



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:55 AM UTC

PDB ID : 2Q04 / pdb_00002q04
Title : Crystal structure of acetoin utilization protein (ZP_00540088.1) from *Exiguobacterium sibiricum* 255-15 at 2.33 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-05-18
Resolution : 2.33 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:

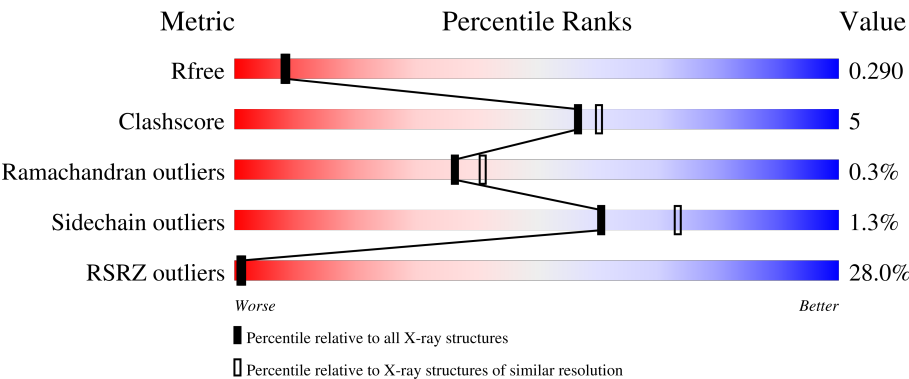
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	211	18% 90% 10%
1	B	211	16% 87% 11% .
1	C	211	43% 89% 8% ..
1	D	211	11% 88% 11% .
1	E	211	11% 88% 10% .

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Mol	Chain	Length	Quality of chain
1	F	211	61% 89% 6% . .

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	ACY	E	212	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10133 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 Acetoin utilization protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	Se	0	2	0
			1691	1092	284	307	1	7			
1	B	207	Total	C	N	O	S	Se	0	2	0
			1645	1058	282	298	1	6			
1	C	208	Total	C	N	O	S	Se	0	2	0
			1608	1030	272	297	1	8			
1	D	210	Total	C	N	O	S	Se	0	1	0
			1678	1083	280	306	1	8			
1	E	210	Total	C	N	O	S	Se	0	0	0
			1660	1072	277	302	1	8			
1	F	204	Total	C	N	O	S	Se	0	1	0
			1560	997	267	288	1	7			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q41BL0
A	1	MSE	MET	modified residue	UNP Q41BL0
A	120	MSE	MET	modified residue	UNP Q41BL0
A	125	MSE	MET	modified residue	UNP Q41BL0
A	155	MSE	MET	modified residue	UNP Q41BL0
A	158	MSE	MET	modified residue	UNP Q41BL0
A	159	MSE	MET	modified residue	UNP Q41BL0
A	183	MSE	MET	modified residue	UNP Q41BL0
A	208	MSE	MET	modified residue	UNP Q41BL0
B	0	GLY	-	expression tag	UNP Q41BL0
B	1	MSE	MET	modified residue	UNP Q41BL0
B	120	MSE	MET	modified residue	UNP Q41BL0
B	125	MSE	MET	modified residue	UNP Q41BL0
B	155	MSE	MET	modified residue	UNP Q41BL0
B	158	MSE	MET	modified residue	UNP Q41BL0
B	159	MSE	MET	modified residue	UNP Q41BL0
B	183	MSE	MET	modified residue	UNP Q41BL0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	208	MSE	MET	modified residue	UNP Q41BL0
C	0	GLY	-	expression tag	UNP Q41BL0
C	1	MSE	MET	modified residue	UNP Q41BL0
C	120	MSE	MET	modified residue	UNP Q41BL0
C	125	MSE	MET	modified residue	UNP Q41BL0
C	155	MSE	MET	modified residue	UNP Q41BL0
C	158	MSE	MET	modified residue	UNP Q41BL0
C	159	MSE	MET	modified residue	UNP Q41BL0
C	183	MSE	MET	modified residue	UNP Q41BL0
C	208	MSE	MET	modified residue	UNP Q41BL0
D	0	GLY	-	expression tag	UNP Q41BL0
D	1	MSE	MET	modified residue	UNP Q41BL0
D	120	MSE	MET	modified residue	UNP Q41BL0
D	125	MSE	MET	modified residue	UNP Q41BL0
D	155	MSE	MET	modified residue	UNP Q41BL0
D	158	MSE	MET	modified residue	UNP Q41BL0
D	159	MSE	MET	modified residue	UNP Q41BL0
D	183	MSE	MET	modified residue	UNP Q41BL0
D	208	MSE	MET	modified residue	UNP Q41BL0
E	0	GLY	-	expression tag	UNP Q41BL0
E	1	MSE	MET	modified residue	UNP Q41BL0
E	120	MSE	MET	modified residue	UNP Q41BL0
E	125	MSE	MET	modified residue	UNP Q41BL0
E	155	MSE	MET	modified residue	UNP Q41BL0
E	158	MSE	MET	modified residue	UNP Q41BL0
E	159	MSE	MET	modified residue	UNP Q41BL0
E	183	MSE	MET	modified residue	UNP Q41BL0
E	208	MSE	MET	modified residue	UNP Q41BL0
F	0	GLY	-	expression tag	UNP Q41BL0
F	1	MSE	MET	modified residue	UNP Q41BL0
F	120	MSE	MET	modified residue	UNP Q41BL0
F	125	MSE	MET	modified residue	UNP Q41BL0
F	155	MSE	MET	modified residue	UNP Q41BL0
F	158	MSE	MET	modified residue	UNP Q41BL0
F	159	MSE	MET	modified residue	UNP Q41BL0
F	183	MSE	MET	modified residue	UNP Q41BL0
F	208	MSE	MET	modified residue	UNP Q41BL0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

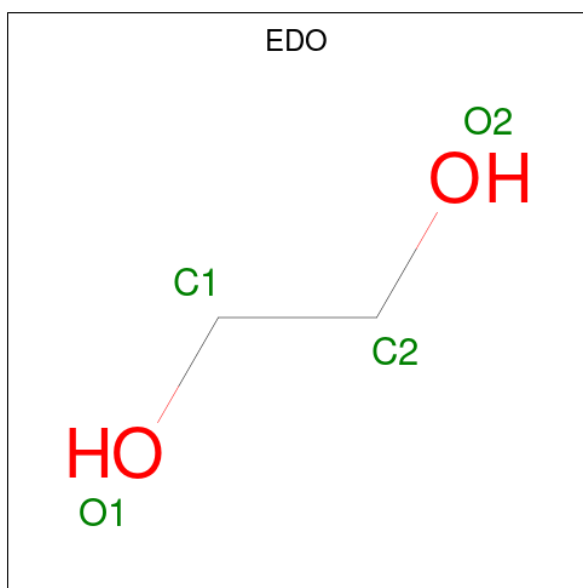
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total 2 Ca 2	0	0
2	B	1	Total 1 Ca 1	0	0
2	C	1	Total 1 Ca 1	0	0
2	D	1	Total 1 Ca 1	0	0
2	E	1	Total 1 Ca 1	0	0
2	F	1	Total 1 Ca 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



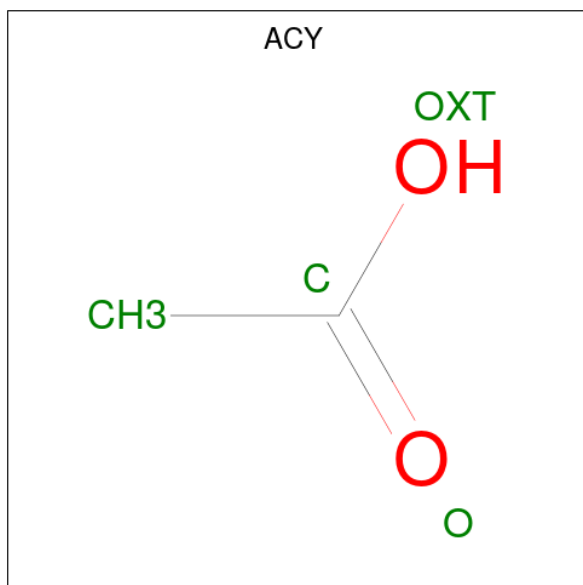
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total 4 C 2 O 2	0	0
3	A	1	Total 4 C 2 O 2	0	0
3	A	1	Total 4 C 2 O 2	0	0
3	C	1	Total 4 C 2 O 2	0	0

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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		
5	B	45	Total	O	0	0
			45	45		

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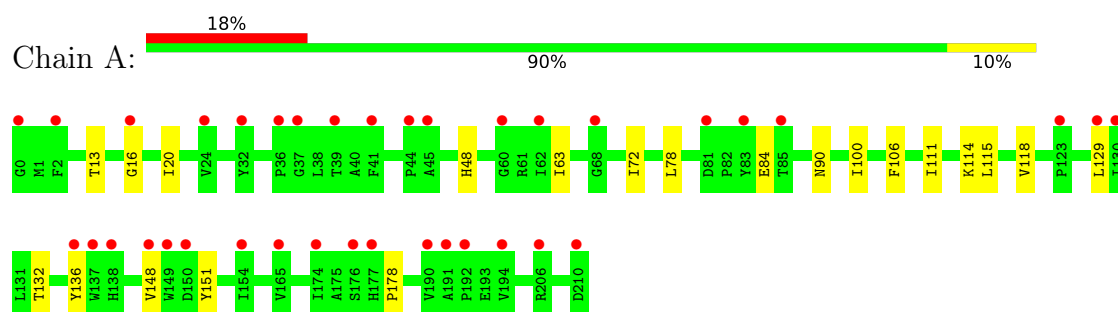
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	23	Total 23	O 23	0	0
5	D	57	Total 57	O 57	0	0
5	E	40	Total 40	O 40	0	0
5	F	18	Total 18	O 18	0	0

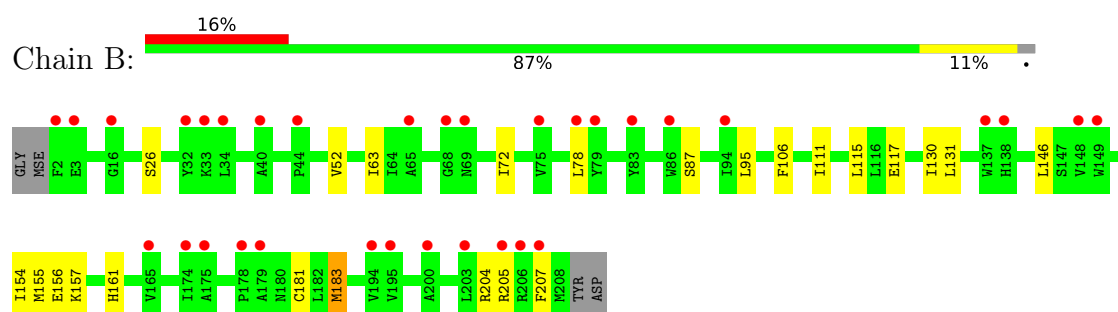
3 Residue-property plots [i](#)

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.

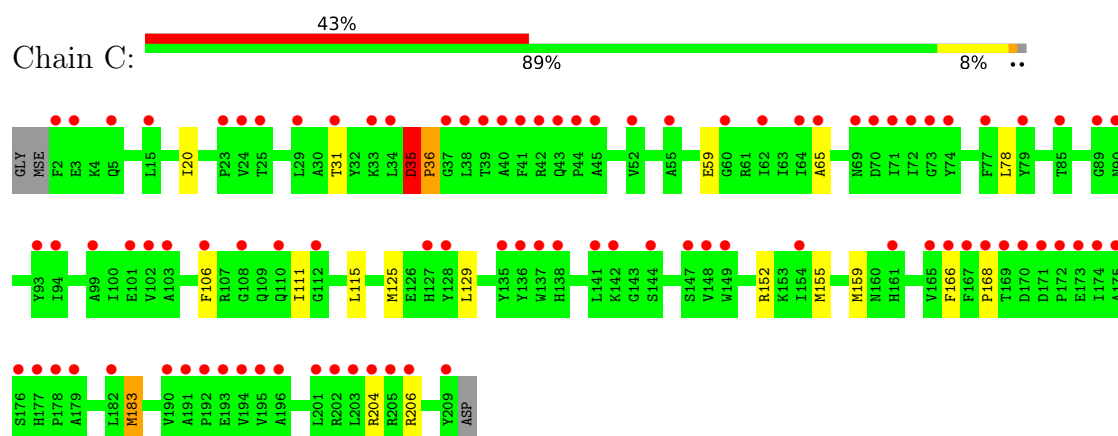
- Molecule 1: Acetoin utilization protein



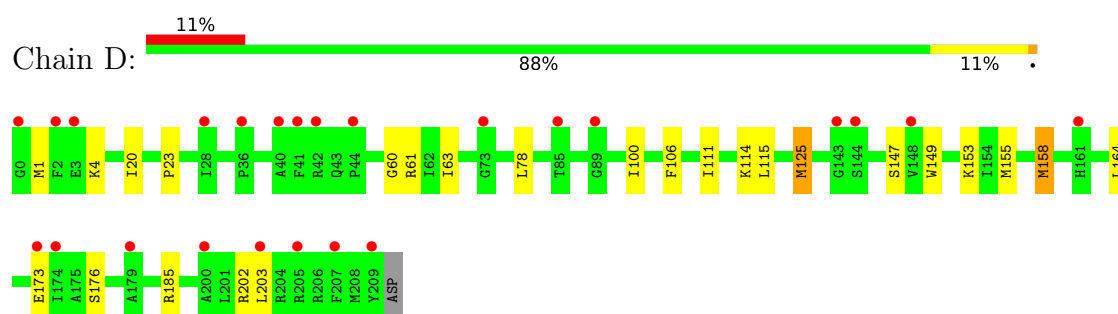
- Molecule 1: Acetoin utilization protein



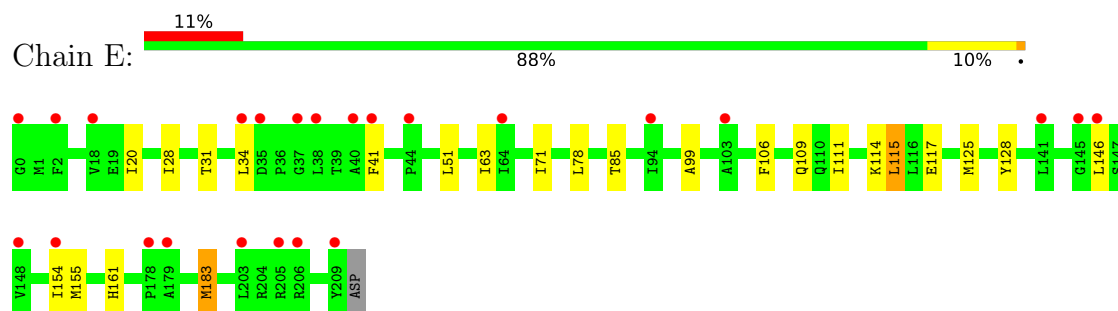
- Molecule 1: Acetoin utilization protein



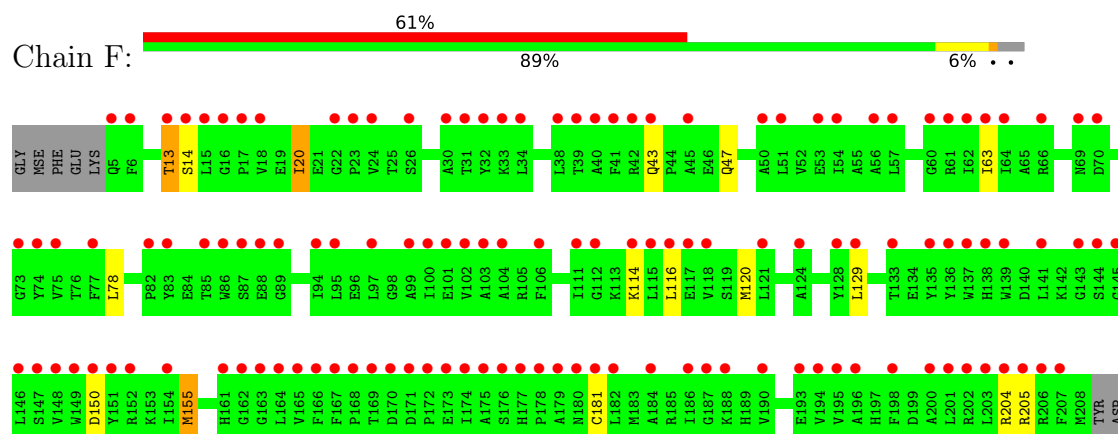
- Molecule 1: Acetoin utilization protein



- Molecule 1: Acetoin utilization protein



- Molecule 1: Acetoin utilization protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.87Å 128.58Å 108.43Å 90.00° 108.43° 90.00°	Depositor
Resolution (Å)	29.34 – 2.33 29.34 – 2.33	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.34-2.33) 93.7 (29.34-2.33)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0005, PHENIX	Depositor
R, R_{free}	0.229 , 0.260 (Not available) , 0.290	Depositor DCC
R_{free} test set	3696 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10133	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.81 % 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 1.0849e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CA, ACY

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	0.81	0/1734	0.63	0/2344
1	B	0.80	1/1689 (0.1%)	0.64	0/2286
1	C	0.72	1/1650 (0.1%)	0.65	2/2235 (0.1%)
1	D	0.95	2/1718 (0.1%)	0.64	0/2319
1	E	0.86	2/1698 (0.1%)	0.65	0/2298
1	F	0.74	1/1598 (0.1%)	0.65	0/2168
All	All	0.82	7/10087 (0.1%)	0.64	2/13650 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	158	MSE	SE-CE	10.47	2.26	1.95
1	E	183	MSE	SE-CE	-9.64	1.66	1.95
1	C	183	MSE	SE-CE	-8.06	1.71	1.95
1	F	155	MSE	SE-CE	-6.84	1.75	1.95
1	D	125	MSE	SE-CE	6.59	2.15	1.95
1	B	183	MSE	SE-CE	-6.36	1.76	1.95
1	E	125	MSE	SE-CE	5.89	2.13	1.95

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	ASP	CA-C-N	5.10	139.23	127.00
1	C	35	ASP	C-N-CA	5.10	139.23	127.00

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	1691	0	1622	18	0
1	B	1645	0	1586	15	0
1	C	1608	0	1486	15	0
1	D	1678	0	1633	19	0
1	E	1660	0	1597	15	0
1	F	1560	0	1440	12	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	12	0	18	2	0
3	C	4	0	6	1	0
3	D	8	0	12	0	0
3	F	4	0	6	0	0
4	A	4	0	3	1	0
4	E	8	0	6	2	0
4	F	4	0	3	0	0
5	A	57	0	0	0	0
5	B	45	0	0	0	0
5	C	23	0	0	0	0
5	D	57	0	0	1	0
5	E	40	0	0	1	0
5	F	18	0	0	0	0
All	All	10133	0	9418	88	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 5.

All (88) 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:125:MSE:SE	1:D:125:MSE:CE	2.15	1.44
1:D:158:MSE:CE	1:D:158:MSE:SE	2.26	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:MSE:SE	1:E:183:MSE:HE1	2.20	0.92
1:B:157:LYS:NZ	1:F:150:ASP:OD2	2.12	0.82
1:A:178:PRO:HG2	1:D:149:TRP:CH2	2.22	0.75
1:C:65:ALA:HB2	1:C:115:LEU:HD11	1.70	0.72
1:E:146:LEU:HD21	1:E:154:ILE:HD12	1.74	0.69
1:B:181:CYS:SG	1:B:183:MSE:HE3	2.32	0.68
1:E:117:GLU:OE2	1:E:161:HIS:NE2	2.27	0.67
1:E:128:TYR:OH	4:E:212:ACY:H3	1.97	0.65
1:C:159:MSE:HG3	1:C:183:MSE:HE1	1.78	0.64
1:C:125:MSE:HA	1:C:125:MSE:HE2	1.85	0.58
1:B:106:PHE:HB3	1:B:111:ILE:HD12	1.86	0.57
1:F:155:MSE:HE1	1:F:181:CYS:SG	2.45	0.56
1:C:20:ILE:HG23	1:C:115:LEU:HD12	1.88	0.55
1:F:20:ILE:CD1	1:F:114:LYS:HB3	2.37	0.55
1:C:35:ASP:CG	1:C:36:PRO:CA	2.81	0.54
1:B:117:GLU:OE2	1:B:161[B]:HIS:NE2	2.42	0.53
1:A:13:THR:OG1	1:A:16:GLY:N	2.41	0.53
1:D:173:GLU:O	1:D:176:SER:OG	2.26	0.52
1:E:85:THR:HG21	5:E:233:HOH:O	2.09	0.52
1:C:166:PHE:HA	1:C:183:MSE:HG2	1.93	0.51
1:A:136:TYR:C	1:A:136:TYR:CD1	2.90	0.50
1:D:4:LYS:NZ	1:D:60:GLY:O	2.30	0.49
1:E:20:ILE:HD13	1:E:114:LYS:HB3	1.94	0.49
1:C:168:PRO:HB3	1:D:147:SER:HA	1.94	0.49
1:D:106:PHE:HB3	1:D:111:ILE:HD12	1.94	0.48
1:A:84:GLU:O	1:B:204:ARG:NH2	2.47	0.48
1:C:35:ASP:CB	1:C:36:PRO:CA	2.92	0.47
1:F:204:ARG:O	1:F:205:ARG:C	2.57	0.47
1:D:202:ARG:HG3	1:D:203:LEU:HG	1.97	0.47
1:A:100:ILE:O	1:A:100:ILE:HG23	2.15	0.46
1:B:156:GLU:HA	1:B:183:MSE:HE1	1.97	0.46
1:C:78:LEU:HD23	1:C:78:LEU:N	2.30	0.46
1:F:155:MSE:CE	1:F:181:CYS:SG	3.04	0.46
1:A:48:HIS:CG	4:A:216:ACY:H3	2.51	0.45
1:D:4:LYS:HB3	1:D:23:PRO:CG	2.46	0.45
1:D:61:ARG:CZ	1:D:125:MSE:HE3	2.47	0.45
1:F:78:LEU:N	1:F:78:LEU:HD23	2.31	0.45
1:F:63:ILE:HD12	1:F:63:ILE:N	2.32	0.45
1:F:129:LEU:C	1:F:129:LEU:HD23	2.42	0.45
1:A:20:ILE:HG22	1:A:118:VAL:HG21	1.99	0.45
1:C:106:PHE:HB3	1:C:111:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:MSE:SE	1:C:183:MSE:HE1	2.67	0.44
1:D:63:ILE:HD12	1:D:63:ILE:N	2.32	0.44
1:C:206:ARG:HB3	3:C:212:EDO:H12	1.99	0.44
1:C:20:ILE:CG2	1:C:115:LEU:HD12	2.47	0.44
1:D:78:LEU:HD23	1:D:78:LEU:N	2.33	0.44
1:A:106:PHE:HB3	1:A:111:ILE:HD12	1.98	0.44
1:B:146:LEU:HD21	1:B:154:ILE:HD12	1.99	0.44
1:F:43:GLN:O	1:F:47:GLN:N	2.46	0.44
1:A:151:TYR:HH	3:A:214:EDO:C1	2.31	0.43
1:C:129:LEU:C	1:C:129:LEU:HD23	2.44	0.43
1:F:155:MSE:SE	1:F:155:MSE:C	3.11	0.43
1:B:63:ILE:HD12	1:B:63:ILE:N	2.34	0.43
1:A:148:VAL:HG23	5:D:235:HOH:O	2.18	0.43
1:A:78:LEU:N	1:A:78:LEU:HD23	2.33	0.43
1:D:100:ILE:O	1:D:100:ILE:HG23	2.19	0.43
1:B:131:LEU:C	1:B:131:LEU:HD12	2.43	0.43
1:E:78:LEU:HD23	1:E:78:LEU:N	2.34	0.43
1:D:164:LEU:HD12	1:D:185:ARG:HB2	2.00	0.43
1:B:26:SER:OG	1:B:52:VAL:HG13	2.19	0.42
1:E:63:ILE:HD12	1:E:63:ILE:N	2.34	0.42
1:E:106:PHE:HB3	1:E:111:ILE:HD12	2.02	0.42
1:B:155:MSE:SE	1:B:155:MSE:C	3.12	0.42
1:D:20:ILE:HD13	1:D:114:LYS:HB3	2.01	0.42
1:B:95:LEU:O	1:B:130:ILE:HA	2.19	0.42
1:E:128:TYR:CZ	4:E:212:ACY:H3	2.54	0.42
1:A:151:TYR:OH	3:A:214:EDO:C1	2.68	0.42
1:A:20:ILE:HD13	1:A:114:LYS:HB3	2.02	0.42
1:B:72:ILE:C	1:B:72:ILE:HD12	2.45	0.42
1:D:149:TRP:O	1:D:153:LYS:HG3	2.20	0.41
1:E:155:MSE:SE	1:E:183:MSE:CE	3.08	0.41
1:B:78:LEU:N	1:B:78:LEU:HD23	2.35	0.41
1:D:4:LYS:HB3	1:D:23:PRO:HG2	2.02	0.41
1:D:155:MSE:SE	1:D:155:MSE:C	3.13	0.41
1:A:178:PRO:HG2	1:D:149:TRP:CZ2	2.52	0.41
1:F:116:LEU:O	1:F:120:MSE:HG2	2.21	0.41
1:E:34:LEU:HD12	1:E:71:ILE:HB	2.01	0.41
1:A:63:ILE:HD12	1:A:63:ILE:N	2.34	0.41
1:E:115:LEU:HD12	1:E:115:LEU:HA	1.94	0.41
1:C:59:GLU:OE1	1:C:59:GLU:N	2.50	0.41
1:E:41:PHE:CZ	1:E:99:ALA:HB1	2.55	0.41
1:F:13:THR:OG1	1:F:14:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:HB2	1:B:87:SER:O	2.21	0.40
1:A:129:LEU:HD23	1:A:129:LEU:C	2.46	0.40
1:E:28:ILE:O	1:E:31:THR:OG1	2.36	0.40
1:A:72:ILE:C	1:A:72:ILE:HD12	2.47	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	211/211 (100%)	206 (98%)	5 (2%)	0	100	100
1	B	207/211 (98%)	201 (97%)	4 (2%)	2 (1%)	12	11
1	C	208/211 (99%)	196 (94%)	10 (5%)	2 (1%)	12	11
1	D	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
1	E	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
1	F	203/211 (96%)	198 (98%)	5 (2%)	0	100	100
All	All	1246/1266 (98%)	1208 (97%)	34 (3%)	4 (0%)	36	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	PHE
1	C	35	ASP
1	C	36	PRO
1	B	205	ARG

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	172/170 (101%)	170 (99%)	2 (1%)	63	75
1	B	167/170 (98%)	166 (99%)	1 (1%)	78	86
1	C	154/170 (91%)	151 (98%)	3 (2%)	50	63
1	D	173/170 (102%)	171 (99%)	2 (1%)	63	75
1	E	169/170 (99%)	166 (98%)	3 (2%)	51	64
1	F	150/170 (88%)	148 (99%)	2 (1%)	61	73
All	All	985/1020 (97%)	972 (99%)	13 (1%)	61	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	132	THR
1	B	115	LEU
1	C	31	THR
1	C	152	ARG
1	C	204	ARG
1	D	1	MSE
1	D	115	LEU
1	E	51	LEU
1	E	109	GLN
1	E	115	LEU
1	F	13	THR
1	F	20	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	ASN
1	A	69	ASN
1	A	160	ASN

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Mol	Chain	Res	Type
1	C	160	ASN
1	D	69	ASN
1	D	160	ASN
1	D	189	HIS
1	E	160	ASN
1	F	189	HIS
1	F	197	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	D	212	-	3,3,3	0.39	0	2,2,2	0.30	0
4	ACY	E	213	2	3,3,3	1.02	0	3,3,3	0.67	0
4	ACY	E	212	-	3,3,3	0.77	0	3,3,3	1.06	0
4	ACY	A	216	-	3,3,3	0.85	0	3,3,3	0.78	0
3	EDO	A	214	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	C	212	-	3,3,3	0.49	0	2,2,2	0.24	0
3	EDO	D	213	-	3,3,3	0.49	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	213	-	3,3,3	0.49	0	2,2,2	0.32	0
3	EDO	F	212	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	A	215	-	3,3,3	0.61	0	2,2,2	0.26	0
4	ACY	F	213	-	3,3,3	0.75	0	3,3,3	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	212	-	-	0/1/1/1	-
3	EDO	A	214	-	-	1/1/1/1	-
3	EDO	C	212	-	-	0/1/1/1	-
3	EDO	D	213	-	-	1/1/1/1	-
3	EDO	A	213	-	-	0/1/1/1	-
3	EDO	F	212	-	-	1/1/1/1	-
3	EDO	A	215	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	213	EDO	O1-C1-C2-O2
3	F	212	EDO	O1-C1-C2-O2
3	A	214	EDO	O1-C1-C2-O2
3	A	215	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	212	ACY	2	0
4	A	216	ACY	1	0
3	A	214	EDO	2	0
3	C	212	EDO	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	203/211 (96%)	1.22	37 (18%) 3 4	26, 57, 67, 82	2 (0%)
1	B	200/211 (94%)	1.26	33 (16%) 4 5	32, 57, 69, 76	2 (1%)
1	C	201/211 (95%)	1.99	91 (45%) 0 0	33, 57, 66, 83	1 (0%)
1	D	202/211 (95%)	1.25	24 (11%) 9 10	36, 57, 71, 90	1 (0%)
1	E	202/211 (95%)	1.14	24 (11%) 9 10	48, 57, 67, 85	0
1	F	197/211 (93%)	2.55	128 (64%) 0 0	30, 57, 64, 85	1 (0%)
All	All	1205/1266 (95%)	1.56	337 (27%) 1 1	26, 57, 69, 90	7 (0%)

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	PHE	7.7
1	D	209	TYR	6.0
1	F	135	TYR	6.0
1	C	148	VAL	5.4
1	F	18	VAL	5.2
1	F	175	ALA	5.1
1	E	44	PRO	5.0
1	F	149	TRP	5.0
1	F	172	PRO	4.8
1	F	22	GLY	4.8
1	D	41	PHE	4.8
1	F	31	THR	4.8
1	F	41	PHE	4.8
1	F	39	THR	4.8
1	C	2	PHE	4.7
1	C	34	LEU	4.7
1	A	16	GLY	4.7
1	F	176	SER	4.7
1	F	174	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	148	VAL	4.5
1	D	143	GLY	4.5
1	F	205	ARG	4.5
1	F	139	TRP	4.5
1	C	149	TRP	4.4
1	F	178	PRO	4.3
1	B	2	PHE	4.3
1	F	167	PHE	4.3
1	A	37	GLY	4.3
1	A	154	ILE	4.2
1	B	83	TYR	4.2
1	F	112	GLY	4.2
1	F	6	PHE	4.2
1	F	171	ASP	4.1
1	F	182	LEU	4.1
1	F	17	PRO	4.1
1	F	137	TRP	4.1
1	C	40	ALA	4.0
1	F	73	GLY	4.0
1	F	103	ALA	3.9
1	F	166	PHE	3.9
1	A	44	PRO	3.9
1	C	209	TYR	3.9
1	F	101	GLU	3.9
1	F	154	ILE	3.9
1	C	194	VAL	3.9
1	F	179	ALA	3.8
1	C	203	LEU	3.8
1	C	169	THR	3.8
1	C	70	ASP	3.8
1	F	170	ASP	3.8
1	C	77	PHE	3.8
1	F	198	PHE	3.8
1	C	193	GLU	3.8
1	F	26	SER	3.8
1	C	136	TYR	3.7
1	F	74	TYR	3.7
1	F	207	PHE	3.7
1	F	62	ILE	3.7
1	F	145	GLY	3.7
1	F	150	ASP	3.7
1	B	86	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	41	PHE	3.6
1	F	30	ALA	3.5
1	C	172	PRO	3.5
1	C	137	TRP	3.5
1	C	73	GLY	3.5
1	B	34	LEU	3.4
1	C	43	GLN	3.4
1	B	179	ALA	3.4
1	A	138[A]	HIS	3.4
1	C	89	GLY	3.4
1	C	170	ASP	3.4
1	F	164	LEU	3.4
1	F	168	PRO	3.4
1	E	0	GLY	3.4
1	F	57	LEU	3.4
1	F	64	ILE	3.4
1	F	89	GLY	3.4
1	C	178	PRO	3.3
1	F	147	SER	3.3
1	B	68	GLY	3.3
1	F	69	ASN	3.3
1	B	206	ARG	3.3
1	F	114	LYS	3.3
1	F	121	LEU	3.3
1	C	206	ARG	3.3
1	F	173	GLU	3.2
1	A	2	PHE	3.2
1	C	135	TYR	3.2
1	F	56	ALA	3.2
1	F	124	ALA	3.2
1	E	145	GLY	3.2
1	F	201	LEU	3.2
1	C	102	VAL	3.2
1	F	16	GLY	3.2
1	F	70	ASP	3.2
1	C	174	ILE	3.2
1	C	39	THR	3.2
1	C	85	THR	3.2
1	C	93	TYR	3.1
1	C	24	VAL	3.1
1	B	203	LEU	3.1
1	C	176	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	144	SER	3.1
1	F	163	GLY	3.1
1	F	50	ALA	3.1
1	F	97	LEU	3.1
1	C	177	HIS	3.1
1	F	177	HIS	3.1
1	B	200	ALA	3.1
1	C	127	HIS	3.0
1	C	138	HIS	3.0
1	F	77	PHE	3.0
1	F	94	ILE	3.0
1	B	69	ASN	3.0
1	C	37	GLY	3.0
1	C	45	ALA	3.0
1	A	194	VAL	3.0
1	F	146	LEU	3.0
1	C	90[A]	ASN	3.0
1	E	41	PHE	3.0
1	C	144	SER	3.0
1	F	14	SER	3.0
1	A	60	GLY	3.0
1	F	104	ALA	2.9
1	F	95	LEU	2.9
1	A	148	VAL	2.9
1	C	74	TYR	2.9
1	C	128	TYR	2.9
1	F	151	TYR	2.9
1	C	106	PHE	2.9
1	D	203	LEU	2.9
1	D	205	ARG	2.9
1	C	69	ASN	2.9
1	C	179	ALA	2.9
1	C	196	ALA	2.9
1	F	61	ARG	2.9
1	F	202	ARG	2.9
1	F	186	ILE	2.9
1	F	85	THR	2.9
1	F	83	TYR	2.9
1	F	136	TYR	2.9
1	C	5	GLN	2.9
1	C	182	LEU	2.9
1	E	40	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	40	ALA	2.9
1	B	149	TRP	2.9
1	F	24	VAL	2.9
1	F	181	CYS	2.9
1	F	169	THR	2.9
1	C	44	PRO	2.8
1	D	44	PRO	2.8
1	F	102	VAL	2.8
1	D	173	GLU	2.8
1	C	31	THR	2.8
1	C	142	LYS	2.8
1	F	206	ARG	2.8
1	C	175	ALA	2.8
1	F	200	ALA	2.8
1	F	88	GLU	2.8
1	C	94	ILE	2.8
1	A	150	ASP	2.8
1	F	165	VAL	2.8
1	B	137	TRP	2.8
1	A	83	TYR	2.8
1	A	62	ILE	2.7
1	A	130	ILE	2.7
1	B	94	ILE	2.7
1	B	174	ILE	2.7
1	E	146	LEU	2.7
1	B	138[A]	HIS	2.7
1	C	64	ILE	2.7
1	C	108	GLY	2.7
1	F	203	LEU	2.7
1	A	39	THR	2.7
1	D	85	THR	2.7
1	C	55	ALA	2.7
1	F	161	HIS	2.7
1	D	3	GLU	2.7
1	C	60	GLY	2.7
1	C	72	ILE	2.7
1	F	111	ILE	2.7
1	A	206	ARG	2.7
1	F	66	ARG	2.7
1	A	129	LEU	2.7
1	C	65	ALA	2.6
1	B	207	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	195	VAL	2.6
1	F	60	GLY	2.6
1	E	205	ARG	2.6
1	F	129	LEU	2.6
1	F	138[A]	HIS	2.6
1	F	86	TRP	2.6
1	B	175	ALA	2.6
1	C	103	ALA	2.6
1	A	136	TYR	2.6
1	A	24	VAL	2.6
1	A	0	GLY	2.6
1	C	62	ILE	2.6
1	F	116	LEU	2.6
1	D	40	ALA	2.6
1	A	41	PHE	2.6
1	C	190	VAL	2.6
1	F	51	LEU	2.6
1	B	65	ALA	2.6
1	E	179	ALA	2.6
1	D	2	PHE	2.6
1	A	174	ILE	2.6
1	F	115	LEU	2.5
1	A	210	ASP	2.5
1	F	133	THR	2.5
1	D	148	VAL	2.5
1	F	54	ILE	2.5
1	F	100	ILE	2.5
1	C	110	GLN	2.5
1	F	87	SER	2.5
1	B	40	ALA	2.5
1	D	200	ALA	2.5
1	C	112	GLY	2.5
1	D	36	PRO	2.5
1	C	38	LEU	2.5
1	F	34	LEU	2.5
1	D	89	GLY	2.5
1	F	43	GLN	2.5
1	E	206	ARG	2.4
1	C	167	PHE	2.4
1	E	2	PHE	2.4
1	A	149	TRP	2.4
1	E	38	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	123	PRO	2.4
1	C	191	ALA	2.4
1	C	204	ARG	2.4
1	F	106	PHE	2.4
1	B	33	LYS	2.4
1	B	79	TYR	2.4
1	C	205	ARG	2.4
1	D	73	GLY	2.4
1	F	99	ALA	2.4
1	F	196	ALA	2.4
1	B	148	VAL	2.4
1	B	165	VAL	2.4
1	B	194	VAL	2.4
1	E	64	ILE	2.4
1	C	141	LEU	2.4
1	C	79	TYR	2.4
1	B	44	PRO	2.4
1	F	184	ALA	2.4
1	F	188	LYS	2.4
1	C	71	ILE	2.4
1	F	128	TYR	2.3
1	A	192	PRO	2.3
1	C	165	VAL	2.3
1	E	18	VAL	2.3
1	C	3	GLU	2.3
1	C	173	GLU	2.3
1	C	23	PRO	2.3
1	F	143	GLY	2.3
1	C	99	ALA	2.3
1	F	204	ARG	2.3
1	C	161	HIS	2.3
1	E	154	ILE	2.3
1	C	166	PHE	2.3
1	C	195	VAL	2.3
1	D	179	ALA	2.3
1	C	147	SER	2.3
1	B	75	VAL	2.3
1	C	15	LEU	2.3
1	E	203	LEU	2.3
1	F	15	LEU	2.3
1	D	0	GLY	2.3
1	D	144	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	34	LEU	2.2
1	F	75	VAL	2.3
1	F	82	PRO	2.2
1	E	37	GLY	2.2
1	F	152	ARG	2.2
1	A	191	ALA	2.2
1	C	101	GLU	2.2
1	F	32	TYR	2.2
1	A	137	TRP	2.2
1	F	63	ILE	2.2
1	C	201	LEU	2.2
1	F	38	LEU	2.2
1	F	141	LEU	2.2
1	E	178	PRO	2.2
1	A	176	SER	2.2
1	E	209	TYR	2.2
1	C	171	ASP	2.2
1	C	202	ARG	2.2
1	B	3	GLU	2.2
1	A	85	THR	2.2
1	F	13	THR	2.2
1	B	205	ARG	2.2
1	F	195	VAL	2.2
1	F	23	PRO	2.2
1	F	33	LYS	2.2
1	F	53	GLU	2.2
1	B	32	TYR	2.1
1	E	94	ILE	2.1
1	F	194	VAL	2.1
1	A	177	HIS	2.1
1	D	161	HIS	2.1
1	F	162	GLY	2.1
1	E	103	ALA	2.1
1	F	45	ALA	2.1
1	D	28	ILE	2.1
1	A	36	PRO	2.1
1	B	178	PRO	2.1
1	F	118	VAL	2.1
1	C	25	THR	2.1
1	D	42	ARG	2.1
1	A	45	ALA	2.1
1	C	29	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	193	GLU	2.1
1	A	32	TYR	2.1
1	F	180	ASN	2.1
1	C	33	LYS	2.1
1	F	117	GLU	2.1
1	B	78	LEU	2.1
1	D	174	ILE	2.1
1	C	192	PRO	2.1
1	C	52	VAL	2.1
1	F	190	VAL	2.1
1	B	16	GLY	2.1
1	F	42	ARG	2.1
1	F	5	GLN	2.0
1	E	35	ASP	2.0
1	C	168	PRO	2.0
1	A	165	VAL	2.0
1	A	190	VAL	2.0
1	E	148	VAL	2.0
1	A	68	GLY	2.0
1	F	187	GLY	2.0
1	A	81	ASP	2.0
1	E	141	LEU	2.0
1	C	42	ARG	2.0
1	C	154	ILE	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	EDO	A	213	4/4	0.72	0.22	82,83,83,83	0
4	ACY	F	213	4/4	0.73	0.27	88,88,88,89	0
4	ACY	E	213	4/4	0.80	0.24	56,56,57,58	0
3	EDO	A	214	4/4	0.83	0.17	76,79,80,81	0
3	EDO	F	212	4/4	0.85	0.17	69,71,73,75	0
4	ACY	A	216	4/4	0.85	0.22	79,79,80,80	0
3	EDO	D	213	4/4	0.87	0.21	44,45,49,53	0
3	EDO	C	212	4/4	0.88	0.22	62,65,67,68	0
4	ACY	E	212	4/4	0.91	0.25	48,49,49,50	0
3	EDO	A	215	4/4	0.93	0.17	38,48,48,55	0
3	EDO	D	212	4/4	0.93	0.19	37,40,43,48	0
2	CA	F	211	1/1	0.95	0.09	68,68,68,68	0
2	CA	C	211	1/1	0.95	0.10	73,73,73,73	0
2	CA	E	211	1/1	0.96	0.06	51,51,51,51	0
2	CA	D	211	1/1	0.98	0.10	39,39,39,39	0
2	CA	A	211	1/1	0.99	0.11	48,48,48,48	0
2	CA	A	212	1/1	0.99	0.09	68,68,68,68	0
2	CA	B	211	1/1	0.99	0.11	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.