:55:VAL:CG1	2:F:433:LEU:HD21	2.34	0.57
1:A:239:GLU:OE1	1:A:335:GLU:OE1	2.23	0.56
2:C:506:GLU:OE1	2:D:475:LEU:HD11	2.05	0.56
1:B:217:HIS:N	1:B:217:HIS:CD2	2.72	0.56
2:D:135:VAL:HG12	2:D:135:VAL:O	2.06	0.56
2:F:396:GLU:HG3	2:F:396:GLU:O	2.05	0.56
2:D:119:MET:HE1	2:D:376:ALA:HA	1.86	0.56
1:B:50:ASN:HD22	1:B:52:GLY:H	1.54	0.56
2:E:441:ARG:HG3	2:E:442:ASN:N	2.20	0.56
1:A:50:ASN:HD22	1:A:52:GLY:H	1.53	0.56
2:D:414:VAL:HG12	2:D:417:LEU:HB2	1.87	0.55
1:A:78:HIS:HD2	1:A:80:GLY:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:HIS:CD2	1:A:217:HIS:N	2.74	0.55
2:C:608:ASP:OD2	2:C:608:ASP:C	2.49	0.55
2:E:146:THR:HG22	2:E:147:THR:N	2.21	0.55
1:A:462:ILE:HD12	2:C:499:VAL:HG11	1.89	0.55
2:F:38:VAL:HG21	2:F:40:TYR:CE2	2.42	0.55
1:A:66:VAL:O	1:A:70:VAL:HG23	2.06	0.55
2:F:88:LEU:C	2:F:429:MET:CE	2.80	0.55
2:C:88:LEU:C	2:C:429:MET:HE2	2.32	0.55
2:C:305:SER:HB3	2:C:317:MET:HE1	1.88	0.55
2:D:595:VAL:HG21	2:D:615:GLN:HG3	1.88	0.55
2:C:534:SER:O	2:C:542:ARG:HG2	2.06	0.55
2:D:605:VAL:HG13	2:D:611:LEU:HD21	1.89	0.55
2:F:150:VAL:HG21	2:F:378:SER:HB2	1.87	0.54
2:F:605:VAL:HG13	2:F:611:LEU:HD21	1.89	0.54
2:C:9:VAL:HG21	2:C:239:LEU:CD1	2.36	0.54
2:E:421:ALA:O	2:E:424:VAL:HB	2.07	0.54
2:C:491:GLY:O	2:C:495:ARG:CB	2.55	0.54
1:B:221:ILE:HD11	1:B:322:TYR:O	2.08	0.54
2:C:494:GLN:O	2:C:496:PRO:HD3	2.08	0.54
2:C:88:LEU:C	2:C:429:MET:CE	2.81	0.54
2:C:135:VAL:HG12	2:C:135:VAL:O	2.07	0.54
1:A:241:ALA:CB	1:A:298:VAL:HG13	2.37	0.54
1:B:77:LEU:HD23	1:B:77:LEU:C	2.33	0.54
2:C:582:MET:CE	2:D:364:GLU:HG3	2.38	0.54
2:C:115:ILE:HG22	2:C:125:LEU:HD22	1.90	0.54
2:C:423:ASP:CG	2:C:441:ARG:NH2	2.66	0.54
2:E:135:VAL:O	2:E:135:VAL:HG12	2.08	0.54
2:C:595:VAL:HG21	2:C:615:GLN:HG3	1.89	0.54
2:D:73:LEU:N	2:D:74:PRO:CD	2.71	0.53
1:B:38:HIS:O	1:B:43:LYS:HE2	2.08	0.53
2:C:430:PHE:CD1	2:C:433:LEU:HD23	2.43	0.53
2:C:423:ASP:OD2	2:C:441:ARG:NH2	2.41	0.53
3:C:2000:BTI:N2	2:D:300:MET:HG3	2.23	0.53
2:C:574:VAL:HG13	2:C:612:LEU:HD11	1.90	0.53
1:B:222:HIS:CD2	1:B:324:GLN:NE2	2.76	0.53
2:E:185:THR:HG21	2:E:214:SER:CB	2.38	0.53
2:E:476:HIS:CE1	2:F:506:GLU:HB3	2.43	0.53
1:B:222:HIS:CG	1:B:324:GLN:HE22	2.26	0.53
2:D:119:MET:CE	2:D:376:ALA:HA	2.39	0.53
2:D:119:MET:SD	2:D:368:TYR:HE2	2.31	0.53
2:E:382:PRO:O	2:E:386:ASN:N	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:VAL:HG12	2:F:135:VAL:O	2.08	0.53
2:D:323:GLU:OE2	2:D:357:ARG:NH1	2.37	0.52
2:F:562:VAL:HG12	2:F:597:ILE:HD11	1.91	0.52
1:A:301:GLN:OE1	1:A:301:GLN:HA	2.09	0.52
2:C:252:THR:HG22	2:D:183:GLN:NE2	2.25	0.52
2:D:331:LEU:HD13	2:D:368:TYR:CD1	2.44	0.52
1:A:34:ASP:OD1	1:A:37:ARG:NH2	2.43	0.52
2:D:396:GLU:HG3	2:D:396:GLU:O	2.09	0.52
1:A:416:THR:HG22	1:A:417:THR:N	2.25	0.52
2:E:119:MET:HE2	2:E:334:PRO:HB3	1.92	0.52
2:D:18:LEU:HD23	2:D:285:THR:CG2	2.39	0.52
2:D:87:LEU:HB3	2:D:429:MET:HE1	1.91	0.52
2:F:557:ILE:HD12	2:F:575:LEU:CD2	2.40	0.51
1:B:241:ALA:CB	1:B:298:VAL:HG13	2.40	0.51
2:C:472:ASN:ND2	2:D:513:LEU:HD11	2.25	0.51
2:F:396:GLU:O	2:F:396:GLU:CG	2.58	0.51
2:D:83:ARG:O	2:D:86:ASN:HB2	2.11	0.51
2:D:557:ILE:HD12	2:D:575:LEU:CD2	2.41	0.51
2:F:24:ARG:NH2	2:F:449:GLU:O	2.44	0.51
2:C:140:GLU:OE1	2:C:201:HIS:HD2	1.93	0.51
2:D:562:VAL:HG12	2:D:597:ILE:HD11	1.91	0.51
2:E:22:ARG:CG	2:E:280:PHE:CE1	2.89	0.51
2:E:153:ILE:O	2:E:157:VAL:HG13	2.11	0.51
2:E:119:MET:HE2	2:E:334:PRO:HB2	1.92	0.51
2:F:119:MET:SD	2:F:368:TYR:HE2	2.34	0.51
1:B:301:GLN:HA	1:B:301:GLN:OE1	2.10	0.51
2:C:291:VAL:HG12	2:C:291:VAL:O	2.11	0.50
2:C:119:MET:SD	2:C:368:TYR:HE2	2.34	0.50
2:D:176:MET:HG2	2:D:337:VAL:HG22	1.93	0.50
2:C:153:ILE:O	2:C:157:VAL:HG13	2.12	0.50
2:D:279:GLN:HE22	2:D:452:LEU:HG	1.77	0.50
2:D:115:ILE:HG22	2:D:125:LEU:HD22	1.93	0.50
2:D:140:GLU:CD	2:D:201:HIS:HD1	2.20	0.50
2:E:254:TYR:O	2:E:255:ASP:C	2.55	0.50
1:B:251:ARG:CZ	1:B:251:ARG:HB2	2.41	0.50
1:B:419:PRO:HB2	1:B:449:TYR:CE2	2.46	0.50
2:D:411:ARG:HB3	2:D:411:ARG:CZ	2.42	0.50
2:F:254:TYR:O	2:F:255:ASP:C	2.55	0.50
2:C:254:TYR:O	2:C:255:ASP:C	2.55	0.49
2:D:540:ARG:HG3	2:D:541:PRO:CD	2.42	0.49
2:E:5:HIS:HB3	2:E:41:TRP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:HD21	1:B:281:ASN:HA	1.95	0.49
2:D:70:ARG:CZ	2:D:78:LEU:HD12	2.43	0.49
2:D:232:SER:OG	2:D:267:SER:O	2.30	0.49
1:A:14:ALA:O	1:A:18:VAL:HG23	2.12	0.49
1:A:328:GLN:HB2	1:B:330:ARG:NH2	2.28	0.49
2:F:88:LEU:C	2:F:429:MET:HE2	2.37	0.49
1:A:254:ILE:HD13	1:A:283:PHE:CG	2.48	0.49
2:F:38:VAL:CG2	2:F:40:TYR:CD2	2.95	0.49
2:C:42:SER:OG	2:C:79:GLN:NE2	2.46	0.49
1:A:43:LYS:NZ	1:B:358:TYR:OH	2.45	0.48
1:B:62:ALA:O	1:B:66:VAL:HG23	2.13	0.48
2:D:8:ASP:HB2	2:D:40:TYR:CE1	2.48	0.48
1:A:332:PHE:HB2	1:A:398:VAL:HG21	1.96	0.48
1:B:14:ALA:O	1:B:18:VAL:HG23	2.13	0.48
2:C:73:LEU:N	2:C:74:PRO:CD	2.76	0.48
2:D:540:ARG:HD2	2:D:598:ASN:O	2.13	0.48
2:E:102:VAL:HG21	2:E:131:SER:CB	2.44	0.48
2:D:252:THR:HG22	2:D:253:GLU:N	2.28	0.48
2:D:254:TYR:O	2:D:255:ASP:C	2.56	0.48
2:D:345:GLY:O	2:D:349:VAL:HG23	2.14	0.48
1:A:62:ALA:O	1:A:66:VAL:HG23	2.13	0.48
1:B:400:GLU:OE2	1:B:431:ARG:NH1	2.47	0.47
2:C:305:SER:CB	2:C:317:MET:CE	2.92	0.47
2:C:279:GLN:HE22	2:C:452:LEU:HG	1.79	0.47
2:E:98:VAL:O	2:E:102:VAL:HG13	2.14	0.47
2:E:119:MET:HE3	2:E:119:MET:HA	1.96	0.47
2:F:8:ASP:HB2	2:F:40:TYR:CE1	2.50	0.47
2:F:70:ARG:HA	2:F:70:ARG:HD3	1.74	0.47
1:A:127:ILE:CD1	1:A:261:ALA:HB2	2.44	0.47
1:B:78:HIS:CD2	1:B:80:GLY:H	2.30	0.47
2:C:364:GLU:HG2	2:C:373:TYR:OH	2.15	0.47
2:C:513:LEU:HB2	2:D:470:GLU:HG3	1.95	0.47
2:D:175:ASP:OD2	2:D:180:LEU:HG	2.14	0.47
2:C:358:TYR:HB2	2:C:387:LEU:HD23	1.95	0.47
2:D:337:VAL:HG12	2:D:338:THR:N	2.30	0.47
1:A:96:ARG:HH12	2:F:587:GLN:HE22	1.62	0.47
1:B:332:PHE:HB2	1:B:398:VAL:HG21	1.95	0.47
2:C:362:THR:HG22	2:C:364:GLU:N	2.29	0.47
2:C:441:ARG:HD2	2:C:442:ASN:OD1	2.15	0.47
1:A:51:ILE:HG13	1:A:58:GLY:HA3	1.95	0.47
2:E:476:HIS:NE2	2:F:506:GLU:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:438:LEU:O	2:F:442:ASN:OD1	2.32	0.47
1:A:251:ARG:HB2	1:A:251:ARG:CZ	2.44	0.47
2:C:207:THR:CG2	2:C:288:ASP:HB3	2.44	0.47
2:C:338:THR:HG22	2:C:342:GLN:OE1	2.15	0.47
2:F:83:ARG:O	2:F:86:ASN:HB2	2.15	0.47
2:F:290:ARG:HH11	2:F:290:ARG:HB2	1.79	0.47
1:A:104:PRO:HB2	1:A:108:VAL:CG2	2.45	0.47
2:F:9:VAL:CG1	2:F:13:ASP:HB2	2.45	0.47
2:F:279:GLN:HG2	2:F:452:LEU:HD12	1.96	0.47
2:D:116:PHE:HE1	2:D:337:VAL:CG1	2.28	0.47
2:D:605:VAL:CG1	2:D:611:LEU:HD21	2.45	0.47
2:E:86:ASN:ND2	2:E:339:PRO:HG3	2.30	0.47
2:F:185:THR:HG21	2:F:214:SER:HB3	1.96	0.47
2:E:205:HIS:HD2	2:E:237:ALA:O	1.98	0.46
1:A:345:ASN:O	1:A:348:LEU:HG	2.16	0.46
1:A:419:PRO:HB2	1:A:449:TYR:CE2	2.50	0.46
2:C:232:SER:OG	2:C:267:SER:O	2.29	0.46
2:C:535:ALA:C	2:C:542:ARG:HD3	2.40	0.46
2:C:611:LEU:O	2:C:612:LEU:HD23	2.15	0.46
2:E:70:ARG:HA	2:E:70:ARG:HD3	1.76	0.46
2:F:177:ALA:HB3	2:F:179:LEU:HG	1.98	0.46
2:F:605:VAL:CG1	2:F:611:LEU:HD21	2.45	0.46
1:A:225:GLU:OE1	1:A:225:GLU:N	2.42	0.46
1:B:127:ILE:CD1	1:B:261:ALA:HB2	2.46	0.46
2:D:324:ILE:N	2:D:325:PRO:HD2	2.30	0.46
2:F:119:MET:HA	2:F:119:MET:HE3	1.96	0.46
1:B:293:GLN:O	1:B:294:VAL:C	2.58	0.46
2:C:485:THR:HG22	2:C:486:GLY:N	2.29	0.46
2:C:514:ASN:O	2:D:469:THR:N	2.44	0.46
2:D:328:ARG:HG2	2:D:334:PRO:HD2	1.98	0.46
1:A:43:LYS:NZ	2:F:478:GLU:OE2	2.47	0.46
2:E:119:MET:CE	2:E:334:PRO:HB2	2.45	0.46
1:A:335:GLU:OE2	1:A:387:LYS:HD3	2.16	0.46
1:B:464:ALA:CB	2:F:508:VAL:HG11	2.46	0.46
2:D:18:LEU:HD23	2:D:285:THR:HG21	1.97	0.46
2:C:9:VAL:CG1	2:C:13:ASP:HB2	2.45	0.45
2:C:97:VAL:HG22	2:C:407:MET:SD	2.56	0.45
2:C:598:ASN:ND2	2:C:610:ALA:O	2.48	0.45
2:D:218:ALA:HB1	2:D:223:VAL:HG21	1.98	0.45
2:F:279:GLN:HG2	2:F:452:LEU:HB2	1.96	0.45
1:B:382:ASP:C	1:B:382:ASP:OD1	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:GLU:CD	2:D:541:PRO:HG3	2.42	0.45
2:D:155:TYR:C	2:D:155:TYR:CD2	2.94	0.45
2:E:8:ASP:HB2	2:E:40:TYR:CE1	2.51	0.45
2:E:252:THR:HG22	2:E:253:GLU:N	2.32	0.45
2:F:592:GLY:HA3	2:F:615:GLN:O	2.16	0.45
1:B:345:ASN:O	1:B:346:ASP:C	2.58	0.45
2:E:146:THR:HG22	2:E:147:THR:H	1.81	0.45
1:A:349:PRO:HB3	1:A:351:PHE:HE2	1.80	0.45
2:C:289:THR:HG21	2:D:243:GLU:HB2	1.98	0.45
2:C:560:VAL:HA	2:C:575:LEU:HD12	1.97	0.45
2:F:474:THR:HG22	2:F:479:THR:CG2	2.37	0.45
2:D:605:VAL:HG12	2:D:606:THR:N	2.31	0.45
2:E:205:HIS:HA	2:E:239:LEU:CD2	2.47	0.45
1:A:406:LEU:HB3	1:A:418:ILE:HG23	1.98	0.45
1:B:348:LEU:HG	1:B:349:PRO:HD2	1.98	0.45
2:D:237:ALA:HB3	2:D:285:THR:HG23	1.97	0.45
2:D:591:SER:O	2:D:616:PRO:HA	2.17	0.45
2:F:5:HIS:HB3	2:F:41:TRP:HB2	1.99	0.45
2:F:414:VAL:HG12	2:F:417:LEU:HB2	1.98	0.45
2:C:70:ARG:CZ	2:C:78:LEU:HD12	2.46	0.45
2:C:582:MET:CE	2:D:343:ILE:CG1	2.95	0.45
1:B:267:TYR:CE1	1:B:288:MET:HE2	2.51	0.44
2:C:176:MET:SD	2:C:176:MET:O	2.75	0.44
2:F:73:LEU:N	2:F:74:PRO:CD	2.80	0.44
1:A:19:ARG:HE	1:B:408:ASP:CG	2.25	0.44
2:C:8:ASP:HB2	2:C:40:TYR:CE1	2.52	0.44
2:E:181:THR:O	2:E:185:THR:HG23	2.18	0.44
1:A:75:ASP:OD2	1:A:75:ASP:N	2.50	0.44
1:A:293:GLN:O	1:A:294:VAL:C	2.60	0.44
2:F:218:ALA:HB1	2:F:223:VAL:HG21	2.00	0.44
2:C:324:ILE:N	2:C:325:PRO:HD2	2.33	0.44
2:C:331:LEU:HD13	2:C:368:TYR:CD1	2.53	0.44
2:D:581:LYS:CG	2:D:581:LYS:O	2.66	0.44
2:E:73:LEU:N	2:E:74:PRO:CD	2.80	0.44
2:E:411:ARG:HG2	2:E:411:ARG:HH11	1.83	0.44
2:E:86:ASN:HA	2:E:91:ARG:O	2.18	0.44
1:A:29:VAL:HG22	1:A:47:GLU:HB2	2.00	0.44
2:C:291:VAL:O	2:C:295:GLN:HA	2.18	0.44
2:C:345:GLY:O	2:C:349:VAL:HG23	2.18	0.44
1:A:278:ASP:OD2	1:A:279:SER:N	2.51	0.44
1:B:29:VAL:HG22	1:B:47:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:611:LEU:C	2:C:612:LEU:HD23	2.43	0.44
2:D:86:ASN:HA	2:D:91:ARG:O	2.18	0.44
2:F:138:HIS:HE1	2:F:170:THR:OG1	2.01	0.44
2:C:385:ARG:HD2	2:C:394:VAL:HG21	2.00	0.43
2:C:582:MET:CE	2:D:343:ILE:HG13	2.48	0.43
1:A:345:ASN:O	1:A:346:ASP:C	2.60	0.43
2:D:221:ASN:N	2:D:221:ASN:HD22	2.16	0.43
2:E:230:ILE:HD11	2:E:266:ILE:HG13	2.00	0.43
1:A:37:ARG:HH12	2:E:507:GLU:CD	2.23	0.43
1:B:96:ARG:HH12	2:D:587:GLN:HE22	1.66	0.43
1:B:400:GLU:OE1	1:B:403:ARG:NH1	2.51	0.43
2:C:249:LEU:O	2:C:252:THR:OG1	2.34	0.43
2:C:591:SER:O	2:C:616:PRO:HA	2.18	0.43
2:D:8:ASP:HB2	2:D:40:TYR:CZ	2.53	0.43
1:A:254:ILE:HD13	1:A:283:PHE:CD2	2.54	0.43
1:A:404:ARG:HG2	1:A:405:ALA:N	2.32	0.43
1:B:75:ASP:OD2	1:B:75:ASP:N	2.52	0.43
2:C:189:VAL:CG1	2:C:223:VAL:HG23	2.47	0.43
2:C:328:ARG:HG2	2:C:334:PRO:HD2	2.01	0.43
2:D:581:LYS:O	2:D:581:LYS:HG2	2.19	0.43
1:A:335:GLU:OE2	1:A:387:LYS:CD	2.67	0.43
1:A:416:THR:HG22	1:A:418:ILE:H	1.84	0.43
2:C:5:HIS:HB3	2:C:41:TRP:HB2	2.00	0.43
2:C:441:ARG:NH1	2:C:442:ASN:OD1	2.40	0.43
2:D:573:ALA:HB2	2:D:585:GLU:OE1	2.18	0.43
2:E:34:LYS:HD3	2:E:34:LYS:N	2.34	0.43
2:E:509:VAL:HB	2:F:474:THR:OG1	2.19	0.43
1:B:226:ARG:HB3	1:B:241:ALA:HB2	1.99	0.43
2:D:101:PHE:CE1	2:D:429:MET:HE3	2.53	0.43
2:D:411:ARG:HB3	2:D:411:ARG:NH1	2.34	0.43
1:B:298:VAL:HG23	1:B:335:GLU:HB3	2.00	0.43
2:D:5:HIS:HB3	2:D:41:TRP:HB2	2.00	0.43
1:A:324:GLN:HE21	1:A:324:GLN:HA	1.84	0.43
2:E:218:ALA:HB1	2:E:223:VAL:HG21	2.01	0.43
2:F:70:ARG:NH2	2:F:111:ASP:OD2	2.51	0.43
2:F:605:VAL:HG12	2:F:606:THR:N	2.33	0.43
2:C:83:ARG:O	2:C:86:ASN:HB2	2.19	0.42
2:C:218:ALA:HB1	2:C:223:VAL:HG21	2.00	0.42
2:E:474:THR:HA	2:E:479:THR:HA	2.01	0.42
2:C:155:TYR:CD2	2:C:155:TYR:C	2.96	0.42
2:C:201:HIS:HE1	2:C:227:ASP:OD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:LEU:HB3	2:D:368:TYR:HE1	1.82	0.42
2:E:119:MET:HE3	2:E:119:MET:CA	2.49	0.42
2:F:221:ASN:N	2:F:221:ASN:HD22	2.18	0.42
2:C:452:LEU:HD13	2:C:457:VAL:HG21	2.02	0.42
2:D:83:ARG:HG2	2:D:116:PHE:CZ	2.54	0.42
1:B:285:PHE:CD1	1:B:285:PHE:C	2.97	0.42
1:B:406:LEU:HB3	1:B:418:ILE:HG23	2.01	0.42
2:D:284:PHE:HE2	2:D:314:LEU:HD22	1.84	0.42
2:E:3:LYS:O	2:E:3:LYS:HG3	2.18	0.42
2:F:119:MET:HE3	2:F:119:MET:CA	2.50	0.42
1:B:222:HIS:NE2	1:B:324:GLN:NE2	2.68	0.42
2:D:176:MET:SD	2:D:337:VAL:CG2	3.08	0.42
2:E:324:ILE:N	2:E:325:PRO:HD2	2.34	0.42
2:F:35:LEU:O	2:F:38:VAL:HG22	2.19	0.42
2:F:86:ASN:HA	2:F:91:ARG:O	2.19	0.42
2:C:59:ARG:HD3	2:C:59:ARG:HA	1.72	0.42
2:D:176:MET:HB2	2:D:297:PRO:HB3	2.02	0.42
2:E:253:GLU:O	2:E:253:GLU:HG2	2.20	0.42
2:C:474:THR:HA	2:C:479:THR:HA	2.02	0.42
2:E:221:ASN:N	2:E:221:ASN:HD22	2.18	0.42
1:A:340:ALA:HB2	1:A:385:CYS:SG	2.59	0.42
2:E:70:ARG:NH2	2:E:111:ASP:OD2	2.52	0.42
2:E:232:SER:OG	2:E:267:SER:O	2.31	0.42
2:F:8:ASP:HB2	2:F:40:TYR:CZ	2.54	0.42
1:A:382:ASP:OD1	1:A:382:ASP:C	2.62	0.42
1:A:7:ILE:HG21	1:A:14:ALA:HA	2.02	0.41
1:A:78:HIS:CD2	1:A:80:GLY:H	2.35	0.41
1:A:91:ALA:HB3	1:A:106:ALA:HB2	2.00	0.41
2:E:337:VAL:C	2:E:341:SER:OG	2.63	0.41
2:E:350:LEU:O	2:E:353:MET:N	2.53	0.41
2:F:9:VAL:HG23	2:F:228:GLY:O	2.20	0.41
2:F:414:VAL:HG12	2:F:414:VAL:O	2.19	0.41
1:B:350:SER:O	1:B:414:VAL:HG13	2.19	0.41
2:C:582:MET:HE3	2:D:343:ILE:HG12	2.02	0.41
2:D:557:ILE:HD13	2:D:577:ILE:HD13	2.01	0.41
1:A:280:ASP:OD2	1:A:280:ASP:C	2.62	0.41
1:B:225:GLU:OE1	1:B:225:GLU:N	2.46	0.41
1:B:254:ILE:HD13	1:B:283:PHE:CG	2.55	0.41
1:B:298:VAL:O	1:B:301:GLN:HB2	2.21	0.41
1:B:301:GLN:NE2	1:B:366:ARG:HD2	2.34	0.41
2:C:175:ASP:OD2	2:C:180:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:338:THR:HG22	2:C:342:GLN:CD	2.45	0.41
2:E:201:HIS:HE1	2:E:227:ASP:OD1	2.04	0.41
2:F:573:ALA:HB2	2:F:585:GLU:OE1	2.20	0.41
2:C:56:ARG:HD2	2:C:57:TYR:CZ	2.56	0.41
2:C:331:LEU:HD23	2:C:331:LEU:N	2.35	0.41
2:D:250:LYS:HA	2:D:255:ASP:OD2	2.20	0.41
1:A:350:SER:O	1:A:414:VAL:HG13	2.21	0.41
2:E:153:ILE:CB	2:E:188:LEU:CD2	2.98	0.41
1:A:408:ASP:OD2	1:B:44:LYS:NZ	2.45	0.41
2:E:411:ARG:HH11	2:E:411:ARG:CG	2.34	0.41
1:B:206:ARG:CZ	1:B:277:LEU:HD22	2.50	0.41
1:B:340:ALA:HB2	1:B:385:CYS:SG	2.61	0.41
2:C:153:ILE:N	2:C:154:PRO:HD2	2.36	0.41
1:A:285:PHE:CD1	1:A:285:PHE:C	2.98	0.41
1:A:408:ASP:CG	1:B:19:ARG:HE	2.26	0.41
1:B:31:ILE:O	1:B:31:ILE:HG13	2.20	0.41
1:B:335:GLU:HB3	1:B:389:THR:HG23	2.03	0.41
2:C:86:ASN:HA	2:C:91:ARG:O	2.21	0.41
2:C:337:VAL:HG12	2:C:338:THR:N	2.36	0.41
2:C:584:ASN:HD22	2:C:584:ASN:HA	1.65	0.41
2:F:9:VAL:CG1	2:F:13:ASP:CB	2.99	0.41
1:A:31:ILE:O	1:A:31:ILE:HG13	2.19	0.41
1:B:7:ILE:HG21	1:B:14:ALA:HA	2.02	0.41
1:A:362:GLY:HA2	1:B:366:ARG:HE	1.86	0.40
2:D:324:ILE:N	2:D:325:PRO:CD	2.84	0.40
2:C:582:MET:HE1	2:D:343:ILE:HG13	2.02	0.40
2:D:323:GLU:OE2	2:D:357:ARG:HD2	2.21	0.40
2:F:155:TYR:CD2	2:F:155:TYR:C	2.99	0.40
2:C:291:VAL:HG22	2:C:298:GLY:H	1.86	0.40
2:C:536:ALA:N	2:C:542:ARG:HD3	2.36	0.40
2:D:70:ARG:NH1	2:D:78:LEU:HD12	2.36	0.40
2:D:297:PRO:HG3	2:D:336:LEU:O	2.21	0.40
2:D:354:THR:HG21	2:D:359:LYS:HB3	2.02	0.40
1:A:21:CYS:O	1:A:22:SER:C	2.64	0.40
1:A:427:HIS:CE1	1:A:429:ASP:HB2	2.57	0.40
1:A:16:ARG:O	1:A:19:ARG:HB2	2.22	0.40
1:A:462:ILE:HD11	2:C:501:VAL:CG2	2.52	0.40
1:B:327:VAL:O	1:B:327:VAL:HG23	2.22	0.40
2:D:381:ASN:HA	2:D:382:PRO:HD3	1.95	0.40
2:F:12:ARG:NE	2:F:44:GLU:OE2	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149:PRO:O	2:F:193:ARG:NH2[4_555]	2.07	0.13

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	402/405 (99%)	375 (93%)	27 (7%)	0	100	100
1	B	402/405 (99%)	372 (92%)	30 (8%)	0	100	100
2	C	599/617 (97%)	572 (96%)	27 (4%)	0	100	100
2	D	574/617 (93%)	553 (96%)	21 (4%)	0	100	100
2	E	416/617 (67%)	397 (95%)	19 (5%)	0	100	100
2	F	468/617 (76%)	445 (95%)	23 (5%)	0	100	100
All	All	2861/3278 (87%)	2714 (95%)	147 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	327/332 (98%)	307 (94%)	20 (6%)	17	47
1	B	329/332 (99%)	304 (92%)	25 (8%)	12	39
2	C	491/513 (96%)	451 (92%)	40 (8%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	479/513 (93%)	443 (92%)	36 (8%)	12	39
2	E	242/513 (47%)	221 (91%)	21 (9%)	9	34
2	F	360/513 (70%)	330 (92%)	30 (8%)	10	35
All	All	2228/2716 (82%)	2056 (92%)	172 (8%)	12	38

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	43	LYS
1	A	50	ASN
1	A	53	SER
1	A	75	ASP
1	A	97	ARG
1	A	99	ILE
1	A	120	THR
1	A	216	SER
1	A	217	HIS
1	A	223	LEU
1	A	298	VAL
1	A	299	THR
1	A	301	GLN
1	A	319	ARG
1	A	337	ARG
1	A	407	ASN
1	A	423	GLU
1	A	445	GLU
1	A	451	THR
1	B	12	GLU
1	B	50	ASN
1	B	51	ILE
1	B	53	SER
1	B	75	ASP
1	B	99	ILE
1	B	102	ILE
1	B	115	LYS
1	B	116	ILE
1	B	216	SER
1	B	217	HIS
1	B	221	ILE
1	B	223	LEU

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	252	GLU
1	B	268	LYS
1	B	298	VAL
1	B	299	THR
1	B	327	VAL
1	B	335	GLU
1	B	337	ARG
1	B	407	ASN
1	B	423	GLU
1	B	445	GLU
1	B	451	THR
2	C	7	THR
2	C	10	VAL
2	C	24	ARG
2	C	31	ILE
2	C	46	TRP
2	C	126	LYS
2	C	146	THR
2	C	157	VAL
2	C	219	VAL
2	C	230	ILE
2	C	232	SER
2	C	250	LYS
2	C	331	LEU
2	C	363	ASN
2	C	364	GLU
2	C	375	LYS
2	C	383	ASP
2	C	389	VAL
2	C	391	ASN
2	C	402	LEU
2	C	404	THR
2	C	409	LYS
2	C	415	GLU
2	C	430	PHE
2	C	438	LEU
2	C	447	LYS
2	C	449	GLU
2	C	472	ASN
2	C	531	LYS
2	C	542	ARG

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Mol	Chain	Res	Type
2	C	562	VAL
2	C	563	ASN
2	C	569	SER
2	C	574	VAL
2	C	575	LEU
2	C	577	ILE
2	C	584	ASN
2	C	587	GLN
2	C	598	ASN
2	C	612	LEU
2	D	7	THR
2	D	10	VAL
2	D	31	ILE
2	D	46	TRP
2	D	176	MET
2	D	190	LYS
2	D	221	ASN
2	D	230	ILE
2	D	232	SER
2	D	250	LYS
2	D	293	VAL
2	D	331	LEU
2	D	338	THR
2	D	342	GLN
2	D	353	MET
2	D	364	GLU
2	D	375	LYS
2	D	386	ASN
2	D	389	VAL
2	D	404	THR
2	D	411	ARG
2	D	414	VAL
2	D	430	PHE
2	D	449	GLU
2	D	479	THR
2	D	540	ARG
2	D	545	HIS
2	D	562	VAL
2	D	569	SER
2	D	574	VAL
2	D	575	LEU
2	D	577	ILE

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Mol	Chain	Res	Type
2	D	581	LYS
2	D	582	MET
2	D	586	ILE
2	D	612	LEU
2	E	31	ILE
2	E	99	ARG
2	E	102	VAL
2	E	104	LYS
2	E	117	ASP
2	E	119	MET
2	E	127	VAL
2	E	157	VAL
2	E	163	LEU
2	E	188	LEU
2	E	219	VAL
2	E	221	ASN
2	E	230	ILE
2	E	232	SER
2	E	381	ASN
2	E	411	ARG
2	E	430	PHE
2	E	438	LEU
2	E	479	THR
2	E	484	LEU
2	E	511	GLU
2	F	9	VAL
2	F	10	VAL
2	F	46	TRP
2	F	104	LYS
2	F	119	MET
2	F	133	LYS
2	F	221	ASN
2	F	230	ILE
2	F	243	GLU
2	F	364	GLU
2	F	365	VAL
2	F	381	ASN
2	F	396	GLU
2	F	404	THR
2	F	408	GLU
2	F	430	PHE
2	F	442	ASN

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Mol	Chain	Res	Type
2	F	449	GLU
2	F	470	GLU
2	F	540	ARG
2	F	562	VAL
2	F	563	ASN
2	F	569	SER
2	F	574	VAL
2	F	575	LEU
2	F	580	MET
2	F	582	MET
2	F	586	ILE
2	F	612	LEU
2	F	615	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	78	HIS
1	A	117	GLN
1	A	234	ASN
1	A	245	GLN
1	A	309	GLN
1	A	318	GLN
1	A	328	GLN
1	A	407	ASN
1	A	443	HIS
1	A	448	ASN
1	B	38	HIS
1	B	50	ASN
1	B	61	ASN
1	B	63	HIS
1	B	78	HIS
1	B	245	GLN
1	B	282	ASN
1	B	309	GLN
1	B	318	GLN
1	B	324	GLN
1	B	407	ASN
1	B	443	HIS
2	C	79	GLN
2	C	85	GLN

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Mol	Chain	Res	Type
2	C	92	HIS
2	C	201	HIS
2	C	264	GLN
2	C	279	GLN
2	C	311	GLN
2	C	391	ASN
2	C	472	ASN
2	C	584	ASN
2	C	598	ASN
2	D	85	GLN
2	D	86	ASN
2	D	183	GLN
2	D	221	ASN
2	D	279	GLN
2	D	307	GLN
2	D	439	GLN
2	D	587	GLN
2	E	86	ASN
2	E	201	HIS
2	E	205	HIS
2	E	221	ASN
2	E	279	GLN
2	E	381	ASN
2	F	85	GLN
2	F	138	HIS
2	F	183	GLN
2	F	201	HIS
2	F	221	ASN
2	F	587	GLN

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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
4	PYR	D	2001	-	5,5,5	1.73	2 (40%)	3,6,6	2.22	1 (33%)
4	PYR	C	2001	-	5,5,5	1.38	1 (20%)	3,6,6	1.65	1 (33%)
3	BTI	C	2000	2	15,16,16	1.88	2 (13%)	20,21,21	2.47	7 (35%)

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
4	PYR	D	2001	-	-	3/4/4/4	-
4	PYR	C	2001	-	-	3/4/4/4	-
3	BTI	C	2000	2	-	2/6/27/27	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2000	BTI	C2-S1	-6.45	1.72	1.82
4	D	2001	PYR	OXT-C	-2.32	1.24	1.30
4	D	2001	PYR	CB-CA	2.24	1.54	1.50
4	C	2001	PYR	CA-C	-2.16	1.47	1.54
3	C	2000	BTI	C6-S1	-2.03	1.75	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2000	BTI	C2-C4-N2	5.26	118.91	113.34
3	C	2000	BTI	C4-C2-S1	-5.01	99.35	105.03
3	C	2000	BTI	C6-S1-C2	4.84	100.04	89.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2000	BTI	C6-C5-N3	-3.44	108.74	113.18
4	D	2001	PYR	OXT-C-O	-3.28	116.09	123.90
3	C	2000	BTI	C5-C6-S1	-2.75	102.28	106.06
3	C	2000	BTI	O3-C3-N3	-2.60	122.16	125.89
4	C	2001	PYR	OXT-C-CA	2.26	119.84	113.59
3	C	2000	BTI	C2-C4-C5	2.10	111.47	108.89

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2000	BTI	C9-C10-C11-O11
4	C	2001	PYR	OXT-C-CA-O3
4	C	2001	PYR	OXT-C-CA-CB
4	D	2001	PYR	O-C-CA-CB
4	D	2001	PYR	OXT-C-CA-CB
3	C	2000	BTI	C7-C8-C9-C10
4	C	2001	PYR	O-C-CA-CB
4	D	2001	PYR	O-C-CA-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2000	BTI	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/405 (99%)	-0.02	0 100 100	55, 94, 126, 158	0
1	B	404/405 (99%)	-0.31	1 (0%) 91 83	54, 78, 132, 198	0
2	C	603/617 (97%)	-0.01	7 (1%) 76 55	52, 94, 137, 214	0
2	D	580/617 (94%)	-0.23	2 (0%) 90 79	47, 74, 138, 194	0
2	E	430/617 (69%)	0.72	29 (6%) 24 12	95, 169, 222, 253	0
2	F	482/617 (78%)	0.52	9 (1%) 66 43	97, 156, 196, 229	0
All	All	2903/3278 (88%)	0.10	48 (1%) 69 46	47, 101, 191, 253	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	43	LEU	5.0
2	E	45	ALA	4.6
2	E	211	ALA	4.5
2	E	46	TRP	4.4
2	E	78	LEU	4.0
2	E	212	SER	3.9
2	E	81	LEU	3.2
2	C	298	GLY	3.2
2	E	337	VAL	3.1
2	E	80	MET	3.1
2	E	79	GLN	3.0
2	C	307	GLN	2.9
2	E	242	THR	2.9
2	E	171	ILE	2.7
2	E	66	LEU	2.6
2	E	188	LEU	2.6
2	E	110	ILE	2.5
2	F	212	SER	2.5
2	E	85	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	50	THR	2.5
2	F	424	VAL	2.5
2	C	304	LEU	2.4
2	E	122	LEU	2.4
2	C	293	VAL	2.4
2	F	89	GLY	2.4
2	E	228	GLY	2.4
2	E	143	ILE	2.4
2	E	166	PHE	2.3
1	B	458	VAL	2.3
2	E	114	ARG	2.3
2	C	300	MET	2.3
2	C	285	THR	2.2
2	E	184	VAL	2.2
2	E	7	THR	2.2
2	F	562	VAL	2.2
2	D	616	PRO	2.2
2	E	113	PHE	2.2
2	F	143	ILE	2.2
2	C	490	HIS	2.2
2	F	8	ASP	2.1
2	F	63	TRP	2.1
2	E	425	LEU	2.1
2	E	128	SER	2.1
2	E	182	PRO	2.1
2	E	180	LEU	2.0
2	F	262	LEU	2.0
2	E	28	MET	2.0
2	D	595	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PYR	C	2001	6/6	0.84	0.20	84,98,101,101	0
4	PYR	D	2001	6/6	0.84	0.18	64,71,72,73	0
5	MN	F	701	1/1	0.90	0.07	164,164,164,164	0
3	BTI	C	2000	15/15	0.96	0.09	54,60,81,91	0
5	MN	D	2002	1/1	0.97	0.11	64,64,64,64	0
5	MN	C	2002	1/1	0.97	0.09	92,92,92,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.