



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:56 PM UTC

PDB ID : 5VYJ / pdb_00005vyj
Title : Crystal structure of the photosynthetic phosphoenolpyruvate carboxylase isoenzyme from maize in complex with Gly
Authors : Gonzalez-Segura, L.; Guemez-Toro, R.; Munoz-Clares, R.A.
Deposited on : 2017-05-25
Resolution : 3.30 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

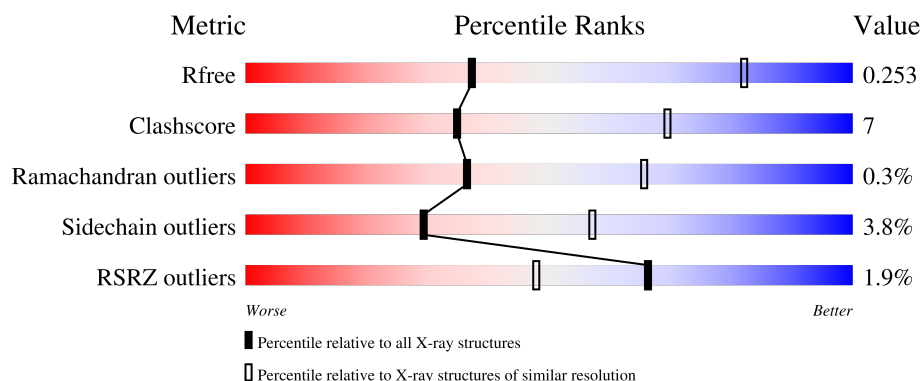
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	970	 2% 72% 21% • 5%
1	B	970	 2% 72% 22% • 5%
1	C	970	 % 74% 20% • 5%
1	D	970	 3% 74% 20% • 5%

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	GLY	B	1001	-	X	-	-

2 Entry composition [i](#)

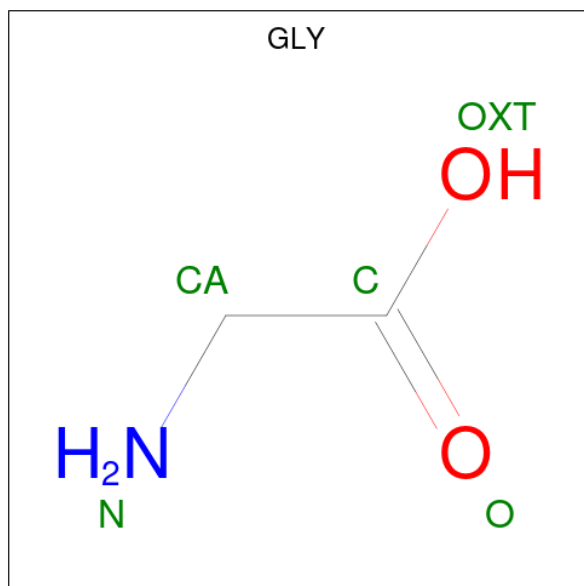
There are 3 unique types of molecules in this entry. The entry contains 29339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoenolpyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	918	Total	C	N	O	S	0	0	0
			7318	4646	1275	1367	30			
1	B	917	Total	C	N	O	S	0	0	0
			7309	4640	1274	1365	30			
1	C	918	Total	C	N	O	S	0	0	0
			7318	4645	1275	1368	30			
1	D	918	Total	C	N	O	S	0	0	0
			7317	4646	1275	1366	30			

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	B	1	Total	C	N	O	0	0
			5	2	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			5	2	1	2		
2	C	1	Total	C	N	O	0	0
			5	2	1	2		
2	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

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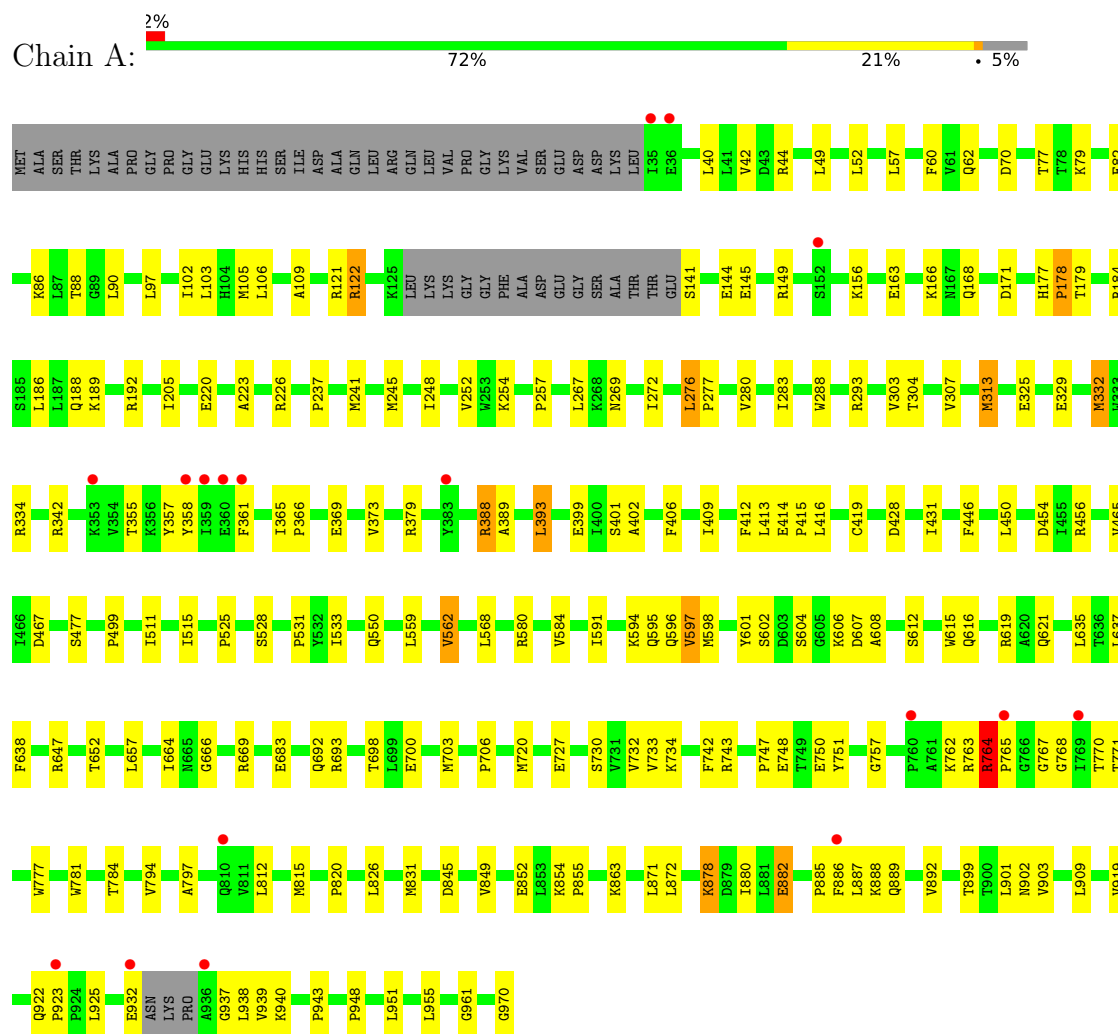
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0

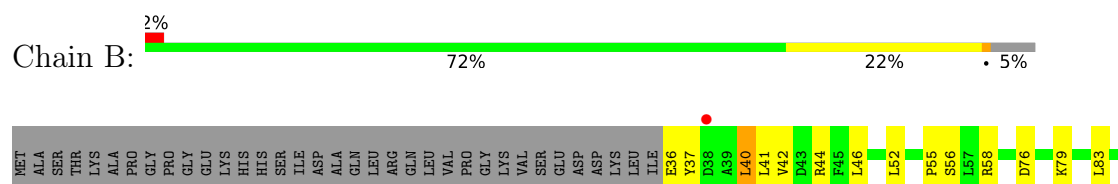
3 Residue-property plots

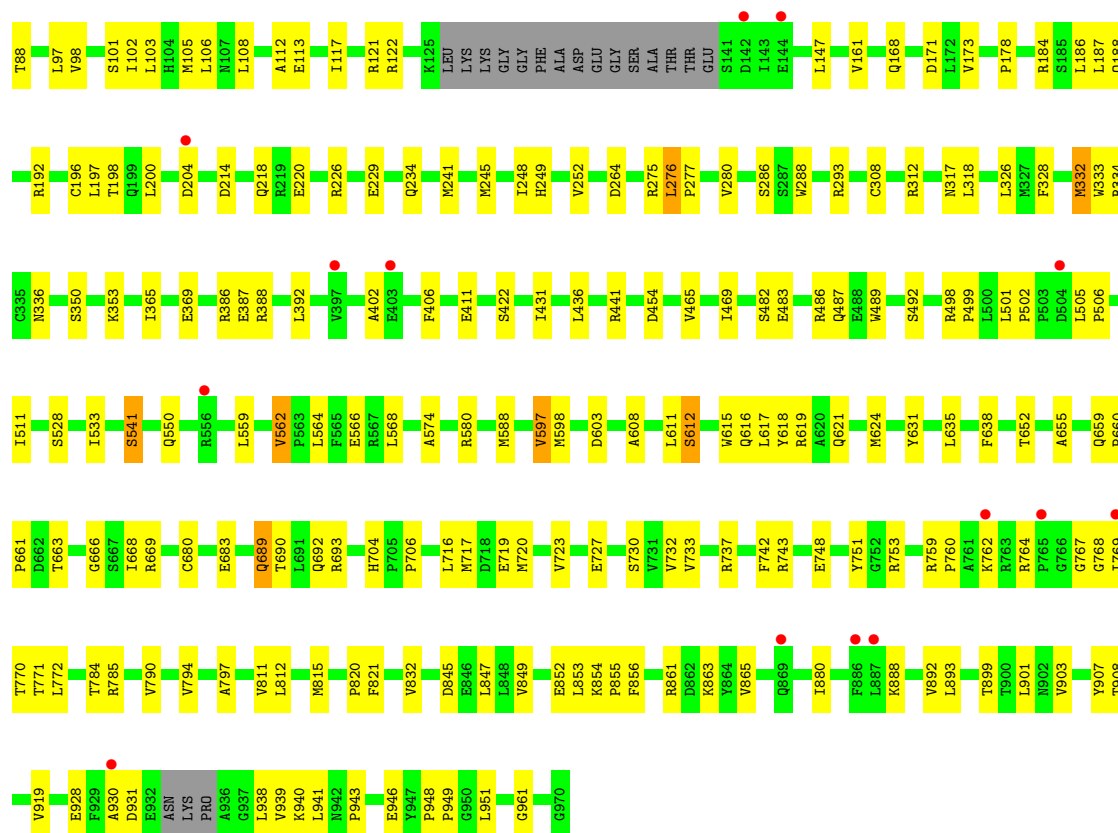
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphoenolpyruvate carboxylase

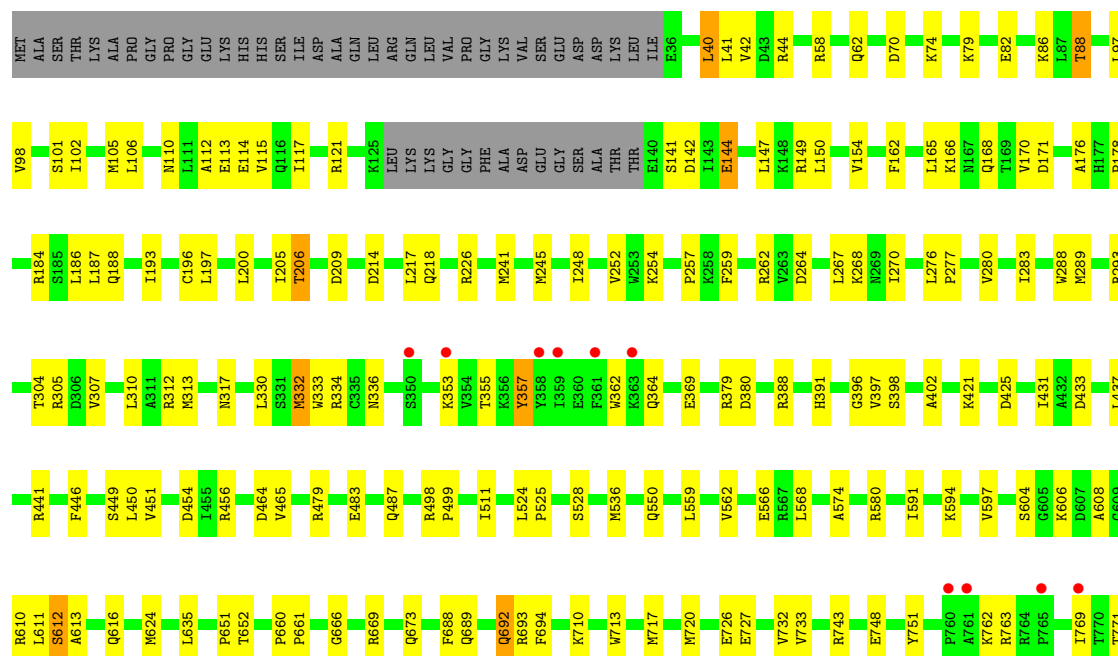
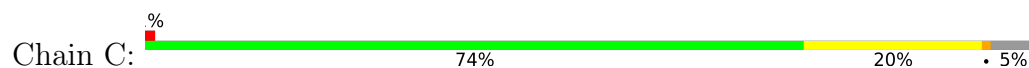


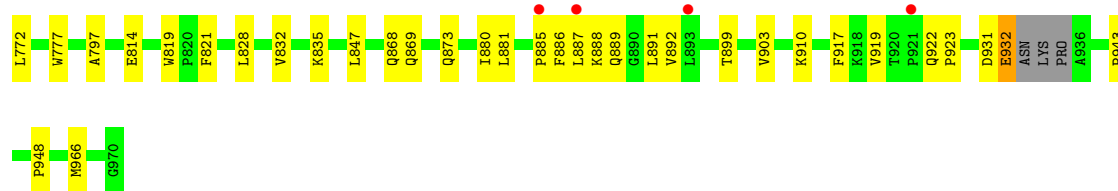
• Molecule 1: Phosphoenolpyruvate carboxylase



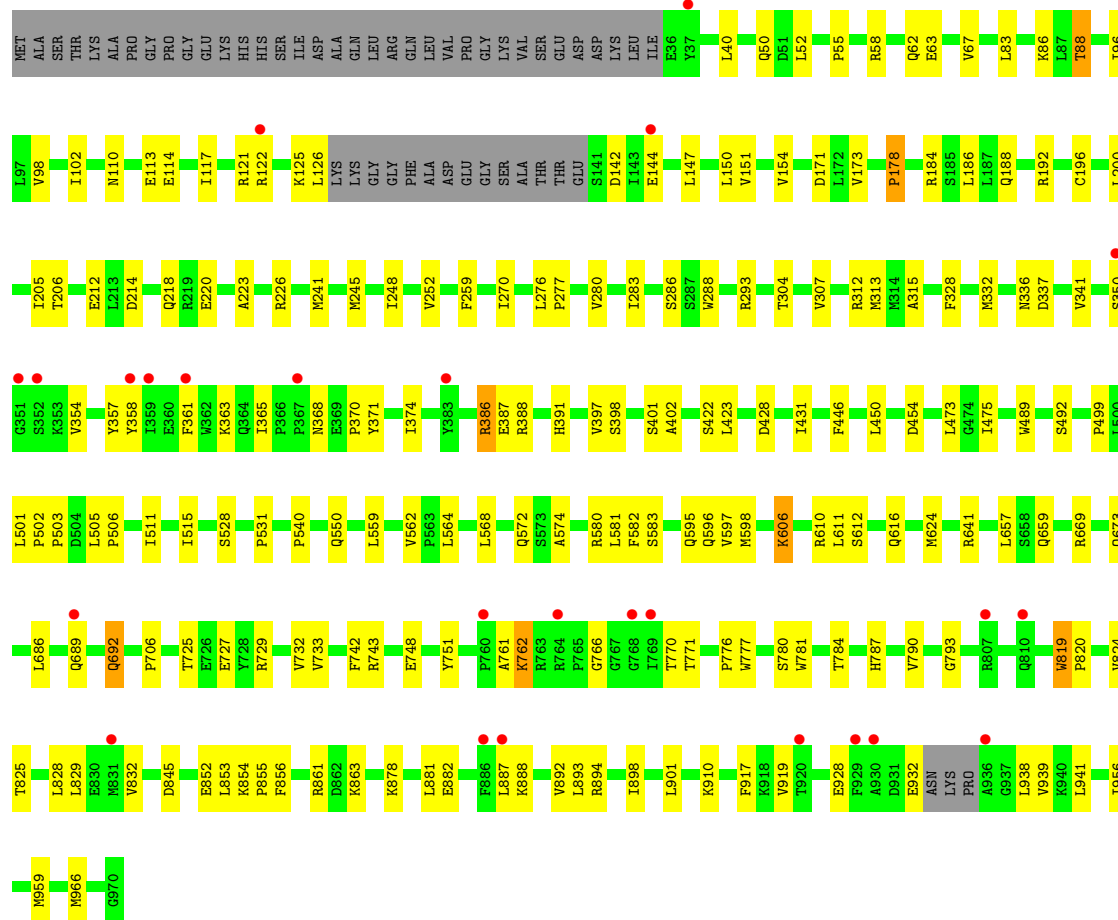
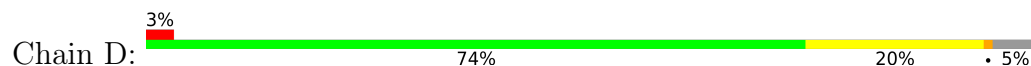


● Molecule 1: Phosphoenolpyruvate carboxylase





● Molecule 1: Phosphoenolpyruvate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	156.95Å 167.24Å 242.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.08 – 3.30 57.08 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.2 (57.08-3.30) 93.2 (57.08-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.210 , 0.253 0.214 , 0.253	Depositor DCC
R_{free} test set	4518 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29339	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4006e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/7473	0.85	4/10119 (0.0%)
1	B	0.47	0/7464	0.88	14/10108 (0.1%)
1	C	0.44	0/7473	0.85	10/10120 (0.1%)
1	D	0.45	0/7472	0.83	6/10119 (0.1%)
All	All	0.45	0/29882	0.85	34/40466 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	354	VAL	N-CA-C	8.19	118.77	110.82
1	B	365	ILE	CA-C-N	7.29	124.91	119.66
1	B	365	ILE	C-N-CA	7.29	124.91	119.66
1	B	941	LEU	N-CA-C	-7.00	104.21	112.89
1	B	234	GLN	CA-C-N	5.76	125.67	119.85
1	B	234	GLN	C-N-CA	5.76	125.67	119.85
1	A	276	LEU	CA-C-N	5.58	126.82	119.84
1	A	276	LEU	C-N-CA	5.58	126.82	119.84
1	C	673	GLN	N-CA-C	5.57	117.61	108.52
1	C	819	TRP	CA-C-N	5.44	126.64	119.84
1	C	819	TRP	C-N-CA	5.44	126.64	119.84
1	B	276	LEU	CA-C-N	5.33	125.33	119.90
1	B	276	LEU	C-N-CA	5.33	125.33	119.90
1	B	794	VAL	N-CA-C	5.33	115.53	110.42
1	B	948	PRO	CA-C-N	5.31	126.47	119.84
1	B	948	PRO	C-N-CA	5.31	126.47	119.84
1	B	704	HIS	CA-C-N	5.28	125.81	120.38
1	B	704	HIS	C-N-CA	5.28	125.81	120.38
1	A	355	THR	N-CA-C	5.26	120.06	113.43
1	D	673	GLN	N-CA-C	5.26	116.87	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	794	VAL	N-CA-C	5.25	115.46	110.42
1	C	948	PRO	CA-C-N	5.17	126.30	119.84
1	C	948	PRO	C-N-CA	5.17	126.30	119.84
1	B	369	GLU	CA-C-N	5.16	124.78	119.05
1	B	369	GLU	C-N-CA	5.16	124.78	119.05
1	D	819	TRP	CA-C-N	5.16	125.20	119.32
1	D	819	TRP	C-N-CA	5.16	125.20	119.32
1	C	357	TYR	N-CA-C	-5.15	102.13	110.32
1	D	365	ILE	CA-C-N	5.12	125.65	120.38
1	D	365	ILE	C-N-CA	5.12	125.65	120.38
1	C	498	ARG	CA-C-N	5.08	125.08	119.89
1	C	498	ARG	C-N-CA	5.08	125.08	119.89
1	C	369	GLU	CA-C-N	5.05	124.23	118.97
1	C	369	GLU	C-N-CA	5.05	124.23	118.97

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	7318	0	7314	120	0
1	B	7309	0	7303	120	0
1	C	7318	0	7309	105	0
1	D	7317	0	7314	103	0
2	A	5	0	2	1	0
2	B	10	0	4	1	0
2	C	5	0	2	1	0
2	D	5	0	2	0	0
3	A	12	0	9	2	0
3	B	12	0	9	0	0
3	C	16	0	12	0	0
3	D	12	0	9	1	0
All	All	29339	0	29289	437	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 7.

All (437) 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:B:388:ARG:HH12	1:B:402:ALA:HA	1.39	0.88
1:D:743:ARG:HH22	1:D:762:LYS:HE3	1.43	0.82
1:B:386:ARG:NH1	1:B:387:GLU:OE1	2.17	0.77
1:C:362:TRP:NE1	1:C:380:ASP:OD2	2.19	0.75
1:C:835:LYS:HB3	1:C:966:MET:HE1	1.69	0.74
1:B:568:LEU:HD22	1:B:608:ALA:HB2	1.67	0.74
1:A:465:VAL:HG22	1:A:511:ILE:HG23	1.69	0.74
1:B:276:LEU:HD12	1:B:277:PRO:HD2	1.71	0.72
1:C:720:MET:HB3	1:C:797:ALA:HB1	1.70	0.72
1:D:88:THR:HB	1:D:919:VAL:HG21	1.72	0.72
1:C:487:GLN:OE1	1:C:580:ARG:NH1	2.24	0.71
1:B:465:VAL:HG22	1:B:511:ILE:HG23	1.72	0.70
1:C:568:LEU:HD22	1:C:608:ALA:HB2	1.73	0.69
1:C:574:ALA:HB1	1:C:624:MET:HE2	1.75	0.67
1:B:574:ALA:HB1	1:B:624:MET:HE2	1.77	0.66
1:C:88:THR:HB	1:C:919:VAL:HG11	1.75	0.66
1:A:293:ARG:NH2	1:A:304:THR:OG1	2.27	0.66
1:D:312:ARG:HH21	1:D:528:SER:HB3	1.60	0.66
1:A:332:MET:HE2	1:A:431:ILE:HD13	1.78	0.66
1:C:41:LEU:HD12	1:C:112:ALA:HB2	1.79	0.65
1:A:192:ARG:NH1	1:A:220:GLU:OE1	2.30	0.65
1:A:103:LEU:HD13	1:A:961:GLY:HA2	1.78	0.65
1:D:259:PHE:HE1	1:D:692:GLN:HE21	1.45	0.64
1:A:937:GLY:HA2	1:A:940:LYS:HD2	1.79	0.64
1:B:812:LEU:HA	1:B:815:MET:HE3	1.79	0.64
1:C:40:LEU:HG	1:C:44:ARG:HH21	1.62	0.63
1:D:171:ASP:HB3	1:D:669:ARG:HG2	1.80	0.63
1:A:720:MET:HB3	1:A:797:ALA:HB1	1.81	0.63
1:D:288:TRP:CD1	1:D:454:ASP:HB2	2.35	0.62
1:D:564:LEU:HD13	1:D:598:MET:HG2	1.80	0.62
1:D:659:GLN:HA	3:D:1004:ACT:H1	1.81	0.62
1:C:332:MET:HE2	1:C:431:ILE:HD13	1.81	0.61
1:C:293:ARG:NH2	1:C:304:THR:OG1	2.32	0.61
1:C:178:PRO:O	1:C:751:TYR:OH	2.17	0.61
1:D:574:ALA:HB1	1:D:624:MET:HE2	1.83	0.61
1:A:606:LYS:HG3	1:A:777:TRP:CD1	2.36	0.60
1:B:811:VAL:HG12	1:B:815:MET:HE2	1.81	0.60
1:C:206:THR:HB	1:C:209:ASP:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LEU:HD12	1:B:506:PRO:HD2	1.83	0.60
1:D:336:ASN:HD22	1:D:422:SER:HA	1.66	0.60
1:A:361:PHE:HD2	1:A:379:ARG:HH12	1.49	0.60
1:B:501:LEU:HD12	1:B:502:PRO:HD2	1.84	0.60
1:A:706:PRO:HB3	1:A:820:PRO:HG2	1.84	0.59
1:C:276:LEU:HD12	1:C:277:PRO:HD2	1.84	0.59
1:A:499:PRO:HB2	1:C:499:PRO:HB2	1.84	0.59
1:C:743:ARG:NH1	1:C:748:GLU:OE2	2.35	0.59
1:D:428:ASP:HB3	1:D:431:ILE:HD12	1.82	0.59
1:A:241:MET:HG3	1:A:307:VAL:HG13	1.84	0.59
1:A:764:ARG:HG3	1:A:765:PRO:HD2	1.84	0.59
1:A:657:LEU:HG	1:A:820:PRO:HB3	1.86	0.58
1:A:428:ASP:HB3	1:A:431:ILE:HD12	1.84	0.58
1:B:173:VAL:HG22	1:B:286:SER:HB2	1.84	0.58
1:D:790:VAL:HG11	1:D:832:VAL:HG21	1.85	0.58
1:B:487:GLN:OE1	1:B:580:ARG:NH1	2.36	0.58
1:C:536:MET:HE3	1:C:763:ARG:HH12	1.67	0.58
1:B:103:LEU:HD13	1:B:961:GLY:HA2	1.86	0.58
1:A:171:ASP:HB3	1:A:669:ARG:HG2	1.85	0.57
1:C:421:LYS:NZ	1:C:425:ASP:OD2	2.35	0.57
1:C:597:VAL:HG12	1:C:635:LEU:HD11	1.87	0.57
1:C:355:THR:HG22	1:C:357:TYR:HB3	1.86	0.57
1:D:568:LEU:HD12	1:D:616:GLN:HG2	1.86	0.57
1:B:248:ILE:HA	1:B:252:VAL:HB	1.87	0.57
1:C:115:VAL:HG21	1:C:197:LEU:HD23	1.86	0.57
1:D:63:GLU:OE1	1:D:86:LYS:NZ	2.34	0.57
1:D:147:LEU:HB3	1:D:270:ILE:HD13	1.87	0.57
1:B:88:THR:HB	1:B:919:VAL:HG21	1.85	0.57
1:C:604:SER:HB3	1:C:613:ALA:HB1	1.87	0.57
1:A:49:LEU:HD11	1:A:57:LEU:HD22	1.87	0.57
1:B:770:THR:HG23	1:B:771:THR:HG23	1.87	0.56
1:B:727:GLU:OE2	1:B:863:LYS:NZ	2.38	0.56
1:C:550:GLN:OE1	1:C:559:LEU:N	2.38	0.56
1:C:248:ILE:HA	1:C:252:VAL:HB	1.88	0.56
1:C:312:ARG:HH21	1:C:528:SER:HB3	1.70	0.56
1:A:767:GLY:O	1:A:770:THR:HG22	2.05	0.56
1:B:184:ARG:O	1:B:188:GLN:HG3	2.06	0.56
1:C:110:ASN:O	1:C:114:GLU:HG3	2.06	0.56
1:D:96:ILE:HG21	1:D:938:LEU:HD21	1.87	0.55
1:D:725:THR:HG22	1:D:729:ARG:HD2	1.86	0.55
1:A:288:TRP:CD1	1:A:454:ASP:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:NH1	1:B:928:GLU:OE2	2.38	0.55
1:D:388:ARG:HH12	1:D:402:ALA:HA	1.71	0.55
1:A:52:LEU:HD13	1:A:226:ARG:NH1	2.21	0.55
1:B:716:LEU:HD23	1:B:815:MET:HE1	1.89	0.55
1:C:101:SER:O	1:C:105:MET:HG3	2.06	0.55
1:A:88:THR:HB	1:A:919:VAL:HG21	1.89	0.55
1:B:930:ALA:HB3	1:B:931:ASP:HA	1.88	0.55
1:A:178:PRO:O	1:A:751:TYR:OH	2.24	0.55
1:C:241:MET:O	1:C:245:MET:HG2	2.06	0.55
1:D:67:VAL:HG11	1:D:83:LEU:HB2	1.89	0.55
1:D:121:ARG:NH1	1:D:689:GLN:OE1	2.41	0.54
1:B:550:GLN:OE1	1:B:559:LEU:N	2.40	0.54
1:A:652:THR:HB	1:A:693:ARG:HD3	1.90	0.54
1:B:288:TRP:CD1	1:B:454:ASP:HB2	2.42	0.54
1:A:730:SER:HA	1:A:734:LYS:HE3	1.88	0.54
1:B:499:PRO:HB2	1:D:499:PRO:HB2	1.88	0.54
1:A:727:GLU:OE2	1:A:863:LYS:NZ	2.40	0.54
1:D:501:LEU:HD12	1:D:502:PRO:HD2	1.90	0.54
1:C:196:CYS:O	1:C:200:LEU:HB2	2.08	0.53
1:A:602:SER:HB2	3:A:1002:ACT:H1	1.90	0.53
1:A:189:LYS:HG2	1:A:192:ARG:HH12	1.73	0.53
1:A:743:ARG:NH1	1:A:748:GLU:OE2	2.41	0.53
1:C:165:LEU:HD12	1:C:267:LEU:HD21	1.91	0.53
1:A:568:LEU:HD12	1:A:616:GLN:HG2	1.91	0.53
1:B:171:ASP:HB3	1:B:669:ARG:HG2	1.90	0.53
1:C:184:ARG:O	1:C:188:GLN:HG3	2.09	0.52
1:A:621:GLN:HG2	1:A:637:LEU:HD13	1.92	0.52
1:C:70:ASP:HB3	1:C:79:LYS:HE3	1.91	0.52
1:A:149:ARG:NH1	1:A:700:GLU:OE1	2.42	0.52
1:A:742:PHE:CZ	1:A:748:GLU:HG3	2.43	0.52
1:A:872:LEU:HD21	1:A:880:ILE:HD12	1.91	0.52
1:D:241:MET:HE3	1:D:307:VAL:HG13	1.91	0.52
1:B:312:ARG:HH21	1:B:528:SER:HB3	1.74	0.52
1:C:141:SER:OG	1:C:149:ARG:NH2	2.41	0.52
1:A:467:ASP:OD1	1:A:477:SER:OG	2.26	0.52
1:B:214:ASP:O	1:B:218:GLN:HG2	2.09	0.52
1:C:142:ASP:HB2	1:C:692:GLN:OE1	2.09	0.52
1:A:550:GLN:OE1	1:A:559:LEU:N	2.42	0.52
1:B:336:ASN:HD22	1:B:422:SER:HB2	1.75	0.52
1:B:249:HIS:CD2	1:B:318:LEU:HD21	2.44	0.52
1:A:144:GLU:CD	1:A:269:ASN:HD22	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:MET:HG3	1:C:307:VAL:HG13	1.92	0.51
1:C:465:VAL:HG22	1:C:511:ILE:HG23	1.91	0.51
1:B:615:TRP:CZ2	1:B:619:ARG:HD2	2.46	0.51
1:D:113:GLU:O	1:D:117:ILE:HG12	2.11	0.51
1:B:498:ARG:HD2	1:D:473:LEU:HD13	1.92	0.51
1:B:717:MET:HE2	1:B:821:PHE:HE2	1.75	0.51
1:A:568:LEU:HD22	1:A:608:ALA:HB2	1.93	0.51
1:D:388:ARG:NH1	1:D:401:SER:O	2.43	0.51
1:A:276:LEU:HD12	1:A:277:PRO:HD2	1.92	0.51
1:B:652:THR:HB	1:B:693:ARG:HD3	1.93	0.51
1:C:433:ASP:HA	1:C:437:LEU:HB2	1.92	0.51
1:B:333:TRP:CZ3	1:B:334:ARG:HG2	2.45	0.51
1:B:52:LEU:HD13	1:B:226:ARG:HH11	1.76	0.50
1:B:566:GLU:HG2	1:B:603:ASP:HB2	1.92	0.50
1:B:732:VAL:HG23	1:B:733:VAL:HG23	1.92	0.50
1:A:595:GLN:NE2	1:A:596:GLN:O	2.43	0.50
1:D:489:TRP:O	1:D:492:SER:OG	2.25	0.50
1:C:226:ARG:NE	1:D:428:ASP:OD1	2.43	0.50
1:A:237:PRO:HB2	1:A:303:VAL:HG11	1.94	0.50
1:B:102:ILE:HG21	1:B:901:LEU:HG	1.94	0.50
1:D:184:ARG:O	1:D:188:GLN:HG3	2.12	0.50
1:D:241:MET:O	1:D:245:MET:HG2	2.11	0.50
1:D:248:ILE:HA	1:D:252:VAL:HB	1.93	0.50
1:C:606:LYS:HG3	1:C:777:TRP:CD1	2.47	0.50
1:C:168:GLN:HG3	1:C:666:GLY:HA2	1.93	0.50
1:D:910:LYS:HE2	1:D:917:PHE:CD1	2.46	0.50
1:C:710:LYS:NZ	1:C:814:GLU:OE1	2.45	0.50
1:A:52:LEU:HD13	1:A:226:ARG:HH11	1.77	0.49
1:A:812:LEU:HA	1:A:815:MET:HE2	1.94	0.49
1:B:196:CYS:O	1:B:200:LEU:HB2	2.12	0.49
1:C:446:PHE:HB3	1:C:450:LEU:HD12	1.94	0.49
1:D:761:ALA:HB1	1:D:776:PRO:HG3	1.93	0.49
1:A:168:GLN:HG3	1:A:666:GLY:HA2	1.94	0.49
1:A:241:MET:HE3	1:A:307:VAL:HG13	1.94	0.49
1:A:747:PRO:HB3	1:A:909:LEU:HD11	1.94	0.49
1:A:102:ILE:HG21	1:A:901:LEU:HG	1.94	0.49
1:B:326:LEU:HD21	1:B:436:LEU:HD13	1.94	0.49
1:D:276:LEU:HD12	1:D:277:PRO:HD2	1.93	0.49
1:C:171:ASP:HB3	1:C:669:ARG:HG2	1.95	0.49
1:A:241:MET:O	1:A:245:MET:HG2	2.13	0.49
1:B:680:CYS:HB3	1:B:690:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:ILE:HB	1:C:594:LYS:O	2.13	0.49
1:D:277:PRO:HG2	1:D:280:VAL:HG23	1.94	0.49
1:D:337:ASP:O	1:D:341:VAL:HG23	2.13	0.49
1:A:184:ARG:O	1:A:188:GLN:HG3	2.13	0.49
1:D:386:ARG:NH1	1:D:387:GLU:OE2	2.46	0.49
1:A:388:ARG:NH1	1:A:401:SER:O	2.45	0.49
1:B:55:PRO:O	1:B:56:SER:OG	2.23	0.49
1:C:568:LEU:HD12	1:C:616:GLN:HG2	1.95	0.49
1:A:357:TYR:HD2	1:A:358:TYR:N	2.11	0.48
1:B:483:GLU:OE1	1:B:541:SER:HB3	2.13	0.48
1:A:42:VAL:HG13	1:A:105:MET:HE2	1.95	0.48
1:A:248:ILE:HA	1:A:252:VAL:HB	1.95	0.48
1:A:948:PRO:HB2	1:A:951:LEU:HD12	1.96	0.48
1:B:564:LEU:HD13	1:B:598:MET:HG2	1.96	0.48
1:B:706:PRO:HB3	1:B:820:PRO:HG2	1.94	0.48
1:C:922:GLN:HB3	1:C:923:PRO:HD2	1.95	0.48
1:D:178:PRO:O	1:D:751:TYR:OH	2.31	0.48
1:A:854:LYS:N	1:A:855:PRO:HD2	2.28	0.48
1:B:113:GLU:O	1:B:117:ILE:HG12	2.14	0.48
1:C:313:MET:HE3	1:C:313:MET:HB2	1.68	0.48
1:D:110:ASN:O	1:D:114:GLU:HG3	2.14	0.48
1:D:894:ARG:HG2	1:D:898:ILE:HD11	1.94	0.48
1:B:42:VAL:HG13	1:B:105:MET:HE2	1.96	0.48
1:B:742:PHE:CZ	1:B:748:GLU:HG3	2.48	0.48
1:A:122:ARG:NH1	1:B:204:ASP:OD2	2.45	0.47
1:C:652:THR:HB	1:C:693:ARG:HD3	1.96	0.47
1:D:595:GLN:NE2	1:D:596:GLN:O	2.47	0.47
1:C:888:LYS:O	1:C:892:VAL:HG23	2.13	0.47
1:D:641:ARG:HH12	1:D:659:GLN:NE2	2.12	0.47
1:A:313:MET:HE1	1:A:393:LEU:HD12	1.97	0.47
1:B:719:GLU:O	1:B:723:VAL:HG23	2.15	0.47
1:B:767:GLY:O	1:B:770:THR:HG22	2.13	0.47
1:B:743:ARG:NH1	1:B:748:GLU:OE2	2.47	0.47
1:D:173:VAL:HG22	1:D:286:SER:HB2	1.96	0.47
1:D:776:PRO:O	1:D:780:SER:OG	2.33	0.47
1:B:83:LEU:HD23	1:B:903:VAL:HG21	1.97	0.47
1:B:264:ASP:CG	1:B:275:ARG:HB3	2.40	0.47
1:B:502:PRO:HG2	1:B:505:LEU:HB2	1.97	0.47
1:C:868:GLN:NE2	1:C:880:ILE:HD12	2.29	0.47
1:A:525:PRO:O	1:A:528:SER:OG	2.33	0.47
1:C:162:PHE:CE2	1:C:166:LYS:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:TRP:CD1	1:C:454:ASP:HB2	2.50	0.47
1:D:770:THR:HG23	1:D:771:THR:HG23	1.96	0.47
1:A:70:ASP:HB3	1:A:79:LYS:HE3	1.97	0.47
1:A:293:ARG:HG2	1:A:456:ARG:O	2.15	0.47
1:B:41:LEU:HD21	1:B:197:LEU:HD13	1.97	0.47
1:B:178:PRO:O	1:B:751:TYR:OH	2.33	0.47
1:B:655:ALA:O	1:B:659:GLN:HG3	2.14	0.47
1:A:750:GLU:HG3	1:A:955:LEU:HD21	1.97	0.47
1:C:464:ASP:OD1	1:C:479:ARG:NH2	2.45	0.47
1:A:267:LEU:O	1:A:272:ILE:HB	2.15	0.47
1:A:388:ARG:HH12	1:A:402:ALA:HA	1.80	0.47
1:A:826:LEU:HB3	1:A:871:LEU:HD11	1.97	0.47
1:B:618:TYR:CD2	1:B:660:PRO:HD3	2.50	0.47
1:B:720:MET:HB3	1:B:797:ALA:HB1	1.96	0.47
1:D:956:ILE:HA	1:D:959:MET:HE3	1.97	0.47
1:A:86:LYS:O	1:A:922:GLN:NE2	2.48	0.46
1:B:574:ALA:CB	1:B:624:MET:HE2	2.45	0.46
1:D:606:LYS:HG3	1:D:777:TRP:CD1	2.50	0.46
1:D:142:ASP:HB2	1:D:692:GLN:OE1	2.15	0.46
1:C:41:LEU:HD11	1:C:197:LEU:HD22	1.97	0.46
1:C:86:LYS:O	1:C:922:GLN:NE2	2.48	0.46
1:C:388:ARG:HH12	1:C:402:ALA:HA	1.80	0.46
1:C:449:SER:O	1:C:451:VAL:N	2.44	0.46
1:D:196:CYS:O	1:D:200:LEU:HB2	2.15	0.46
1:D:845:ASP:CG	1:D:861:ARG:HH12	2.23	0.46
1:B:121:ARG:NH2	1:B:693:ARG:HH22	2.14	0.46
1:A:845:ASP:HA	1:A:849:VAL:HG23	1.97	0.46
1:B:568:LEU:HD12	1:B:616:GLN:HG2	1.97	0.46
1:A:60:PHE:CE2	1:A:90:LEU:HD11	2.50	0.46
1:A:885:PRO:O	1:A:887:LEU:N	2.49	0.46
1:A:102:ILE:O	1:A:106:LEU:HB2	2.16	0.46
1:A:732:VAL:HG23	1:A:733:VAL:HG23	1.98	0.46
1:C:259:PHE:HA	1:C:688:PHE:HE1	1.81	0.46
1:A:254:LYS:O	1:A:257:PRO:HD2	2.15	0.46
1:B:861:ARG:O	1:B:865:VAL:HG23	2.16	0.46
1:D:781:TRP:HA	1:D:784:THR:HG22	1.98	0.46
1:A:446:PHE:HB3	1:A:450:LEU:HA	1.98	0.45
1:D:505:LEU:HD12	1:D:506:PRO:HD2	1.98	0.45
1:B:406:PHE:HD1	1:B:411:GLU:HG2	1.81	0.45
1:B:617:LEU:O	1:B:621:GLN:HG3	2.17	0.45
1:B:241:MET:O	1:B:245:MET:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:NH2	1:A:693:ARG:HH22	2.14	0.45
1:D:446:PHE:HB3	1:D:450:LEU:HD12	1.99	0.45
1:B:52:LEU:HD13	1:B:226:ARG:NH1	2.32	0.45
1:A:730:SER:HA	1:A:734:LYS:HB2	1.97	0.45
1:C:40:LEU:HG	1:C:44:ARG:NH2	2.31	0.45
1:C:147:LEU:HB3	1:C:270:ILE:HD13	1.98	0.45
1:D:102:ILE:HG21	1:D:901:LEU:HG	1.98	0.45
1:A:598:MET:HA	1:A:638:PHE:HB3	1.99	0.45
1:A:762:LYS:HE3	1:A:771:THR:OG1	2.17	0.45
1:A:79:LYS:O	1:A:82:GLU:HG2	2.17	0.45
1:B:533:ILE:HG12	1:B:562:VAL:HG22	1.99	0.45
1:C:254:LYS:O	1:C:257:PRO:HD2	2.17	0.45
1:C:264:ASP:CG	1:C:441:ARG:HH22	2.22	0.45
1:C:732:VAL:HG23	1:C:733:VAL:HG23	1.99	0.45
1:D:313:MET:HB2	1:D:313:MET:HE3	1.79	0.45
1:D:357:TYR:HD2	1:D:358:TYR:CD2	2.35	0.45
1:B:98:VAL:O	1:B:102:ILE:HG12	2.16	0.45
1:B:106:LEU:HD12	1:B:106:LEU:HA	1.80	0.45
1:B:908:THR:HG23	1:B:951:LEU:HD22	1.99	0.45
1:A:511:ILE:O	1:A:515:ILE:HG13	2.17	0.44
1:A:591:ILE:HB	1:A:594:LYS:O	2.17	0.44
1:B:147:LEU:HD22	1:B:161:VAL:HG11	1.99	0.44
1:D:150:LEU:HD23	1:D:154:VAL:HG21	1.97	0.44
1:D:568:LEU:O	1:D:572:GLN:HG3	2.17	0.44
1:A:597:VAL:CG1	1:A:635:LEU:HD11	2.47	0.44
1:B:888:LYS:O	1:B:892:VAL:HG23	2.17	0.44
1:C:305:ARG:HA	1:C:524:LEU:HD11	1.99	0.44
1:D:657:LEU:HD12	1:D:706:PRO:HG3	1.98	0.44
1:B:336:ASN:HD22	1:B:422:SER:CB	2.30	0.44
1:B:489:TRP:O	1:B:492:SER:OG	2.28	0.44
1:B:598:MET:HA	1:B:638:PHE:HB3	2.00	0.44
1:B:716:LEU:HD23	1:B:815:MET:CE	2.47	0.44
1:B:854:LYS:N	1:B:855:PRO:HD2	2.32	0.44
1:A:416:LEU:O	1:A:419:CYS:HB2	2.18	0.44
1:A:615:TRP:CE2	1:A:619:ARG:HD2	2.52	0.44
1:C:717:MET:HE2	1:C:821:PHE:HE2	1.82	0.44
1:A:533:ILE:HG12	1:A:562:VAL:HG22	1.99	0.44
1:A:734:LYS:HE3	1:A:734:LYS:HB2	1.83	0.44
1:C:334:ARG:NH1	1:D:928:GLU:OE2	2.51	0.44
1:D:454:ASP:OD1	1:D:531:PRO:HD2	2.18	0.44
1:A:601:TYR:HE2	3:A:1004:ACT:H1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:MET:HE1	1:B:631:TYR:HB3	1.99	0.44
1:D:828:LEU:O	1:D:832:VAL:HG23	2.18	0.44
1:A:177:HIS:O	1:A:179:THR:N	2.50	0.44
1:A:342:ARG:HH22	1:A:414:GLU:CD	2.24	0.44
1:B:168:GLN:HG3	1:B:666:GLY:HA2	2.00	0.44
1:B:277:PRO:HG2	1:B:280:VAL:CG2	2.48	0.44
1:C:391:HIS:HB2	1:C:398:SER:HB2	2.00	0.44
1:A:40:LEU:O	1:A:44:ARG:HG3	2.18	0.44
1:A:277:PRO:HG2	1:A:280:VAL:HG23	2.00	0.44
1:A:604:SER:O	1:A:607:ASP:N	2.50	0.44
1:A:141:SER:HB2	1:A:145:GLU:OE1	2.18	0.43
1:A:406:PHE:CE1	1:A:412:PHE:HA	2.53	0.43
1:C:41:LEU:HD21	1:C:197:LEU:HD13	2.00	0.43
1:D:147:LEU:O	1:D:151:VAL:HG23	2.18	0.43
1:D:657:LEU:HG	1:D:820:PRO:HB3	2.00	0.43
1:A:647:ARG:NE	1:A:970:GLY:OXT	2.51	0.43
1:A:888:LYS:O	1:A:892:VAL:HG23	2.17	0.43
1:B:469:ILE:HD11	1:B:501:LEU:HD13	1.99	0.43
2:A:1001:GLY:N	1:B:229:GLU:OE1	2.52	0.43
1:B:40:LEU:O	1:B:44:ARG:HG3	2.18	0.43
1:B:406:PHE:CD1	1:B:411:GLU:HG2	2.52	0.43
1:B:737:ARG:HB3	1:B:853:LEU:HD21	2.00	0.43
1:C:113:GLU:O	1:C:117:ILE:HG12	2.17	0.43
1:C:305:ARG:HH22	1:C:396:GLY:HA2	1.83	0.43
1:D:540:PRO:HB3	1:D:581:LEU:HG	1.99	0.43
1:B:97:LEU:HD11	1:B:938:LEU:HD13	1.99	0.43
1:C:193:ILE:HG23	1:C:217:LEU:HD11	1.99	0.43
1:A:178:PRO:HB3	1:A:757:GLY:HA3	2.01	0.43
1:A:365:ILE:HG21	1:A:373:VAL:HG22	2.00	0.43
1:C:885:PRO:O	1:C:887:LEU:N	2.48	0.43
1:D:727:GLU:OE2	1:D:863:LYS:NZ	2.52	0.43
1:D:742:PHE:CZ	1:D:748:GLU:HG3	2.54	0.43
1:A:886:PHE:HA	1:A:889:GLN:HB2	2.00	0.43
1:B:597:VAL:HG12	1:B:635:LEU:HD11	2.00	0.43
1:B:608:ALA:HB1	1:B:612:SER:HB2	2.00	0.43
1:C:931:ASP:OD1	1:C:931:ASP:N	2.50	0.43
1:D:610:ARG:HA	1:D:610:ARG:HD2	1.90	0.43
1:C:70:ASP:O	1:C:74:LYS:HG2	2.17	0.43
1:C:176:ALA:HB2	1:C:289:MET:HG2	2.01	0.43
1:D:766:GLY:O	1:D:771:THR:HG21	2.19	0.43
1:A:781:TRP:HA	1:A:784:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:HIS:HD2	1:B:318:LEU:HD21	1.84	0.43
1:C:886:PHE:HA	1:C:889:GLN:HB2	2.00	0.43
1:D:50:GLN:HG3	1:D:55:PRO:HA	1.99	0.43
1:D:727:GLU:HG2	1:D:793:GLY:HA2	2.00	0.43
1:D:956:ILE:HA	1:D:959:MET:CE	2.49	0.43
1:A:223:ALA:HA	1:B:431:ILE:HD11	2.01	0.43
1:A:899:THR:O	1:A:903:VAL:HG23	2.19	0.43
1:A:922:GLN:HB3	1:A:923:PRO:HD2	2.01	0.43
1:C:98:VAL:O	1:C:102:ILE:HG12	2.19	0.43
1:C:608:ALA:HB1	1:C:612:SER:HB2	2.00	0.43
1:B:753:ARG:NH2	1:B:946:GLU:OE1	2.45	0.43
1:C:293:ARG:HG2	1:C:456:ARG:O	2.19	0.43
1:D:391:HIS:HB2	1:D:398:SER:HB2	2.00	0.43
1:A:762:LYS:NZ	1:A:768:GLY:O	2.41	0.42
1:B:845:ASP:HA	1:B:849:VAL:HG23	2.00	0.42
1:D:214:ASP:O	1:D:218:GLN:HG2	2.19	0.42
1:D:580:ARG:HA	1:D:580:ARG:HD3	1.89	0.42
1:B:76:ASP:HB3	1:B:79:LYS:H	1.84	0.42
1:C:121:ARG:NH1	1:C:689:GLN:OE1	2.52	0.42
1:C:214:ASP:O	1:C:218:GLN:HG2	2.19	0.42
1:D:192:ARG:HD2	1:D:220:GLU:OE2	2.20	0.42
1:A:163:GLU:HA	1:A:166:LYS:HD3	2.00	0.42
1:A:412:PHE:O	1:A:415:PRO:HD2	2.19	0.42
1:B:41:LEU:HD13	1:B:108:LEU:HD22	2.02	0.42
1:D:732:VAL:HG23	1:D:733:VAL:HG23	2.00	0.42
1:A:366:PRO:HD2	1:A:369:GLU:OE2	2.20	0.42
1:C:334:ARG:NH2	2:C:1001:GLY:O	2.52	0.42
1:D:502:PRO:HG2	1:D:505:LEU:HB2	2.00	0.42
1:D:819:TRP:HD1	1:D:820:PRO:HD2	1.84	0.42
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.75	0.42
1:C:262:ARG:NH2	1:D:212:GLU:OE2	2.53	0.42
1:D:820:PRO:O	1:D:824:VAL:HG23	2.20	0.42
1:B:853:LEU:O	1:B:856:PHE:HB3	2.20	0.42
1:D:371:TYR:CE1	1:D:423:LEU:HG	2.55	0.42
1:A:357:TYR:CD2	1:A:358:TYR:N	2.88	0.42
1:A:878:LYS:HE2	1:A:882:GLU:HG3	2.01	0.42
1:B:264:ASP:CG	1:B:441:ARG:HH22	2.27	0.42
1:A:664:ILE:HG21	1:A:698:THR:HG23	2.02	0.42
1:B:759:ARG:HG2	1:B:760:PRO:O	2.20	0.42
1:A:313:MET:HE2	1:A:389:ALA:CB	2.50	0.41
1:C:150:LEU:HD23	1:C:154:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:PRO:HA	1:D:503:PRO:HD3	1.81	0.41
1:C:106:LEU:HA	1:C:106:LEU:HD12	1.75	0.41
1:C:525:PRO:O	1:C:528:SER:OG	2.34	0.41
1:D:336:ASN:ND2	1:D:422:SER:HA	2.32	0.41
1:A:106:LEU:O	1:A:109:ALA:HB3	2.19	0.41
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.79	0.41
1:C:881:LEU:HD23	1:C:881:LEU:HA	1.83	0.41
1:B:483:GLU:CD	1:B:541:SER:HB3	2.45	0.41
1:C:431:ILE:HD11	1:D:223:ALA:HA	2.01	0.41
1:A:156:LYS:HE3	1:A:703:MET:HB3	2.02	0.41
1:A:580:ARG:O	1:A:584:VAL:HG23	2.21	0.41
1:B:689:GLN:OE1	1:B:693:ARG:NH1	2.54	0.41
1:B:785:ARG:NH2	1:B:899:THR:OG1	2.52	0.41
1:D:368:ASN:C	1:D:370:PRO:HD3	2.45	0.41
1:B:101:SER:O	1:B:105:MET:HG3	2.21	0.41
1:C:762:LYS:HD2	1:C:772:LEU:HA	2.02	0.41
1:D:52:LEU:HD13	1:D:226:ARG:HD2	2.02	0.41
1:D:259:PHE:HE1	1:D:692:GLN:NE2	2.16	0.41
1:D:293:ARG:NH2	1:D:304:THR:OG1	2.52	0.41
1:D:881:LEU:HD11	1:D:887:LEU:HD23	2.02	0.41
1:A:409:ILE:HG22	1:A:413:LEU:HD12	2.02	0.41
1:B:790:VAL:HG11	1:B:832:VAL:HG21	2.03	0.41
1:C:170:VAL:HG11	1:C:694:PHE:HB3	2.01	0.41
1:D:582:PHE:O	1:D:583:SER:OG	2.34	0.41
1:A:450:LEU:HA	1:A:450:LEU:HD12	1.90	0.41
1:B:308:CYS:O	1:B:312:ARG:HG3	2.21	0.41
1:C:268:LYS:HE2	1:C:268:LYS:HB3	1.80	0.41
1:C:660:PRO:HA	1:C:661:PRO:HD3	1.92	0.41
1:D:315:ALA:HB2	1:D:450:LEU:HB2	2.02	0.41
1:D:854:LYS:N	1:D:855:PRO:HD2	2.36	0.41
1:D:888:LYS:O	1:D:892:VAL:HG23	2.21	0.41
1:A:313:MET:HB2	1:A:313:MET:HE3	1.64	0.41
1:B:334:ARG:NH2	2:B:1002:GLY:OXT	2.54	0.41
1:C:483:GLU:O	1:C:487:GLN:HG3	2.21	0.41
1:C:828:LEU:O	1:C:832:VAL:HG23	2.21	0.41
1:C:910:LYS:HG2	1:C:917:PHE:CD2	2.56	0.41
1:A:365:ILE:HA	1:A:366:PRO:HD3	1.94	0.41
1:A:938:LEU:HD23	1:A:938:LEU:O	2.21	0.41
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.81	0.41
1:C:102:ILE:O	1:C:106:LEU:HB2	2.21	0.41
1:C:277:PRO:HG2	1:C:280:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:LYS:HD2	1:C:713:TRP:CE2	2.56	0.41
1:D:98:VAL:O	1:D:102:ILE:HG12	2.21	0.41
1:D:550:GLN:OE1	1:D:559:LEU:N	2.51	0.41
1:D:787:HIS:HE1	1:D:966:MET:HE2	1.86	0.41
1:B:277:PRO:HG2	1:B:280:VAL:HG23	2.02	0.40
1:B:661:PRO:O	1:B:663:THR:HG23	2.21	0.40
1:B:762:LYS:HE2	1:B:772:LEU:HD13	2.04	0.40
1:C:144:GLU:OE2	1:C:262:ARG:HD2	2.21	0.40
1:C:899:THR:O	1:C:903:VAL:HG23	2.21	0.40
1:B:192:ARG:HD2	1:B:220:GLU:OE1	2.20	0.40
1:B:638:PHE:CD1	1:B:669:ARG:HB2	2.56	0.40
1:C:932:GLU:H	1:C:932:GLU:HG3	1.52	0.40
1:A:770:THR:HG23	1:A:771:THR:HG23	2.03	0.40
1:C:42:VAL:HG13	1:C:105:MET:HE2	2.03	0.40
1:C:333:TRP:CD2	1:D:941:LEU:HD11	2.56	0.40
1:A:325:GLU:O	1:A:329:GLU:HG3	2.21	0.40
1:B:37:TYR:HB3	1:B:112:ALA:HB1	2.04	0.40
1:B:332:MET:HE2	1:B:431:ILE:HD13	2.03	0.40
1:B:727:GLU:O	1:B:730:SER:OG	2.29	0.40
1:B:847:LEU:HD21	1:B:907:TYR:CZ	2.57	0.40
1:B:930:ALA:N	1:B:931:ASP:HB2	2.37	0.40
1:D:125:LYS:O	1:D:126:LEU:HG	2.22	0.40
1:D:686:LEU:HD23	1:D:686:LEU:HA	1.89	0.40
1:D:853:LEU:O	1:D:856:PHE:HB3	2.21	0.40
1:A:57:LEU:HA	1:A:925:LEU:HD23	2.03	0.40
1:B:482:SER:O	1:B:486:ARG:HG3	2.22	0.40
1:B:660:PRO:HA	1:B:661:PRO:HD3	2.00	0.40
1:C:869:GLN:O	1:C:873:GLN:HG3	2.22	0.40
1:D:511:ILE:O	1:D:515:ILE:HG13	2.21	0.40
1:D:829:LEU:HA	1:D:829:LEU:HD23	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	912/970 (94%)	855 (94%)	53 (6%)	4 (0%)	30	60
1	B	911/970 (94%)	863 (95%)	44 (5%)	4 (0%)	30	60
1	C	912/970 (94%)	867 (95%)	42 (5%)	3 (0%)	36	65
1	D	912/970 (94%)	857 (94%)	54 (6%)	1 (0%)	48	75
All	All	3647/3880 (94%)	3442 (94%)	193 (5%)	12 (0%)	36	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	943	PRO
1	B	943	PRO
1	C	330	LEU
1	A	764	ARG
1	A	943	PRO
1	C	651	PRO
1	A	531	PRO
1	B	764	ARG
1	B	768	GLY
1	B	949	PRO
1	D	178	PRO
1	A	178	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	791/832 (95%)	765 (97%)	26 (3%)	33	59
1	B	790/832 (95%)	761 (96%)	29 (4%)	30	58
1	C	791/832 (95%)	759 (96%)	32 (4%)	28	56
1	D	791/832 (95%)	758 (96%)	33 (4%)	26	55
All	All	3163/3328 (95%)	3043 (96%)	120 (4%)	29	57

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	77	THR
1	A	97	LEU
1	A	122	ARG
1	A	186	LEU
1	A	205	ILE
1	A	283	ILE
1	A	313	MET
1	A	332	MET
1	A	388	ARG
1	A	393	LEU
1	A	399	GLU
1	A	562	VAL
1	A	597	VAL
1	A	612	SER
1	A	683	GLU
1	A	692	GLN
1	A	763	ARG
1	A	764	ARG
1	A	831	MET
1	A	852	GLU
1	A	878	LYS
1	A	882	GLU
1	A	902	ASN
1	A	932	GLU
1	A	939	VAL
1	B	36	GLU
1	B	40	LEU
1	B	58	ARG
1	B	122	ARG
1	B	186	LEU
1	B	198	THR
1	B	293	ARG
1	B	317	ASN
1	B	328	PHE
1	B	332	MET
1	B	350	SER
1	B	353	LYS
1	B	392	LEU
1	B	541	SER
1	B	562	VAL
1	B	597	VAL

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Mol	Chain	Res	Type
1	B	611	LEU
1	B	612	SER
1	B	668	ILE
1	B	683	GLU
1	B	689	GLN
1	B	692	GLN
1	B	769	ILE
1	B	784	THR
1	B	852	GLU
1	B	880	ILE
1	B	893	LEU
1	B	939	VAL
1	B	940	LYS
1	C	40	LEU
1	C	58	ARG
1	C	62	GLN
1	C	82	GLU
1	C	88	THR
1	C	97	LEU
1	C	144	GLU
1	C	186	LEU
1	C	205	ILE
1	C	206	THR
1	C	283	ILE
1	C	310	LEU
1	C	317	ASN
1	C	332	MET
1	C	336	ASN
1	C	353	LYS
1	C	364	GLN
1	C	379	ARG
1	C	397	VAL
1	C	562	VAL
1	C	566	GLU
1	C	610	ARG
1	C	611	LEU
1	C	612	SER
1	C	692	GLN
1	C	726	GLU
1	C	727	GLU
1	C	769	ILE
1	C	771	THR

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Mol	Chain	Res	Type
1	C	847	LEU
1	C	891	LEU
1	C	932	GLU
1	D	40	LEU
1	D	58	ARG
1	D	62	GLN
1	D	88	THR
1	D	122	ARG
1	D	144	GLU
1	D	186	LEU
1	D	205	ILE
1	D	206	THR
1	D	283	ILE
1	D	328	PHE
1	D	332	MET
1	D	350	SER
1	D	361	PHE
1	D	363	LYS
1	D	374	ILE
1	D	386	ARG
1	D	397	VAL
1	D	475	ILE
1	D	562	VAL
1	D	597	VAL
1	D	606	LYS
1	D	611	LEU
1	D	612	SER
1	D	692	GLN
1	D	762	LYS
1	D	825	THR
1	D	852	GLU
1	D	878	LYS
1	D	882	GLU
1	D	893	LEU
1	D	932	GLU
1	D	939	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	507	GLN

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Mol	Chain	Res	Type
1	A	659	GLN
1	A	665	ASN
1	A	873	GLN
1	B	180	GLN
1	B	211	GLN
1	B	249	HIS
1	B	322	GLN
1	B	336	ASN
1	B	377	HIS
1	B	472	HIS
1	B	665	ASN
1	B	895	ASN
1	C	116	GLN
1	C	180	GLN
1	C	188	GLN
1	C	199	GLN
1	C	201	ASN
1	C	211	GLN
1	C	621	GLN
1	C	639	HIS
1	C	659	GLN
1	C	665	ASN
1	D	53	HIS
1	D	336	ASN
1	D	472	HIS
1	D	557	GLN
1	D	665	ASN
1	D	692	GLN
1	D	787	HIS
1	D	868	GLN
1	D	895	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	1002	-	3,3,3	0.80	0	3,3,3	1.38	0
3	ACT	B	1003	-	3,3,3	0.81	0	3,3,3	1.57	0
3	ACT	D	1002	-	3,3,3	0.84	0	3,3,3	1.61	1 (33%)
2	GLY	D	1001	-	4,4,4	0.94	0	3,4,4	1.69	1 (33%)
3	ACT	C	1002	-	3,3,3	0.85	0	3,3,3	1.30	0
3	ACT	C	1003	-	3,3,3	0.82	0	3,3,3	1.38	0
2	GLY	B	1001	-	4,4,4	1.14	1 (25%)	3,4,4	2.11	2 (66%)
3	ACT	B	1004	-	3,3,3	0.82	0	3,3,3	1.35	0
3	ACT	A	1004	-	3,3,3	0.82	0	3,3,3	1.62	1 (33%)
3	ACT	D	1003	-	3,3,3	0.84	0	3,3,3	1.41	0
3	ACT	A	1003	-	3,3,3	0.76	0	3,3,3	1.45	0
3	ACT	D	1004	-	3,3,3	0.80	0	3,3,3	1.17	0
2	GLY	C	1001	-	4,4,4	1.04	0	3,4,4	1.52	0
3	ACT	C	1004	-	3,3,3	0.80	0	3,3,3	1.53	0
3	ACT	B	1005	-	3,3,3	0.78	0	3,3,3	1.60	1 (33%)
2	GLY	B	1002	-	4,4,4	1.09	0	3,4,4	1.43	0
2	GLY	A	1001	-	4,4,4	1.17	1 (25%)	3,4,4	1.60	1 (33%)
3	ACT	C	1005	-	3,3,3	0.87	0	3,3,3	1.36	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
2	GLY	D	1001	-	-	0/2/2/2	-
2	GLY	B	1001	-	-	2/2/2/2	-
2	GLY	C	1001	-	-	1/2/2/2	-
2	GLY	B	1002	-	-	2/2/2/2	-
2	GLY	A	1001	-	-	0/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	GLY	OXT-C	-2.17	1.23	1.30
2	A	1001	GLY	OXT-C	-2.11	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	GLY	OXT-C-O	-2.93	115.79	123.33
2	A	1001	GLY	OXT-C-O	-2.42	117.11	123.33
2	D	1001	GLY	OXT-C-CA	2.26	122.38	113.38
2	B	1001	GLY	OXT-C-CA	2.19	122.07	113.38
3	A	1004	ACT	OXT-C-O	-2.09	114.28	122.03
3	D	1002	ACT	OXT-C-O	-2.07	114.33	122.03
3	B	1005	ACT	OXT-C-CH3	2.01	123.49	115.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	GLY	O-C-CA-N
2	B	1001	GLY	OXT-C-CA-N
2	B	1002	GLY	OXT-C-CA-N
2	B	1002	GLY	O-C-CA-N
2	C	1001	GLY	OXT-C-CA-N

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	ACT	1	0
3	A	1004	ACT	1	0
3	D	1004	ACT	1	0
2	C	1001	GLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	GLY	1	0
2	A	1001	GLY	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	918/970 (94%)	0.00	17 (1%)	66 48	3, 24, 57, 85	0
1	B	917/970 (94%)	-0.11	15 (1%)	70 52	0, 17, 50, 88	0
1	C	918/970 (94%)	0.01	14 (1%)	72 53	8, 24, 60, 100	0
1	D	918/970 (94%)	0.12	25 (2%)	56 37	2, 30, 74, 97	0
All	All	3671/3880 (94%)	0.00	71 (1%)	66 48	0, 23, 63, 100	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	765	PRO	4.1
1	D	769	ILE	4.1
1	D	359	ILE	3.9
1	D	351	GLY	3.8
1	A	35	ILE	3.8
1	A	765	PRO	3.7
1	A	361	PHE	3.5
1	D	760	PRO	3.4
1	C	769	ILE	3.3
1	D	920	THR	3.2
1	D	361	PHE	3.1
1	A	886	PHE	3.1
1	A	936	ALA	3.0
1	D	352	SER	3.0
1	A	358	TYR	2.9
1	D	887	LEU	2.9
1	D	810	GLN	2.9
1	D	350	SER	2.8
1	B	403	GLU	2.8
1	B	38	ASP	2.8
1	C	358	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	761	ALA	2.7
1	A	353	LYS	2.7
1	D	358	TYR	2.6
1	B	869	GLN	2.6
1	D	383	TYR	2.6
1	C	893	LEU	2.6
1	B	762	LYS	2.6
1	A	769	ILE	2.6
1	B	769	ILE	2.5
1	A	810	GLN	2.5
1	C	887	LEU	2.5
1	B	504	ASP	2.5
1	C	361	PHE	2.5
1	C	921	PRO	2.5
1	D	37	TYR	2.5
1	A	36	GLU	2.4
1	A	923	PRO	2.4
1	B	556	ARG	2.4
1	D	122	ARG	2.4
1	B	886	PHE	2.4
1	B	142	ASP	2.4
1	D	936	ALA	2.4
1	A	359	ILE	2.3
1	C	353	LYS	2.3
1	A	383	TYR	2.3
1	B	930	ALA	2.3
1	C	350	SER	2.3
1	D	886	PHE	2.3
1	D	930	ALA	2.3
1	D	807	ARG	2.3
1	B	765	PRO	2.2
1	B	887	LEU	2.2
1	D	831	MET	2.2
1	D	929	PHE	2.2
1	A	760	PRO	2.2
1	D	144	GLU	2.2
1	B	397	VAL	2.2
1	C	359	ILE	2.2
1	C	885	PRO	2.2
1	B	204	ASP	2.2
1	A	360	GLU	2.1
1	D	689	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	367	PRO	2.1
1	B	144	GLU	2.1
1	C	363	LYS	2.0
1	A	152	SER	2.0
1	D	768	GLY	2.0
1	C	760	PRO	2.0
1	A	932	GLU	2.0
1	D	764	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

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
3	ACT	D	1002	4/4	0.60	0.18	21,21,21,21	0
3	ACT	C	1005	4/4	0.71	0.26	37,37,37,37	0
3	ACT	A	1003	4/4	0.77	0.28	40,40,40,40	0
3	ACT	C	1003	4/4	0.79	0.21	30,30,30,30	0
2	GLY	B	1001	5/5	0.81	0.20	22,22,22,22	0
3	ACT	B	1005	4/4	0.84	0.16	11,11,11,11	0
2	GLY	C	1001	5/5	0.84	0.17	18,18,18,18	0
2	GLY	D	1001	5/5	0.86	0.15	8,8,8,8	0
2	GLY	B	1002	5/5	0.87	0.14	8,8,8,8	0
3	ACT	B	1003	4/4	0.87	0.16	11,11,11,11	0
3	ACT	A	1004	4/4	0.88	0.14	20,20,20,20	0
3	ACT	D	1003	4/4	0.89	0.19	39,39,39,39	0
2	GLY	A	1001	5/5	0.90	0.13	9,9,9,9	0
3	ACT	A	1002	4/4	0.90	0.15	16,16,16,16	0
3	ACT	D	1004	4/4	0.90	0.15	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	C	1002	4/4	0.91	0.16	17,17,17,17	0
3	ACT	B	1004	4/4	0.95	0.10	10,10,10,10	0
3	ACT	C	1004	4/4	0.95	0.12	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.