



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:57 AM UTC

PDB ID : 3SOT / pdb_00003sot
Title : Crystal structure of a Multidomain protein including DUF1735 (BA-COVA_03322) from Bacteroides ovatus at 2.80 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2011-06-30
Resolution : 2.80 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:

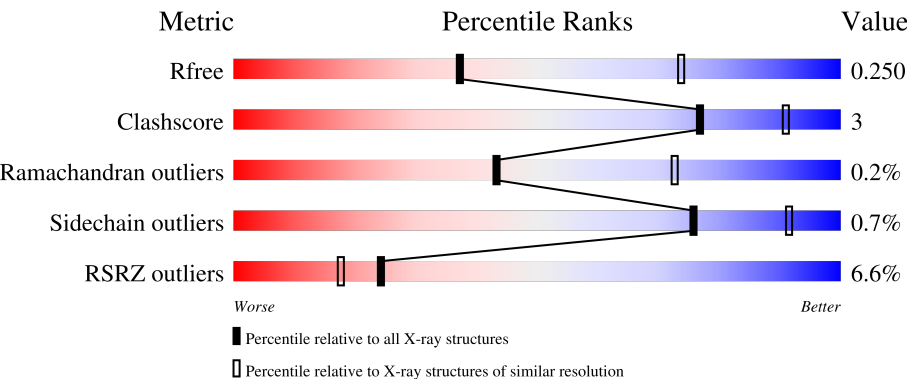
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	319	5% 85%8%7%
1	B	319	3% 82%9%9%
1	C	319	5% 79%11%8%
1	D	319	8% 83%10%7%
1	E	319	9% 80%12%7%

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Mol	Chain	Length	Quality of chain
1	F	319	5% 70% 9% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13888 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 Multidomain protein including DUF1735.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	Se	0	2	0
			2388	1521	380	475	1	11			
1	B	291	Total	C	N	O	S	Se	0	1	0
			2329	1483	372	462	1	11			
1	C	293	Total	C	N	O	S	Se	0	1	0
			2324	1483	371	458	1	11			
1	D	298	Total	C	N	O	S	Se	0	1	0
			2374	1513	377	472	1	11			
1	E	296	Total	C	N	O	S	Se	0	1	0
			2313	1477	368	456	1	11			
1	F	255	Total	C	N	O	Se		0	2	0
			2007	1274	323	399	11				

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A7LZP6
B	0	GLY	-	expression tag	UNP A7LZP6
C	0	GLY	-	expression tag	UNP A7LZP6
D	0	GLY	-	expression tag	UNP A7LZP6
E	0	GLY	-	expression tag	UNP A7LZP6
F	0	GLY	-	expression tag	UNP A7LZP6

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



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

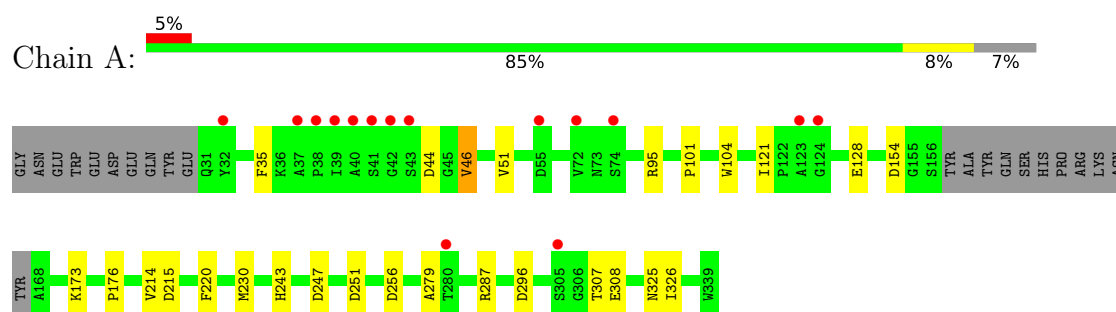
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	38	Total	O	0	0
			38	38		
3	C	36	Total	O	0	0
			36	36		
3	D	16	Total	O	0	0
			16	16		
3	E	8	Total	O	0	0
			8	8		
3	F	1	Total	O	0	0
			1	1		

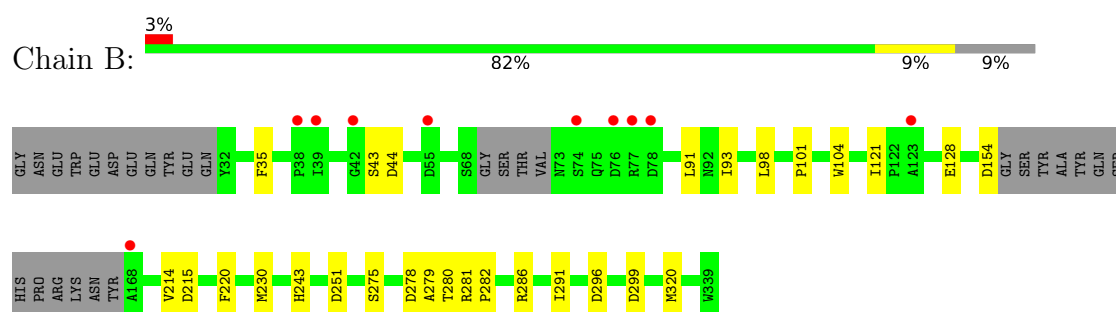
3 Residue-property plots [i](#)

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.

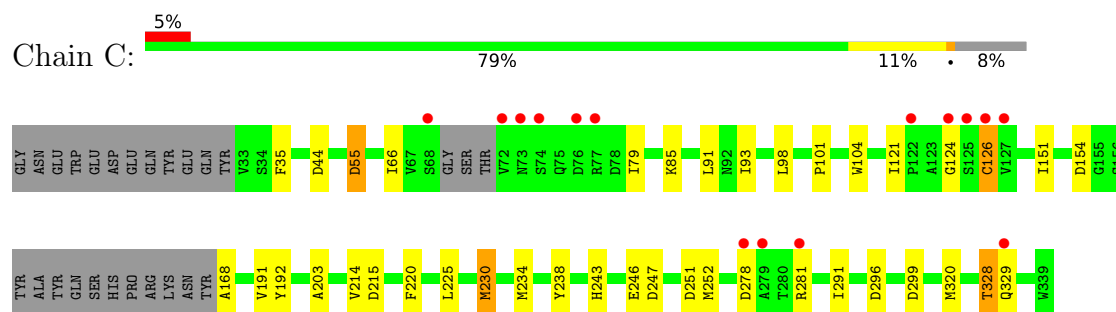
- Molecule 1: Multidomain protein including DUF1735



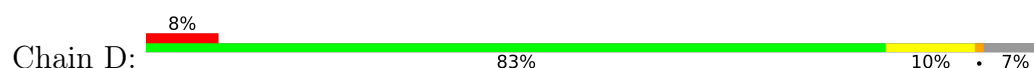
- Molecule 1: Multidomain protein including DUF1735

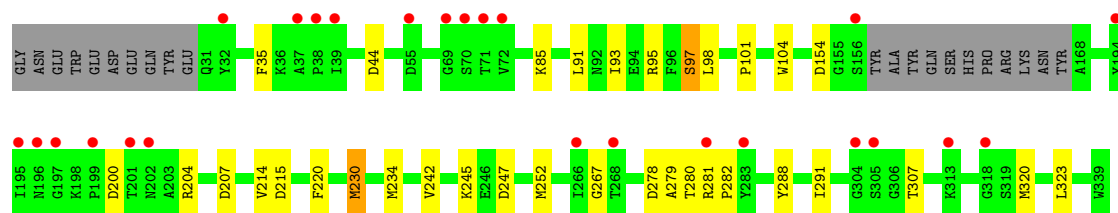


- Molecule 1: Multidomain protein including DUF1735

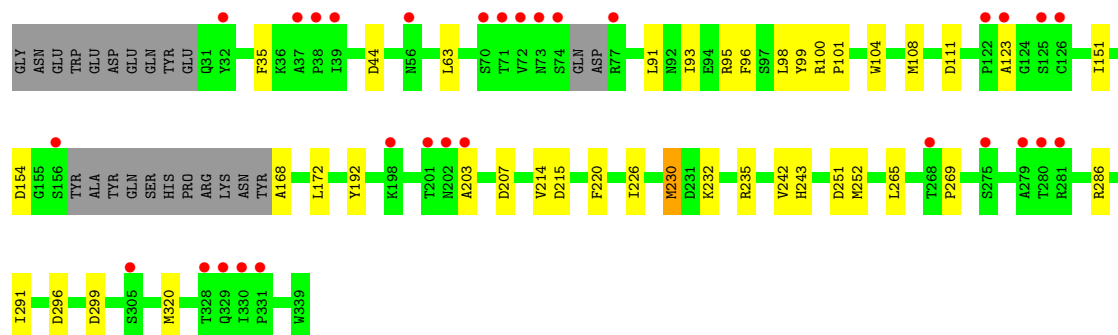
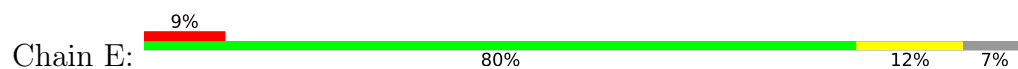


- Molecule 1: Multidomain protein including DUF1735

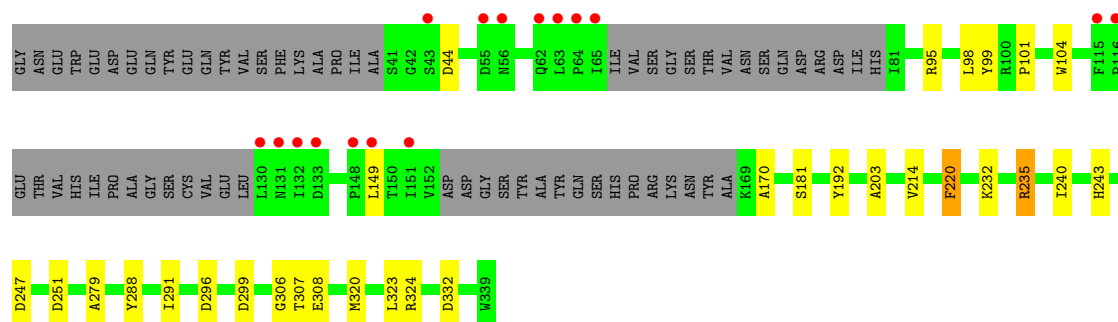




● Molecule 1: Multidomain protein including DUF1735



● Molecule 1: Multidomain protein including DUF1735



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.47Å 123.34Å 189.52Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	29.97 – 2.80 29.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.97-2.80) 98.6 (29.97-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.80Å)	Xtriage
Refinement program	BUSTER-TNT 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.203 , 0.229 0.224 , 0.250	Depositor DCC
R_{free} test set	2460 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13888	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 20.71 % 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 8.2011e-03. 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: EDO

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	0.87	1/2434 (0.0%)	1.18	12/3287 (0.4%)
1	B	0.88	1/2371 (0.0%)	1.15	9/3202 (0.3%)
1	C	0.95	5/2366 (0.2%)	1.20	16/3196 (0.5%)
1	D	0.85	1/2418 (0.0%)	1.16	12/3267 (0.4%)
1	E	0.86	1/2354 (0.0%)	1.15	11/3183 (0.3%)
1	F	0.84	0/2046	1.20	11/2761 (0.4%)
All	All	0.88	9/13989 (0.1%)	1.17	71/18896 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	230	MSE	SE-CE	-13.38	1.55	1.95
1	B	230	MSE	SE-CE	-10.80	1.63	1.95
1	D	230	MSE	SE-CE	-9.05	1.68	1.95
1	E	230	MSE	SE-CE	-8.76	1.69	1.95
1	A	230	MSE	SE-CE	-8.21	1.70	1.95
1	C	328	THR	CA-C	5.49	1.60	1.52
1	C	126	CYS	CA-C	5.47	1.60	1.52
1	C	329	GLN	C-N	5.43	1.38	1.33
1	C	252	MSE	SE-CE	-5.11	1.80	1.95

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	VAL	N-CA-C	-6.94	105.59	111.56
1	E	111	ASP	CA-CB-CG	6.91	119.50	112.60
1	C	214	VAL	N-CA-C	-6.64	105.85	111.56
1	C	296	ASP	CA-CB-CG	6.59	119.19	112.60
1	E	214	VAL	N-CA-C	-6.50	105.97	111.56
1	D	214	VAL	N-CA-C	-6.46	106.01	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	VAL	N-CA-C	-6.42	106.04	111.56
1	F	296	ASP	CA-CB-CG	6.42	119.02	112.60
1	F	214	VAL	N-CA-C	-6.41	105.45	111.48
1	F	279	ALA	CA-C-N	6.33	129.01	120.65
1	F	279	ALA	C-N-CA	6.33	129.01	120.65
1	D	200	ASP	CA-CB-CG	6.32	118.92	112.60
1	D	245	LYS	CA-C-N	6.14	128.51	120.28
1	D	245	LYS	C-N-CA	6.14	128.51	120.28
1	A	279	ALA	CA-C-N	6.14	128.76	120.65
1	A	279	ALA	C-N-CA	6.14	128.76	120.65
1	A	307	THR	CA-C-N	6.10	129.49	120.95
1	A	307	THR	C-N-CA	6.10	129.49	120.95
1	B	35	PHE	CA-CB-CG	6.04	119.84	113.80
1	B	299	ASP	CA-CB-CG	5.94	118.54	112.60
1	C	124	GLY	CA-C-N	5.93	128.15	120.44
1	C	124	GLY	C-N-CA	5.93	128.15	120.44
1	D	154	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	279	ALA	CA-C-N	5.87	128.40	120.65
1	B	279	ALA	C-N-CA	5.87	128.40	120.65
1	C	35	PHE	CA-CB-CG	5.86	119.66	113.80
1	C	234[A]	MSE	CA-C-N	5.85	128.12	120.28
1	C	234[A]	MSE	C-N-CA	5.85	128.12	120.28
1	C	234[B]	MSE	CA-C-N	5.85	128.12	120.28
1	C	234[B]	MSE	C-N-CA	5.85	128.12	120.28
1	B	154	ASP	CA-CB-CG	5.83	118.43	112.60
1	E	296	ASP	CA-CB-CG	5.83	118.42	112.60
1	B	296	ASP	CA-CB-CG	5.82	118.42	112.60
1	F	220	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	154	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	220	PHE	CA-CB-CG	5.67	119.47	113.80
1	D	207	ASP	CA-CB-CG	5.66	118.26	112.60
1	E	35	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	220	PHE	CA-CB-CG	5.64	119.44	113.80
1	E	154	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	296	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	220	PHE	CA-CB-CG	5.59	119.39	113.80
1	D	279	ALA	CA-C-N	5.59	128.03	120.65
1	D	279	ALA	C-N-CA	5.59	128.03	120.65
1	A	35	PHE	CA-CB-CG	5.58	119.38	113.80
1	C	220	PHE	CA-CB-CG	5.54	119.34	113.80
1	E	220	PHE	CA-CB-CG	5.47	119.27	113.80
1	E	207	ASP	CA-CB-CG	5.46	118.06	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	299	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	215	ASP	CA-CB-CG	5.43	118.03	112.60
1	F	299	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	154	ASP	CA-CB-CG	5.41	118.01	112.60
1	D	35	PHE	CA-CB-CG	5.35	119.15	113.80
1	D	215	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	215	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	247	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	247	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	256	ASP	CA-CB-CG	5.28	117.88	112.60
1	E	215	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	215	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	299	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	247	ASP	CA-CB-CG	5.08	117.68	112.60
1	F	332	ASP	CA-C-N	5.07	127.79	120.38
1	F	332	ASP	C-N-CA	5.07	127.79	120.38
1	F	247	ASP	CA-CB-CG	5.07	117.67	112.60
1	F	306	GLY	CA-C-N	5.07	129.32	121.26
1	F	306	GLY	C-N-CA	5.07	129.32	121.26
1	E	108	MSE	CA-C-N	5.04	127.93	120.82
1	E	108	MSE	C-N-CA	5.04	127.93	120.82
1	C	85	LYS	CA-C-N	5.02	127.01	120.28
1	C	85	LYS	C-N-CA	5.02	127.01	120.28

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	2388	0	2272	9	0
1	B	2329	0	2212	11	0
1	C	2324	0	2196	14	0
1	D	2374	0	2262	15	0
1	E	2313	0	2168	19	0
1	F	2007	0	1824	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	8	0	12	0	0
3	A	38	0	0	0	0
3	B	38	0	0	1	0
3	C	36	0	0	2	0
3	D	16	0	0	2	0
3	E	8	0	0	0	0
3	F	1	0	0	0	0
All	All	13888	0	12958	77	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 3.

All (77) 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:E:226:ILE:HG23	1:E:230:MSE:HE2	1.64	0.79
1:D:44:ASP:HB2	1:D:91:LEU:HD11	1.73	0.71
1:E:230:MSE:HE3	1:E:235:ARG:HA	1.72	0.71
1:A:287:ARG:HH11	1:A:326:ILE:HG13	1.69	0.58
1:D:101:PRO:HA	1:D:104:TRP:CD1	2.41	0.56
1:D:204:ARG:HA	3:D:444:HOH:O	2.07	0.54
1:C:328:THR:HA	3:C:469:HOH:O	2.08	0.54
1:E:93:ILE:HD12	1:E:98:LEU:HG	1.91	0.53
1:D:230:MSE:HE3	1:D:234[B]:MSE:HB3	1.89	0.53
1:D:93:ILE:HD12	1:D:98:LEU:HG	1.90	0.53
1:D:267:GLY:HA3	3:D:445:HOH:O	2.09	0.53
1:E:230:MSE:HG3	1:E:235:ARG:HB3	1.90	0.52
1:B:291:ILE:HD11	1:B:320:MSE:HE3	1.91	0.52
1:B:93:ILE:HD12	1:B:98:LEU:HG	1.91	0.52
1:D:291:ILE:HD11	1:D:320:MSE:HE3	1.91	0.51
1:F:291:ILE:HD11	1:F:320:MSE:HE3	1.91	0.51
1:A:308:GLU:CD	1:B:286:ARG:HH12	2.20	0.50
1:E:242:VAL:HG22	1:E:252:MSE:HG2	1.93	0.50
1:E:286:ARG:HH12	1:F:308:GLU:CD	2.21	0.49
1:C:291:ILE:HD11	1:C:320:MSE:HE3	1.94	0.49
1:D:242:VAL:HG22	1:D:252:MSE:HG2	1.94	0.49
1:F:149:LEU:HB2	1:F:170:ALA:HB3	1.95	0.48
1:D:278:ASP:HB3	1:D:281:ARG:O	2.14	0.48
1:C:278:ASP:HB3	1:C:281:ARG:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:ILE:HD11	1:E:320:MSE:HE3	1.96	0.48
1:D:230:MSE:CE	1:D:234[B]:MSE:HB3	2.43	0.48
1:B:43:SER:HB3	3:B:347:HOH:O	2.13	0.47
1:C:230:MSE:HE1	1:C:238:TYR:CE2	2.49	0.47
1:C:55:ASP:HA	3:C:412:HOH:O	2.14	0.47
1:E:95:ARG:HD2	1:F:99:TYR:HB3	1.97	0.47
1:B:44:ASP:HB2	1:B:91:LEU:HD11	1.96	0.47
1:B:98:LEU:H	1:B:98:LEU:HD12	1.80	0.47
1:C:44:ASP:HB2	1:C:91:LEU:HD11	1.97	0.47
1:C:79:ILE:HD12	1:C:121:ILE:HD12	1.97	0.46
1:B:278:ASP:HB3	1:B:281:ARG:O	2.15	0.46
1:E:44:ASP:HB2	1:E:91:LEU:HD11	1.98	0.46
1:D:98:LEU:HD12	1:D:98:LEU:H	1.80	0.45
1:F:98:LEU:H	1:F:98:LEU:HD12	1.80	0.45
1:D:93:ILE:O	1:D:97:SER:HA	2.17	0.45
1:C:151:ILE:HD12	1:C:168:ALA:HB3	1.99	0.45
1:A:287:ARG:NH1	1:A:326:ILE:HG13	2.31	0.45
1:C:93:ILE:HD12	1:C:98:LEU:HG	1.99	0.45
1:F:44:ASP:HB3	1:F:95:ARG:HH11	1.82	0.44
1:F:288:TYR:CE1	1:F:323:LEU:HD13	2.52	0.44
1:C:98:LEU:H	1:C:98:LEU:HD12	1.82	0.44
1:B:121:ILE:HG12	1:B:128:GLU:HB2	1.98	0.44
1:F:243:HIS:HB3	1:F:251:ASP:HB2	2.00	0.43
1:B:101:PRO:HA	1:B:104:TRP:CD1	2.53	0.43
1:E:63:LEU:HD22	1:E:172:LEU:HD11	2.01	0.43
1:A:46:VAL:HG13	1:A:173:LYS:HB2	2.00	0.43
1:C:243:HIS:HB3	1:C:251:ASP:HB2	2.00	0.43
1:F:181:SER:O	1:F:324:ARG:NH2	2.52	0.43
1:A:101:PRO:HA	1:A:104:TRP:CD1	2.54	0.43
1:A:121:ILE:HG12	1:A:128:GLU:HB2	2.01	0.42
1:E:232:LYS:HA	1:E:235:ARG:HG2	2.01	0.42
1:E:243:HIS:HB3	1:E:251:ASP:HB2	2.02	0.42
1:F:101:PRO:HA	1:F:104:TRP:CD1	2.54	0.42
1:E:101:PRO:HA	1:E:104:TRP:CD1	2.55	0.42
1:A:243:HIS:HB3	1:A:251:ASP:HB2	2.00	0.42
1:E:96:PHE:HA	1:E:100:ARG:HH21	1.83	0.42
1:E:98:LEU:HD12	1:E:98:LEU:H	1.85	0.42
1:F:232:LYS:HA	1:F:235:ARG:HG2	2.00	0.42
1:B:280:THR:O	1:B:282:PRO:HD3	2.20	0.42
1:F:192:TYR:CE1	1:F:203:ALA:HB2	2.55	0.42
1:A:51:VAL:O	1:A:176:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:VAL:HG21	1:C:225:LEU:HG	2.02	0.41
1:D:95:ARG:HD2	1:E:99:TYR:HB3	2.03	0.41
1:D:280:THR:O	1:D:282:PRO:HD3	2.21	0.41
1:E:192:TYR:CE1	1:E:203:ALA:HB2	2.54	0.41
1:C:192:TYR:CE1	1:C:203:ALA:HB2	2.56	0.41
1:E:265:LEU:HD11	1:E:269:PRO:HG3	2.03	0.40
1:D:288:TYR:CE2	1:D:323:LEU:HD13	2.56	0.40
1:E:151:ILE:HD12	1:E:168:ALA:HB3	2.04	0.40
1:B:243:HIS:HB3	1:B:251:ASP:HB2	2.03	0.40
1:F:220:PHE:HA	1:F:240:ILE:O	2.22	0.40
1:A:44:ASP:HB3	1:A:95:ARG:CD	2.51	0.40
1:C:101:PRO:HA	1:C:104:TRP:CD1	2.57	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	296/319 (93%)	288 (97%)	8 (3%)	0	100	100
1	B	286/319 (90%)	277 (97%)	9 (3%)	0	100	100
1	C	288/319 (90%)	274 (95%)	13 (4%)	1 (0%)	36	66
1	D	295/319 (92%)	286 (97%)	8 (3%)	1 (0%)	36	66
1	E	291/319 (91%)	279 (96%)	11 (4%)	1 (0%)	36	66
1	F	249/319 (78%)	241 (97%)	8 (3%)	0	100	100
All	All	1705/1914 (89%)	1645 (96%)	57 (3%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	123	ALA

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Mol	Chain	Res	Type
1	D	97	SER
1	C	126	CYS

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	259/280 (92%)	257 (99%)	2 (1%)	73	90
1	B	253/280 (90%)	252 (100%)	1 (0%)	84	94
1	C	248/280 (89%)	245 (99%)	3 (1%)	63	87
1	D	259/280 (92%)	257 (99%)	2 (1%)	73	90
1	E	243/280 (87%)	243 (100%)	0	100	100
1	F	205/280 (73%)	203 (99%)	2 (1%)	68	88
All	All	1467/1680 (87%)	1457 (99%)	10 (1%)	76	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	VAL
1	A	325	ASN
1	B	275	SER
1	C	55	ASP
1	C	66	ILE
1	C	246	GLU
1	D	85	LYS
1	D	307	THR
1	F	235	ARG
1	F	307	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN

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Mol	Chain	Res	Type
1	A	325	ASN
1	B	135	ASN
1	C	135	ASN
1	D	62	GLN
1	D	73	ASN
1	D	202	ASN
1	D	325	ASN
1	D	336	GLN
1	E	62	GLN
1	F	135	ASN
1	F	329	GLN

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](#)

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	EDO	B	341	-	3,3,3	0.51	0	2,2,2	0.16	0
2	EDO	C	343	-	3,3,3	0.46	0	2,2,2	0.43	0
2	EDO	C	342	-	3,3,3	0.55	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	340	-	3,3,3	0.49	0	2,2,2	0.20	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	EDO	B	341	-	-	0/1/1/1	-
2	EDO	C	343	-	-	0/1/1/1	-
2	EDO	C	342	-	-	0/1/1/1	-
2	EDO	A	340	-	-	0/1/1/1	-

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.

No monomer is involved in short contacts.

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	288/319 (90%)	0.07	15 (5%)	33	25	9, 33, 94, 116	1 (0%)
1	B	281/319 (88%)	-0.08	10 (3%)	46	37	8, 27, 67, 98	0
1	C	283/319 (88%)	0.16	15 (5%)	32	24	10, 32, 73, 131	0
1	D	288/319 (90%)	0.43	25 (8%)	16	11	14, 47, 93, 112	0
1	E	286/319 (89%)	0.59	30 (10%)	11	8	25, 53, 89, 122	0
1	F	245/319 (76%)	0.55	16 (6%)	25	18	29, 56, 95, 118	1 (0%)
All	All	1671/1914 (87%)	0.28	111 (6%)	24	18	8, 41, 90, 131	2 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	73	ASN	5.6
1	C	76	ASP	5.5
1	F	131	ASN	4.8
1	D	201	THR	4.6
1	A	38	PRO	4.5
1	B	76	ASP	4.4
1	D	32	TYR	4.4
1	E	329	GLN	4.0
1	A	305	SER	4.0
1	C	72	VAL	3.8
1	D	283	TYR	3.8
1	D	195	ILE	3.8
1	F	116	PRO	3.7
1	A	32	TYR	3.7
1	E	70	SER	3.6
1	A	39	ILE	3.5
1	C	329	GLN	3.4
1	D	55	ASP	3.4
1	F	56	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	74	SER	3.4
1	A	37	ALA	3.4
1	E	202	ASN	3.3
1	E	305	SER	3.3
1	A	74	SER	3.2
1	B	78	ASP	3.2
1	C	279	ALA	3.2
1	E	279	ALA	3.2
1	A	41	SER	3.1
1	E	123	ALA	3.0
1	D	194	TYR	3.0
1	C	125	SER	3.0
1	A	72	VAL	3.0
1	D	199	PRO	3.0
1	E	156	SER	3.0
1	B	168	ALA	3.0
1	C	127	VAL	3.0
1	A	42	GLY	2.9
1	D	196	ASN	2.9
1	D	197	GLY	2.9
1	B	39	ILE	2.9
1	E	268	THR	2.9
1	F	65	ILE	2.8
1	F	130	LEU	2.8
1	E	280	THR	2.8
1	E	125	SER	2.8
1	F	63	LEU	2.7
1	D	202	ASN	2.7
1	D	71	THR	2.7
1	C	126	CYS	2.7
1	E	56	ASN	2.7
1	B	123	ALA	2.7
1	C	74	SER	2.7
1	E	126	CYS	2.6
1	B	38	PRO	2.6
1	E	71	THR	2.6
1	A	55	ASP	2.6
1	E	72	VAL	2.6
1	D	72	VAL	2.6
1	E	201	THR	2.6
1	F	133	ASP	2.6
1	D	39	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	73	ASN	2.5
1	B	74	SER	2.5
1	F	55	ASP	2.5
1	F	149	LEU	2.5
1	D	268	THR	2.5
1	B	77	ARG	2.5
1	D	281	ARG	2.5
1	C	124	GLY	2.5
1	E	281	ARG	2.5
1	E	203	ALA	2.4
1	A	43	SER	2.4
1	D	70	SER	2.4
1	E	38	PRO	2.4
1	E	37	ALA	2.4
1	E	32	TYR	2.3
1	E	331	PRO	2.3
1	C	281	ARG	2.3
1	D	69	GLY	2.3
1	B	42	GLY	2.3
1	D	156	SER	2.3
1	D	38	PRO	2.3
1	A	280	THR	2.3
1	C	122	PRO	2.3
1	C	68	SER	2.2
1	F	151	ILE	2.2
1	F	64	PRO	2.2
1	A	40	ALA	2.2
1	D	37	ALA	2.2
1	E	198	LYS	2.2
1	F	62	GLN	2.2
1	D	313	LYS	2.2
1	E	39	ILE	2.2
1	F	43	SER	2.2
1	F	115	PHE	2.1
1	E	77	ARG	2.1
1	F	132	ILE	2.1
1	B	55	ASP	2.1
1	C	278	ASP	2.1
1	D	304	GLY	2.1
1	D	318	GLY	2.1
1	D	266	ILE	2.1
1	E	328	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	305	SER	2.0
1	E	275	SER	2.0
1	E	122	PRO	2.0
1	F	148	PRO	2.0
1	A	124	GLY	2.0
1	E	330	ILE	2.0
1	C	77	ARG	2.0
1	A	123	ALA	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	EDO	A	340	4/4	0.85	0.15	45,46,47,50	0
2	EDO	C	343	4/4	0.86	0.09	47,47,49,55	0
2	EDO	C	342	4/4	0.87	0.10	41,43,44,45	0
2	EDO	B	341	4/4	0.91	0.16	34,35,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.