



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:50 AM UTC

PDB ID : 3PH1 / pdb_00003ph1
Title : The Crystal Structure of a Pathogenic Protein from the *Xanthomonas campestris* Reveals a New Tetrameric PilZ Domain Self-Assembled via a Unusual Helical Bundle
Authors : Li, T.-N.; Chin, K.-H.; Yang, M.-D.; Chou, S.-H.
Deposited on : 2010-11-03
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)	:	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

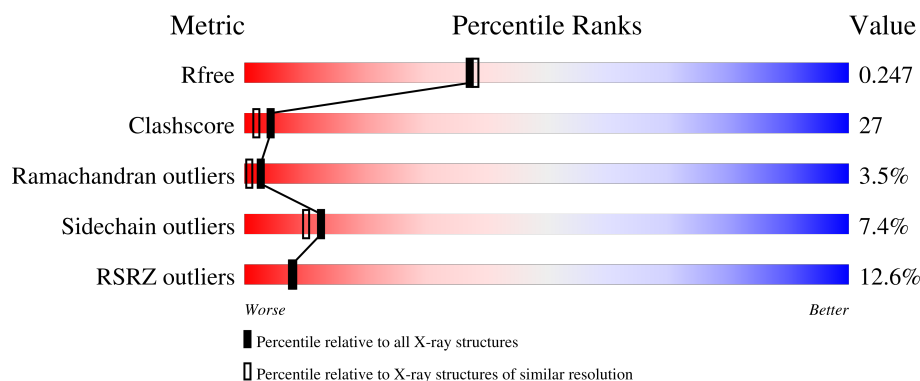
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	191	12% 50% 36% 7% 6%
1	B	191	14% 47% 32% 9% 12%
1	C	191	10% 63% 26% 7% • •
1	D	191	11% 61% 26% 8% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5935 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1384	871	252	259	2			
1	B	168	Total	C	N	O	S	0	0	0
			1295	822	237	234	2			
1	C	185	Total	C	N	O	S	0	0	0
			1421	892	260	266	3			
1	D	182	Total	C	N	O	S	0	0	0
			1403	881	257	263	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B0RT03
A	-1	ASN	-	expression tag	UNP B0RT03
A	0	ALA	-	expression tag	UNP B0RT03
B	-2	SER	-	expression tag	UNP B0RT03
B	-1	ASN	-	expression tag	UNP B0RT03
B	0	ALA	-	expression tag	UNP B0RT03
C	-2	SER	-	expression tag	UNP B0RT03
C	-1	ASN	-	expression tag	UNP B0RT03
C	0	ALA	-	expression tag	UNP B0RT03
D	-2	SER	-	expression tag	UNP B0RT03
D	-1	ASN	-	expression tag	UNP B0RT03
D	0	ALA	-	expression tag	UNP B0RT03

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



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

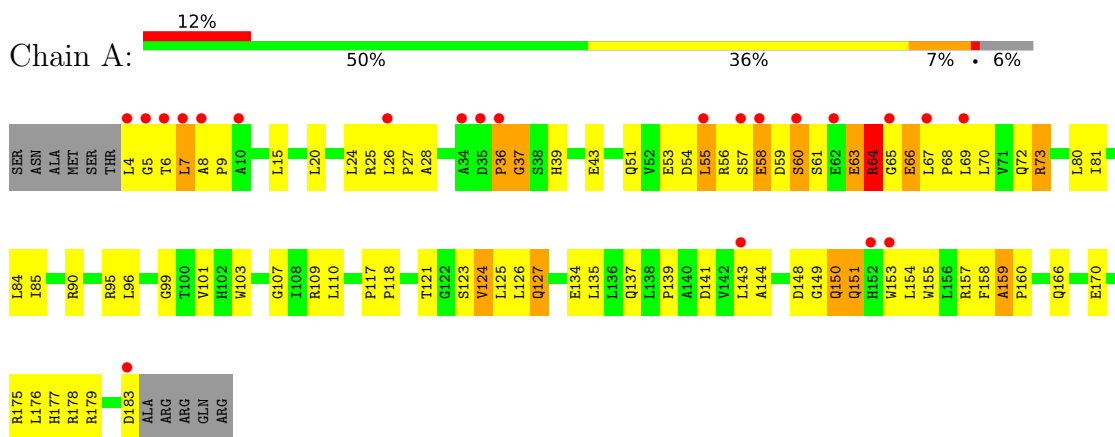
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total	O	0	0
			84	84		
3	B	90	Total	O	0	0
			90	90		
3	C	141	Total	O	0	0
			141	141		
3	D	101	Total	O	0	0
			101	101		

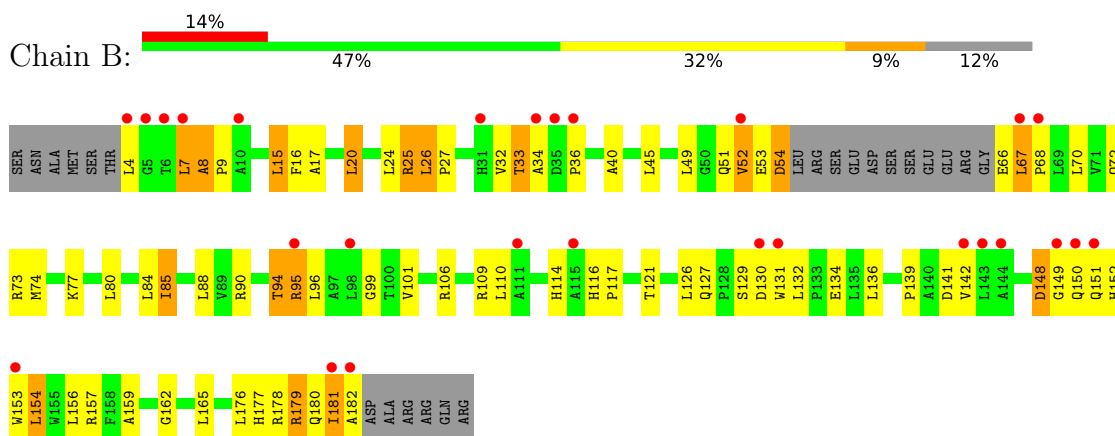
3 Residue-property plots [i](#)

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.

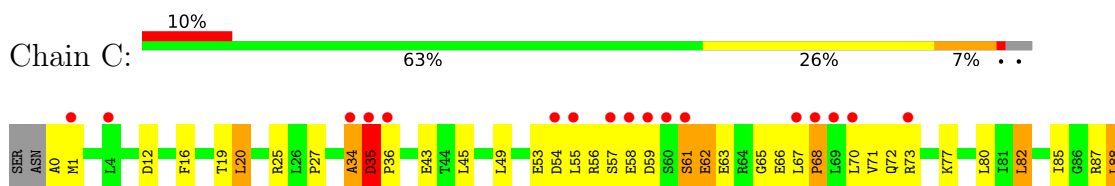
- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein

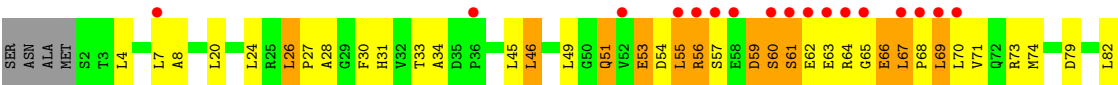


- Molecule 1: Putative uncharacterized protein





● Molecule 1: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.84Å 89.36Å 87.34Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	25.02 – 2.10 25.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.1 (25.02-2.10) 99.4 (25.02-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.229 , 0.259 0.246 , 0.247	Depositor DCC
R_{free} test set	2564 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.0	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	0.93	EDS
Total number of atoms	5935	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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:
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	0.43	0/1414	0.95	10/1929 (0.5%)
1	B	0.44	0/1324	0.95	6/1807 (0.3%)
1	C	0.46	0/1451	0.96	7/1978 (0.4%)
1	D	0.46	0/1433	0.95	8/1954 (0.4%)
All	All	0.45	0/5622	0.95	31/7668 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	ALA	CA-C-N	7.11	126.64	119.24
1	D	8	ALA	C-N-CA	7.11	126.64	119.24
1	A	37	GLY	N-CA-C	7.03	122.01	112.17
1	D	56	ARG	N-CA-C	-6.93	104.78	113.23
1	D	53	GLU	N-CA-C	-6.52	104.59	112.54
1	B	34	ALA	N-CA-C	-6.35	105.57	113.38
1	A	127	GLN	CA-C-N	6.08	125.80	119.05
1	A	127	GLN	C-N-CA	6.08	125.80	119.05
1	D	59	ASP	N-CA-C	-6.06	105.72	112.57
1	B	162	GLY	N-CA-C	-6.03	105.53	112.29
1	A	55	LEU	N-CA-C	-6.01	105.66	112.87
1	B	159	ALA	N-CA-C	-5.93	101.89	110.08
1	A	159	ALA	N-CA-C	-5.82	101.82	110.20
1	C	127	GLN	CA-C-N	5.74	124.94	118.97
1	C	127	GLN	C-N-CA	5.74	124.94	118.97
1	C	16	PHE	N-CA-C	5.74	121.31	113.97
1	B	16	PHE	N-CA-C	5.63	121.57	114.31
1	A	39	HIS	N-CA-C	-5.63	105.22	111.36
1	B	74	MET	N-CA-C	-5.49	105.37	111.36
1	C	53	GLU	N-CA-C	5.49	118.36	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	ASP	N-CA-C	5.47	117.38	110.33
1	A	66	GLU	CB-CA-C	-5.38	109.91	117.23
1	D	162	GLY	N-CA-C	-5.37	105.98	112.48
1	C	159	ALA	N-CA-C	-5.34	102.51	110.20
1	A	124	VAL	N-CA-C	-5.33	100.90	108.58
1	A	8	ALA	CA-C-N	5.28	124.73	119.24
1	A	8	ALA	C-N-CA	5.28	124.73	119.24
1	C	35	ASP	CA-C-N	5.24	124.42	118.97
1	C	35	ASP	C-N-CA	5.24	124.42	118.97
1	B	7	LEU	N-CA-C	-5.12	106.89	112.72
1	D	159	ALA	N-CA-C	-5.05	102.92	110.20

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	1384	0	1380	86	0
1	B	1295	0	1309	101	0
1	C	1421	0	1425	71	0
1	D	1403	0	1403	64	0
2	A	8	0	6	1	0
2	B	4	0	3	1	0
2	C	4	0	3	0	0
3	A	84	0	0	2	0
3	B	90	0	0	10	0
3	C	141	0	0	4	0
3	D	101	0	0	4	0
All	All	5935	0	5529	297	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 27.

All (297) 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:D:71:VAL:HA	1:D:74:MET:HE3	1.40	1.01
1:C:27:PRO:HG2	1:C:127:GLN:HB3	1.46	0.97
1:C:55:LEU:HG	1:C:56:ARG:H	1.30	0.96
1:C:35:ASP:H	1:C:36:PRO:HD3	1.28	0.95
1:A:70:LEU:HD22	1:B:66:GLU:HB2	1.48	0.95
1:A:64:ARG:H	1:A:64:ARG:NE	1.65	0.94
1:A:27:PRO:HG2	1:A:127:GLN:HB3	1.50	0.93
1:B:148:ASP:C	1:B:150:GLN:H	1.75	0.92
1:A:64:ARG:HE	1:A:64:ARG:N	1.69	0.91
1:B:25:ARG:H	1:B:25:ARG:HD2	1.36	0.90
1:B:70:LEU:HD13	1:C:67:LEU:HD22	1.53	0.89
1:A:73:ARG:HH21	1:B:54:ASP:H	1.21	0.88
1:A:73:ARG:HH11	1:A:73:ARG:HB2	1.39	0.87
1:D:64:ARG:HB2	1:D:64:ARG:NH1	1.91	0.86
1:C:36:PRO:HG2	1:C:139:PRO:HG3	1.58	0.85
1:D:64:ARG:HB2	1:D:64:ARG:HH11	1.39	0.85
2:B:1004:ACT:H2	3:B:367:HOH:O	1.77	0.85
1:B:106:ARG:HD3	3:B:1011:HOH:O	1.76	0.84
1:C:35:ASP:N	1:C:36:PRO:HD3	1.91	0.83
1:D:67:LEU:HB2	1:D:68:PRO:HD3	1.61	0.83
1:D:27:PRO:HG2	1:D:127:GLN:HB3	1.61	0.82
1:A:84:LEU:HB3	1:B:85:ILE:HD12	1.61	0.82
1:A:80:LEU:HD22	1:B:132:LEU:HD21	1.62	0.81
1:A:64:ARG:H	1:A:64:ARG:HE	0.86	0.80
1:C:129:SER:O	1:C:130:ASP:HB2	1.81	0.80
1:B:67:LEU:HB3	1:B:68:PRO:CD	2.12	0.80
1:B:126:LEU:HD21	1:B:136:LEU:HD23	1.63	0.79
1:C:35:ASP:H	1:C:36:PRO:CD	1.98	0.77
1:C:73:ARG:NH2	1:C:77:LYS:HZ1	1.81	0.77
1:A:143:LEU:HD22	1:A:157:ARG:HB2	1.68	0.76
1:B:148:ASP:C	1:B:150:GLN:N	2.43	0.75
1:D:70:LEU:HG	1:D:74:MET:HE2	1.67	0.75
1:A:143:LEU:HD23	1:A:155:TRP:O	1.88	0.73
1:B:179:ARG:HG2	1:B:179:ARG:HH21	1.53	0.73
1:A:73:ARG:HB2	1:A:73:ARG:NH1	2.05	0.70
1:C:73:ARG:HG2	1:C:77:LYS:HE3	1.75	0.69
1:A:90:ARG:HB3	1:A:95:ARG:HH12	1.58	0.68
1:A:73:ARG:NH2	1:B:54:ASP:O	2.27	0.68
1:A:73:ARG:NH2	1:B:54:ASP:H	1.89	0.68
1:A:84:LEU:HD11	1:B:132:LEU:HD11	1.75	0.68
1:B:95:ARG:CG	1:B:95:ARG:HH11	2.07	0.68
1:B:131:TRP:HZ2	3:B:210:HOH:O	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HB3	1:B:68:PRO:HD2	1.76	0.67
1:B:179:ARG:HG2	1:B:179:ARG:NH2	2.10	0.67
1:A:121:THR:HG22	1:A:141:ASP:OD2	1.95	0.66
1:D:69:LEU:HB2	3:D:227:HOH:O	1.94	0.66
1:C:36:PRO:HG3	1:C:123:SER:OG	1.96	0.66
1:A:27:PRO:HG2	1:A:127:GLN:CB	2.26	0.65
1:A:73:ARG:HH11	1:A:73:ARG:CB	2.09	0.65
1:D:49:LEU:O	1:D:53:GLU:HG2	1.97	0.65
1:A:7:LEU:HD12	1:A:7:LEU:H	1.62	0.64
1:B:7:LEU:HD23	1:B:7:LEU:H	1.63	0.64
1:B:165:LEU:O	1:B:165:LEU:HD12	1.98	0.64
1:D:56:ARG:O	1:D:56:ARG:HD3	1.98	0.64
1:B:94:THR:O	1:B:95:ARG:HB2	1.96	0.63
1:B:148:ASP:O	1:B:150:GLN:N	2.29	0.63
1:B:85:ILE:HD13	1:B:85:ILE:O	1.98	0.63
1:B:84:LEU:CD2	1:C:134:GLU:HG2	2.29	0.63
1:B:45:LEU:O	1:B:49:LEU:HD13	1.99	0.62
1:A:7:LEU:H	1:A:7:LEU:CD1	2.12	0.62
1:A:24:LEU:N	1:A:24:LEU:HD23	2.14	0.62
1:D:33:THR:HG22	1:D:34:ALA:N	2.14	0.62
1:C:57:SER:O	1:C:58:GLU:HG3	2.00	0.62
1:C:73:ARG:CZ	1:C:77:LYS:HZ1	2.12	0.61
1:C:180:GLN:HG3	3:C:288:HOH:O	1.99	0.61
1:C:67:LEU:HD12	1:C:68:PRO:HD2	1.82	0.61
1:B:84:LEU:HD21	1:C:134:GLU:HG2	1.82	0.61
1:D:33:THR:HG22	1:D:34:ALA:H	1.66	0.60
1:C:88:LEU:O	1:C:91:GLN:HB2	2.02	0.60
1:D:73:ARG:HH21	1:D:73:ARG:HG3	1.67	0.60
1:A:6:THR:O	1:A:9:PRO:HD3	2.01	0.60
1:B:84:LEU:HD12	1:C:89:VAL:HG21	1.84	0.60
1:B:127:GLN:NE2	1:B:130:ASP:HA	2.17	0.60
1:A:36:PRO:HG2	1:A:37:GLY:H	1.68	0.59
1:B:36:PRO:HB2	1:B:139:PRO:HG3	1.85	0.59
1:A:135:LEU:HD21	3:A:1019:HOH:O	2.02	0.59
1:C:55:LEU:CG	1:C:56:ARG:H	2.04	0.59
1:B:114:HIS:HA	1:B:152:HIS:HD2	1.67	0.59
1:D:64:ARG:HH11	1:D:64:ARG:CB	2.14	0.59
1:D:68:PRO:HB2	1:D:71:VAL:HG12	1.83	0.59
1:A:7:LEU:HD12	1:A:7:LEU:N	2.17	0.58
1:B:126:LEU:HD23	1:B:136:LEU:HB3	1.85	0.58
1:B:32:VAL:O	1:B:33:THR:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLN:HE21	1:B:130:ASP:HA	1.68	0.58
1:B:53:GLU:HA	3:B:476:HOH:O	2.03	0.58
1:C:65:GLY:O	1:C:66:GLU:HB3	2.04	0.58
1:A:73:ARG:HH21	1:B:54:ASP:N	1.98	0.58
1:D:56:ARG:HG2	1:D:60:SER:OG	2.03	0.57
1:C:61:SER:C	1:C:63:GLU:H	2.12	0.57
1:B:26:LEU:HD12	1:B:26:LEU:O	2.04	0.57
1:B:127:GLN:HG2	1:B:129:SER:O	2.04	0.57
1:C:112:SER:HB2	1:C:154:LEU:HD22	1.87	0.57
1:D:157:ARG:HH11	1:D:157:ARG:HG3	1.70	0.56
1:B:25:ARG:HD2	1:B:25:ARG:N	2.14	0.56
1:B:73:ARG:O	1:B:77:LYS:HG3	2.05	0.56
1:B:178:ARG:O	1:B:181:ILE:HG22	2.04	0.56
1:C:34:ALA:HB1	1:C:36:PRO:HD3	1.87	0.56
1:C:36:PRO:HA	1:C:137:GLN:HE21	1.70	0.56
1:A:68:PRO:HG2	1:B:67:LEU:HD11	1.87	0.56
1:A:81:ILE:O	1:A:85:ILE:HG22	2.05	0.56
1:D:55:LEU:HD12	3:D:1015:HOH:O	2.05	0.56
1:B:25:ARG:H	1:B:25:ARG:CD	2.14	0.56
1:D:60:SER:O	1:D:62:GLU:N	2.39	0.56
1:D:175:ARG:O	1:D:179:ARG:HD3	2.05	0.56
1:D:33:THR:HG21	3:D:357:HOH:O	2.05	0.56
1:D:131:TRP:CZ3	1:D:132:LEU:HD13	2.41	0.56
1:B:121:THR:HA	1:B:141:ASP:OD1	2.06	0.55
1:A:166:GLN:O	1:A:170:GLU:HG3	2.06	0.55
1:A:144:ALA:HB3	1:A:155:TRP:HB2	1.87	0.55
1:B:150:GLN:HA	1:B:150:GLN:OE1	2.06	0.55
1:C:73:ARG:CG	1:C:77:LYS:HE3	2.36	0.55
1:C:45:LEU:O	1:C:49:LEU:HB2	2.06	0.55
1:B:20:LEU:HD21	1:B:177:HIS:CD2	2.42	0.54
1:B:24:LEU:HD23	1:B:24:LEU:N	2.22	0.54
1:B:52:VAL:HG23	1:B:52:VAL:O	2.07	0.54
1:B:131:TRP:CZ2	3:B:210:HOH:O	2.53	0.54
1:D:71:VAL:HA	1:D:74:MET:CE	2.26	0.54
1:A:90:ARG:HH11	1:A:95:ARG:HH22	1.55	0.54
1:A:24:LEU:HD23	1:A:24:LEU:H	1.72	0.54
1:D:27:PRO:HG2	1:D:127:GLN:CB	2.37	0.54
1:A:143:LEU:HD23	1:A:143:LEU:H	1.72	0.54
1:D:59:ASP:OD2	1:D:63:GLU:HG3	2.08	0.54
1:D:131:TRP:CE3	1:D:132:LEU:HD13	2.43	0.53
1:D:55:LEU:HD13	1:D:63:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PRO:HD2	3:C:507:HOH:O	2.09	0.53
1:B:66:GLU:N	1:B:72:GLN:HG2	2.24	0.53
1:B:178:ARG:HA	1:B:181:ILE:HG22	1.90	0.53
1:A:90:ARG:HB3	1:A:95:ARG:NH1	2.22	0.53
1:B:70:LEU:HD13	1:C:67:LEU:CD2	2.31	0.53
1:C:176:LEU:HD23	1:C:179:ARG:NH2	2.24	0.53
1:C:57:SER:C	1:C:58:GLU:HG3	2.34	0.52
1:D:31:HIS:HD2	1:D:125:LEU:HD23	1.74	0.52
1:C:129:SER:O	1:C:130:ASP:CB	2.55	0.52
1:A:36:PRO:HG2	1:A:37:GLY:N	2.24	0.52
1:A:123:SER:HB3	1:A:137:GLN:HG3	1.92	0.52
1:A:84:LEU:HD11	1:B:132:LEU:CD1	2.40	0.52
1:A:124:VAL:HG12	1:A:126:LEU:HD13	1.91	0.52
1:B:176:LEU:C	1:B:176:LEU:HD23	2.35	0.51
1:B:149:GLY:C	1:B:151:GLN:H	2.17	0.51
1:B:33:THR:HG21	3:B:1007:HOH:O	2.09	0.51
1:A:20:LEU:HD11	1:A:177:HIS:CD2	2.45	0.51
1:B:90:ARG:HD3	3:B:339:HOH:O	2.10	0.51
1:B:149:GLY:HA3	1:B:153:TRP:HE1	1.74	0.51
3:B:397:HOH:O	1:C:43:GLU:HG2	2.11	0.51
1:C:36:PRO:HA	1:C:137:GLN:NE2	2.24	0.51
1:C:82:LEU:O	1:C:85:ILE:HG22	2.10	0.51
1:A:59:ASP:C	1:A:61:SER:H	2.18	0.51
1:B:150:GLN:HG3	1:B:151:GLN:HE21	1.76	0.51
1:C:63:GLU:HG3	1:C:72:GLN:CD	2.36	0.51
1:A:85:ILE:HD11	1:D:85:ILE:N	2.26	0.51
1:B:106:ARG:O	1:B:157:ARG:HD2	2.10	0.51
1:C:67:LEU:CD1	1:C:68:PRO:HD2	2.41	0.51
1:B:154:LEU:HB3	1:B:156:LEU:CD2	2.42	0.50
1:B:178:ARG:HG3	1:B:179:ARG:N	2.25	0.50
1:D:67:LEU:HB2	1:D:68:PRO:CD	2.38	0.50
1:B:4:LEU:N	1:B:4:LEU:HD23	2.27	0.49
1:B:70:LEU:HD23	1:B:70:LEU:O	2.12	0.49
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.77	0.49
1:A:63:GLU:HG3	1:A:66:GLU:HB2	1.93	0.49
1:B:88:LEU:HD21	1:C:89:VAL:HG22	1.94	0.49
1:B:179:ARG:HH21	1:B:179:ARG:CG	2.21	0.49
1:D:27:PRO:CG	1:D:127:GLN:HB3	2.38	0.49
1:A:80:LEU:HD21	1:B:49:LEU:HD12	1.93	0.49
1:A:175:ARG:O	1:A:179:ARG:HG3	2.13	0.49
1:C:55:LEU:CG	1:C:56:ARG:N	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:HG3	1:C:58:GLU:H	1.78	0.48
1:A:80:LEU:HD22	1:B:132:LEU:CD2	2.39	0.48
1:A:63:GLU:CG	1:A:66:GLU:HB2	2.43	0.48
1:D:170:GLU:HG2	3:D:198:HOH:O	2.13	0.48
1:B:154:LEU:HB3	1:B:156:LEU:HD21	1.96	0.48
1:C:19:THR:HG23	1:C:106:ARG:NH2	2.29	0.48
1:D:175:ARG:HG2	1:D:178:ARG:NH1	2.29	0.48
1:C:55:LEU:HG	1:C:56:ARG:N	2.12	0.47
1:D:68:PRO:HB2	1:D:71:VAL:CG1	2.44	0.47
1:A:69:LEU:HA	1:A:72:GLN:OE1	2.13	0.47
1:C:110:LEU:C	1:C:110:LEU:HD12	2.39	0.47
1:D:26:LEU:HD12	1:D:26:LEU:O	2.14	0.47
1:B:95:ARG:CG	1:B:95:ARG:NH1	2.73	0.47
1:C:67:LEU:HD21	1:C:71:VAL:HB	1.95	0.47
1:D:51:GLN:HE21	1:D:51:GLN:HB2	1.54	0.47
1:A:175:ARG:HB3	1:A:179:ARG:NH1	2.30	0.47
1:B:181:ILE:HG23	1:B:181:ILE:O	2.13	0.47
1:B:25:ARG:HB3	3:B:472:HOH:O	2.14	0.46
1:C:59:ASP:OD1	1:C:62:GLU:HB3	2.15	0.46
1:A:54:ASP:C	1:A:56:ARG:N	2.71	0.46
1:B:84:LEU:CD1	1:C:89:VAL:HG21	2.46	0.46
1:A:159:ALA:O	1:A:160:PRO:C	2.59	0.46
1:B:8:ALA:N	1:B:9:PRO:CD	2.79	0.46
1:C:35:ASP:N	1:C:36:PRO:CD	2.62	0.46
1:A:58:GLU:C	1:A:60:SER:H	2.22	0.46
1:B:95:ARG:HG3	1:B:95:ARG:NH1	2.31	0.46
1:C:87:ARG:HD3	3:C:229:HOH:O	2.16	0.46
1:D:55:LEU:HD13	1:D:63:GLU:CD	2.41	0.46
1:D:110:LEU:HD12	1:D:110:LEU:C	2.41	0.46
1:B:114:HIS:HA	1:B:152:HIS:CD2	2.48	0.46
1:C:73:ARG:CZ	1:C:77:LYS:NZ	2.79	0.46
1:A:36:PRO:HG2	1:A:139:PRO:HG3	1.98	0.46
1:A:7:LEU:CD1	1:A:7:LEU:N	2.77	0.45
1:B:126:LEU:CD2	1:B:136:LEU:HB3	2.45	0.45
1:B:67:LEU:CB	1:B:68:PRO:CD	2.86	0.45
1:B:109:ARG:HG3	1:B:109:ARG:HH11	1.80	0.45
1:C:65:GLY:C	1:C:67:LEU:H	2.25	0.45
1:B:24:LEU:HD13	1:B:176:LEU:HD21	1.98	0.45
1:D:177:HIS:NE2	1:D:181:ILE:HD11	2.31	0.45
1:A:28:ALA:HA	1:A:125:LEU:O	2.16	0.45
1:B:27:PRO:HG2	1:B:127:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:HD21	1:C:71:VAL:CG1	2.47	0.45
1:A:54:ASP:C	1:A:56:ARG:H	2.25	0.45
1:A:148:ASP:CG	1:A:149:GLY:H	2.25	0.45
1:B:26:LEU:HD12	1:B:26:LEU:C	2.42	0.45
1:D:131:TRP:H	1:D:131:TRP:CD1	2.35	0.45
1:A:150:GLN:O	1:A:151:GLN:C	2.60	0.44
1:C:77:LYS:NZ	1:D:79:ASP:OD1	2.43	0.44
1:C:20:LEU:HD21	1:C:177:HIS:CD2	2.52	0.44
1:D:4:LEU:HA	1:D:7:LEU:HD23	2.00	0.44
1:D:60:SER:OG	1:D:61:SER:N	2.48	0.44
1:C:49:LEU:HD11	1:C:129:SER:HB2	1.98	0.44
1:C:95:ARG:H	1:C:95:ARG:HD2	1.82	0.44
1:D:82:LEU:O	1:D:85:ILE:HG22	2.17	0.44
1:C:61:SER:C	1:C:63:GLU:N	2.76	0.44
1:A:24:LEU:N	1:A:24:LEU:CD2	2.81	0.44
1:A:157:ARG:HD3	1:A:158:PHE:O	2.17	0.44
1:B:17:ALA:O	1:B:106:ARG:NH2	2.38	0.44
1:C:159:ALA:O	1:C:160:PRO:C	2.60	0.44
1:B:152:HIS:HB3	3:B:1010:HOH:O	2.17	0.44
1:C:0:ALA:O	1:C:1:MET:HB2	2.17	0.44
1:C:70:LEU:HD13	1:C:70:LEU:C	2.43	0.44
2:A:1003:ACT:H2	1:B:40:ALA:HB3	2.00	0.43
1:C:176:LEU:HD23	1:C:179:ARG:HH22	1.83	0.43
1:B:27:PRO:HG2	1:B:127:GLN:CB	2.48	0.43
1:B:67:LEU:O	1:B:68:PRO:C	2.61	0.43
1:C:100:THR:HG21	3:C:434:HOH:O	2.18	0.43
1:C:112:SER:CB	1:C:154:LEU:HD22	2.47	0.43
1:A:90:ARG:NH1	1:A:95:ARG:HH22	2.16	0.43
1:D:73:ARG:HG3	1:D:73:ARG:NH2	2.33	0.43
1:A:58:GLU:O	1:A:59:ASP:CB	2.65	0.43
1:A:67:LEU:HB3	1:A:68:PRO:HD2	1.99	0.43
1:A:121:THR:HG22	1:A:141:ASP:CG	2.43	0.43
1:D:33:THR:CG2	1:D:34:ALA:N	2.82	0.43
1:B:15:LEU:CD1	1:B:157:ARG:HD3	2.49	0.43
1:C:34:ALA:C	1:C:35:ASP:OD1	2.61	0.43
1:D:88:LEU:O	1:D:91:GLN:HB2	2.18	0.43
1:A:103:TRP:CH2	1:A:126:LEU:HD23	2.54	0.42
1:D:30:PHE:CD2	1:D:156:LEU:HG	2.54	0.42
1:B:67:LEU:HB3	1:B:68:PRO:HD3	1.98	0.42
1:D:126:LEU:O	1:D:128:PRO:HD3	2.19	0.42
1:A:25:ARG:HA	1:A:99:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PRO:CG	1:A:37:GLY:N	2.81	0.42
1:A:69:LEU:C	1:A:69:LEU:HD23	2.44	0.42
1:A:4:LEU:HD21	1:A:153:TRP:CE2	2.54	0.42
1:A:90:ARG:CB	1:A:95:ARG:HH12	2.29	0.42
1:A:101:VAL:HG12	1:A:110:LEU:HB3	2.02	0.42
1:B:101:VAL:HG12	1:B:110:LEU:HB3	2.00	0.42
1:C:70:LEU:HD13	1:C:70:LEU:O	2.19	0.42
1:D:93:ASP:OD2	1:D:93:ASP:O	2.37	0.42
1:A:176:LEU:C	1:A:176:LEU:HD13	2.45	0.42
1:B:142:VAL:HG22	1:B:156:LEU:CD1	2.49	0.42
1:D:46:LEU:HD13	1:D:136:LEU:HD13	2.02	0.42
1:D:143:LEU:HG	1:D:157:ARG:HB2	2.02	0.42
1:A:134:GLU:OE2	1:A:134:GLU:HA	2.20	0.42
1:C:25:ARG:HG2	1:C:98:LEU:HD22	2.02	0.42
1:D:26:LEU:CD1	1:D:26:LEU:C	2.92	0.42
1:D:121:THR:HG22	1:D:141:ASP:CG	2.45	0.41
1:A:178:ARG:NH1	3:A:341:HOH:O	2.53	0.41
1:D:68:PRO:O	1:D:71:VAL:HG12	2.20	0.41
1:A:15:LEU:HD22	1:A:107:GLY:HA3	2.01	0.41
1:D:55:LEU:O	1:D:56:ARG:HB3	2.20	0.41
1:A:124:VAL:CG1	1:A:126:LEU:HD13	2.51	0.41
1:D:26:LEU:HD12	1:D:26:LEU:C	2.45	0.41
1:D:45:LEU:O	1:D:49:LEU:HB2	2.20	0.41
1:C:61:SER:O	1:C:63:GLU:N	2.53	0.41
1:B:36:PRO:HB2	1:B:139:PRO:CG	2.50	0.41
1:C:87:ARG:HD2	1:D:89:VAL:HG11	2.02	0.41
1:A:67:LEU:HB3	1:A:68:PRO:CD	2.51	0.41
1:B:84:LEU:HD22	1:C:134:GLU:HG2	2.01	0.41
1:C:175:ARG:HG3	1:C:175:ARG:NH2	2.36	0.41
1:A:27:PRO:HB2	1:A:96:LEU:HB2	2.02	0.41
1:A:51:GLN:HB3	1:D:73:ARG:HD3	2.03	0.41
1:B:181:ILE:HD12	1:B:181:ILE:HA	1.96	0.41
1:C:56:ARG:HG3	1:C:58:GLU:N	2.35	0.41
1:D:26:LEU:CD1	1:D:28:ALA:HB2	2.51	0.41
1:D:49:LEU:CD2	1:D:128:PRO:HB2	2.51	0.41
1:A:90:ARG:HG2	1:A:95:ARG:HH22	1.85	0.41
1:B:25:ARG:HA	1:B:99:GLY:O	2.20	0.40
1:B:45:LEU:HD13	1:B:134:GLU:HG2	2.02	0.40
1:B:51:GLN:HE21	1:B:51:GLN:HB2	1.69	0.40
1:D:49:LEU:HA	1:D:49:LEU:HD12	1.83	0.40
1:A:43:GLU:OE1	1:D:56:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:LEU:HD23	1:D:24:LEU:N	2.36	0.40
1:A:72:GLN:HB3	1:B:51:GLN:OE1	2.21	0.40
1:A:109:ARG:HA	1:A:154:LEU:O	2.21	0.40
1:A:117:PRO:HA	1:A:118:PRO:HD3	1.96	0.40
1:C:107:GLY:HA3	1:C:156:LEU:O	2.22	0.40
1:A:5:GLY:H	1:A:7:LEU:HD13	1.86	0.40
1:A:58:GLU:O	1:A:59:ASP:HB3	2.21	0.40
1:B:116:HIS:HA	1:B:117:PRO:HD3	1.98	0.40
1:B:180:GLN:C	1:B:182:ALA:H	2.30	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	178/191 (93%)	158 (89%)	13 (7%)	7 (4%)	2	0
1	B	164/191 (86%)	149 (91%)	10 (6%)	5 (3%)	3	1
1	C	183/191 (96%)	164 (90%)	13 (7%)	6 (3%)	3	1
1	D	180/191 (94%)	167 (93%)	6 (3%)	7 (4%)	2	0
All	All	705/764 (92%)	638 (90%)	42 (6%)	25 (4%)	3	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	PRO
1	A	151	GLN
1	B	67	LEU
1	C	34	ALA
1	C	35	ASP
1	C	68	PRO

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Mol	Chain	Res	Type
1	D	55	LEU
1	D	60	SER
1	D	61	SER
1	A	64	ARG
1	B	148	ASP
1	C	61	SER
1	C	130	ASP
1	A	63	GLU
1	C	129	SER
1	D	66	GLU
1	D	67	LEU
1	B	8	ALA
1	D	57	SER
1	A	57	SER
1	A	60	SER
1	D	65	GLY
1	B	52	VAL
1	A	65	GLY
1	B	181	ILE

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	147/157 (94%)	138 (94%)	9 (6%)	17	15
1	B	137/157 (87%)	124 (90%)	13 (10%)	8	5
1	C	151/157 (96%)	140 (93%)	11 (7%)	13	10
1	D	150/157 (96%)	140 (93%)	10 (7%)	15	12
All	All	585/628 (93%)	542 (93%)	43 (7%)	13	10

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	26	LEU

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Mol	Chain	Res	Type
1	A	53	GLU
1	A	55	LEU
1	A	58	GLU
1	A	64	ARG
1	A	73	ARG
1	A	150	GLN
1	A	183	ASP
1	B	15	LEU
1	B	20	LEU
1	B	25	ARG
1	B	26	LEU
1	B	33	THR
1	B	54	ASP
1	B	80	LEU
1	B	85	ILE
1	B	94	THR
1	B	95	ARG
1	B	96	LEU
1	B	154	LEU
1	B	179	ARG
1	C	12	ASP
1	C	20	LEU
1	C	54	ASP
1	C	62	GLU
1	C	80	LEU
1	C	82	LEU
1	C	88	LEU
1	C	95	ARG
1	C	126	LEU
1	C	134	GLU
1	C	154	LEU
1	D	20	LEU
1	D	26	LEU
1	D	46	LEU
1	D	51	GLN
1	D	66	GLU
1	D	69	LEU
1	D	132	LEU
1	D	156	LEU
1	D	157	ARG
1	D	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	39	HIS
1	A	51	GLN
1	A	150	GLN
1	A	152	HIS
1	A	177	HIS
1	B	51	GLN
1	B	91	GLN
1	B	102	HIS
1	B	116	HIS
1	B	127	GLN
1	B	137	GLN
1	B	151	GLN
1	B	177	HIS
1	C	31	HIS
1	C	72	GLN
1	C	102	HIS
1	C	137	GLN
1	C	151	GLN
1	D	31	HIS
1	D	51	GLN
1	D	72	GLN
1	D	114	HIS
1	D	116	HIS
1	D	152	HIS

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 [i](#)

4 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	$\# Z > 2$
2	ACT	A	1001	-	3,3,3	0.08	0	3,3,3	0.64	0
2	ACT	A	1003	-	3,3,3	0.08	0	3,3,3	0.64	0
2	ACT	B	1004	-	3,3,3	0.08	0	3,3,3	0.63	0
2	ACT	C	1002	-	3,3,3	0.08	0	3,3,3	0.64	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	ACT	1	0
2	B	1004	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	180/191 (94%)	0.81	22 (12%) 8 8	23, 43, 103, 119	0
1	B	168/191 (87%)	0.96	27 (16%) 4 5	25, 48, 76, 88	0
1	C	185/191 (96%)	0.51	20 (10%) 11 11	19, 35, 92, 108	0
1	D	182/191 (95%)	0.47	21 (11%) 9 10	19, 35, 108, 120	0
All	All	715/764 (93%)	0.68	90 (12%) 8 8	19, 39, 92, 120	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	ALA	5.9
1	C	55	LEU	5.4
1	D	65	GLY	5.1
1	D	55	LEU	4.9
1	C	34	ALA	4.3
1	A	55	LEU	4.1
1	A	35	ASP	4.1
1	D	57	SER	4.0
1	B	6	THR	3.9
1	A	60	SER	3.9
1	A	36	PRO	3.8
1	C	184	ALA	3.8
1	B	4	LEU	3.7
1	C	54	ASP	3.7
1	C	61	SER	3.7
1	D	61	SER	3.7
1	A	5	GLY	3.6
1	B	5	GLY	3.6
1	D	182	ALA	3.5
1	D	67	LEU	3.4
1	A	4	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	60	SER	3.3
1	C	57	SER	3.3
1	A	57	SER	3.2
1	A	6	THR	3.2
1	B	36	PRO	3.1
1	C	67	LEU	3.1
1	D	56	ARG	3.0
1	D	68	PRO	3.0
1	A	7	LEU	3.0
1	D	183	ASP	3.0
1	A	67	LEU	2.9
1	A	183	ASP	2.8
1	B	67	LEU	2.8
1	A	8	ALA	2.8
1	C	36	PRO	2.8
1	C	73	ARG	2.8
1	C	70	LEU	2.8
1	D	69	LEU	2.8
1	B	131	TRP	2.8
1	B	7	LEU	2.7
1	C	182	ALA	2.6
1	B	130	ASP	2.6
1	B	150	GLN	2.6
1	B	182	ALA	2.6
1	D	94	THR	2.6
1	A	152	HIS	2.5
1	C	68	PRO	2.5
1	C	4	LEU	2.5
1	D	58	GLU	2.5
1	B	181	ILE	2.5
1	B	52	VAL	2.4
1	B	142	VAL	2.4
1	B	115	ALA	2.4
1	A	153	TRP	2.4
1	D	36	PRO	2.4
1	D	70	LEU	2.4
1	A	58	GLU	2.3
1	B	10	ALA	2.3
1	B	111	ALA	2.3
1	A	143	LEU	2.3
1	B	143	LEU	2.3
1	B	95	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	62	GLU	2.3
1	D	64	ARG	2.3
1	C	1	MET	2.3
1	D	52	VAL	2.3
1	B	98	LEU	2.3
1	D	63	GLU	2.3
1	B	151	GLN	2.3
1	C	58	GLU	2.2
1	B	35	ASP	2.2
1	A	65	GLY	2.2
1	B	149	GLY	2.2
1	D	7	LEU	2.2
1	C	35	ASP	2.2
1	A	62	GLU	2.2
1	A	26	LEU	2.2
1	B	68	PRO	2.2
1	C	177	HIS	2.1
1	A	69	LEU	2.1
1	B	31	HIS	2.1
1	B	153	TRP	2.1
1	A	10	ALA	2.1
1	C	59	ASP	2.1
1	B	34	ALA	2.1
1	D	60	SER	2.1
1	D	181	ILE	2.0
1	B	144	ALA	2.0
1	C	69	LEU	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
2	ACT	A	1001	4/4	0.87	0.22	10,13,14,15	0
2	ACT	B	1004	4/4	0.87	0.36	10,13,14,15	0
2	ACT	C	1002	4/4	0.88	0.22	10,13,14,15	0
2	ACT	A	1003	4/4	0.89	0.24	10,13,14,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.