



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:36 PM UTC

PDB ID : 7WU1 / pdb_00007wu1
Title : Crystal structure of phospholipase D from Moritella sp. JT01
Authors : Wang, Y.H.; Mao, X.J.; Wang, J.; Wang, F.H.
Deposited on : 2022-02-05
Resolution : 2.30 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

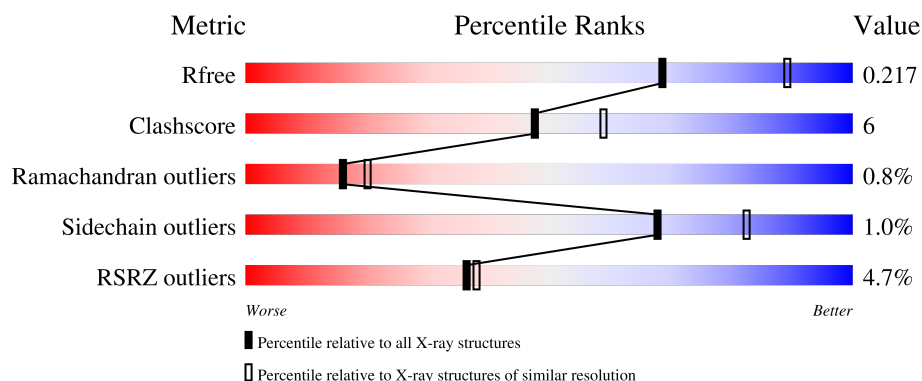
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	557	3% 89% 7% ..
1	B	557	6% 87% 9% ..
1	C	557	6% 88% 7% ..
1	D	557	5% 85% 11% ..
1	E	557	3% 89% 8% .

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Mol	Chain	Length	Quality of chain
1	F	557	 A horizontal bar chart showing the quality of chain 1. The bar is green, indicating a high quality. The chart is labeled with '5%' at the start, '87%' in the middle, and '10%' at the end. There are two small black dots at the end of the bar.

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
3	NA	B	605	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51186 atoms, of which 24695 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 Phospholipase D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	538	Total	C	H	N	O	S	0	0	0
			8294	2661	4085	703	831	14			
1	B	542	Total	C	H	N	O	S	0	0	0
			8351	2679	4113	707	837	15			
1	C	542	Total	C	H	N	O	S	0	0	0
			8354	2682	4111	708	838	15			
1	D	542	Total	C	H	N	O	S	0	0	0
			8346	2677	4108	708	838	15			
1	E	545	Total	C	H	N	O	S	0	0	0
			8395	2694	4133	711	842	15			
1	F	545	Total	C	H	N	O	S	0	0	0
			8395	2694	4133	711	842	15			

There are 42 discrepancies between the modelled and reference sequences:

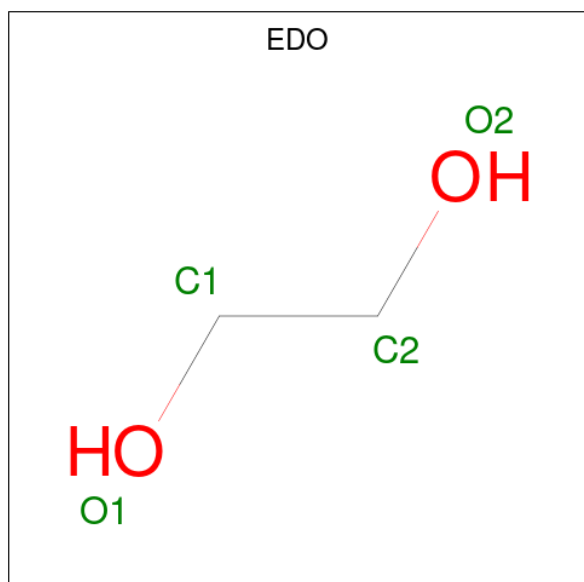
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A0A137SLD1
A	2	HIS	-	expression tag	UNP A0A137SLD1
A	3	HIS	-	expression tag	UNP A0A137SLD1
A	4	HIS	-	expression tag	UNP A0A137SLD1
A	5	HIS	-	expression tag	UNP A0A137SLD1
A	6	HIS	-	expression tag	UNP A0A137SLD1
A	7	HIS	-	expression tag	UNP A0A137SLD1
B	1	MET	-	expression tag	UNP A0A137SLD1
B	2	HIS	-	expression tag	UNP A0A137SLD1
B	3	HIS	-	expression tag	UNP A0A137SLD1
B	4	HIS	-	expression tag	UNP A0A137SLD1
B	5	HIS	-	expression tag	UNP A0A137SLD1
B	6	HIS	-	expression tag	UNP A0A137SLD1
B	7	HIS	-	expression tag	UNP A0A137SLD1
C	1	MET	-	expression tag	UNP A0A137SLD1
C	2	HIS	-	expression tag	UNP A0A137SLD1
C	3	HIS	-	expression tag	UNP A0A137SLD1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	HIS	-	expression tag	UNP A0A137SLD1
C	5	HIS	-	expression tag	UNP A0A137SLD1
C	6	HIS	-	expression tag	UNP A0A137SLD1
C	7	HIS	-	expression tag	UNP A0A137SLD1
D	1	MET	-	expression tag	UNP A0A137SLD1
D	2	HIS	-	expression tag	UNP A0A137SLD1
D	3	HIS	-	expression tag	UNP A0A137SLD1
D	4	HIS	-	expression tag	UNP A0A137SLD1
D	5	HIS	-	expression tag	UNP A0A137SLD1
D	6	HIS	-	expression tag	UNP A0A137SLD1
D	7	HIS	-	expression tag	UNP A0A137SLD1
E	1	MET	-	expression tag	UNP A0A137SLD1
E	2	HIS	-	expression tag	UNP A0A137SLD1
E	3	HIS	-	expression tag	UNP A0A137SLD1
E	4	HIS	-	expression tag	UNP A0A137SLD1
E	5	HIS	-	expression tag	UNP A0A137SLD1
E	6	HIS	-	expression tag	UNP A0A137SLD1
E	7	HIS	-	expression tag	UNP A0A137SLD1
F	1	MET	-	expression tag	UNP A0A137SLD1
F	2	HIS	-	expression tag	UNP A0A137SLD1
F	3	HIS	-	expression tag	UNP A0A137SLD1
F	4	HIS	-	expression tag	UNP A0A137SLD1
F	5	HIS	-	expression tag	UNP A0A137SLD1
F	6	HIS	-	expression tag	UNP A0A137SLD1
F	7	HIS	-	expression tag	UNP A0A137SLD1

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	Na	0	0
			9	9		
3	B	10	Total	Na	0	0
			10	10		
3	C	11	Total	Na	0	0
			11	11		
3	D	8	Total	Na	0	0
			8	8		
3	E	3	Total	Na	0	0
			3	3		
3	F	6	Total	Na	0	0
			6	6		

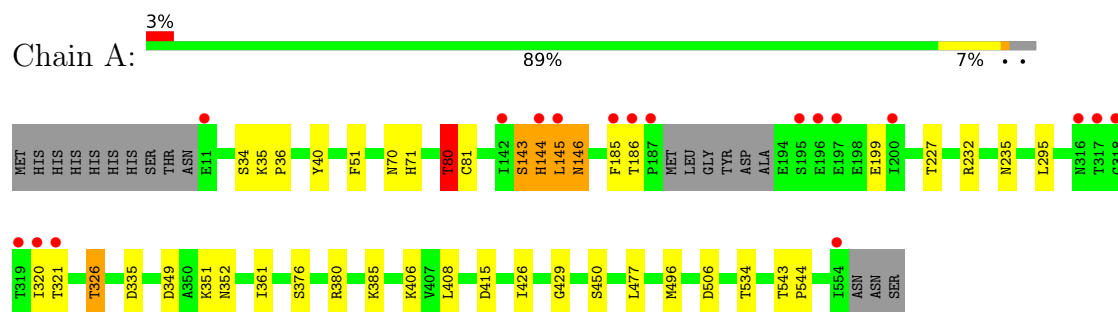
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total	O	0	0
			256	256		
4	B	146	Total	O	0	0
			146	146		
4	C	198	Total	O	0	0
			198	198		
4	D	144	Total	O	0	0
			144	144		
4	E	146	Total	O	0	0
			146	146		
4	F	94	Total	O	0	0
			94	94		

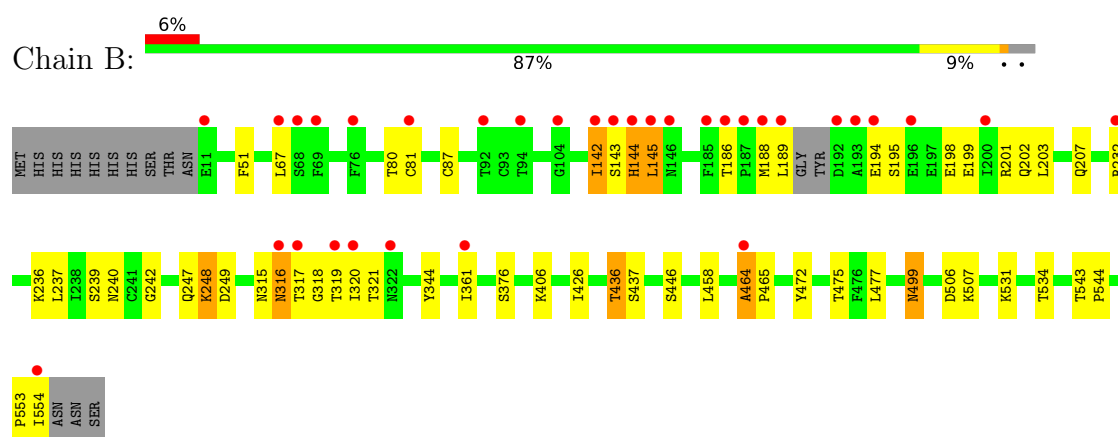
3 Residue-property plots [i](#)

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.

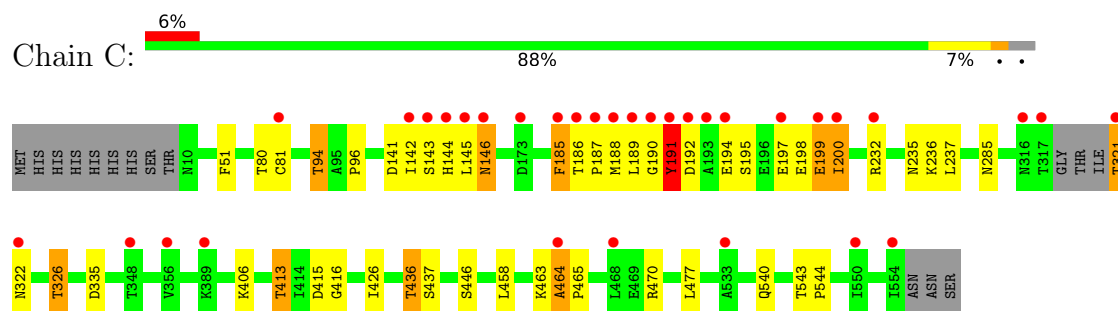
• Molecule 1: Phospholipase D



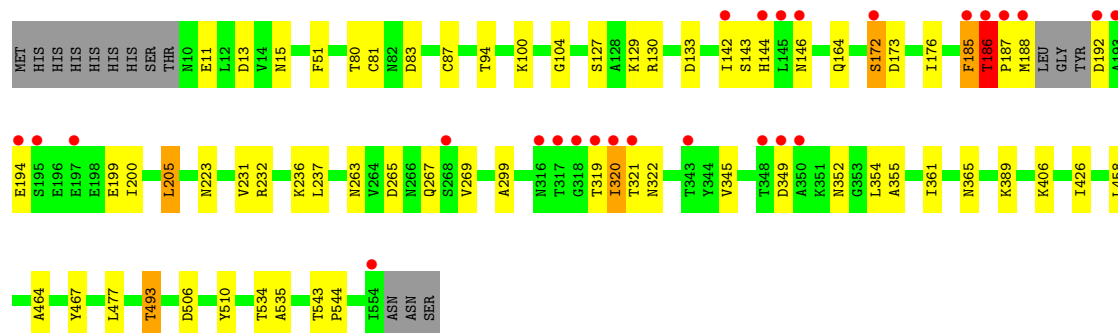
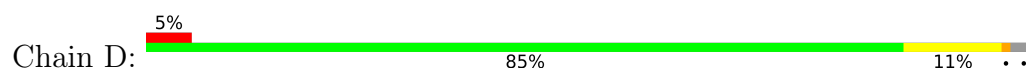
• Molecule 1: Phospholipase D



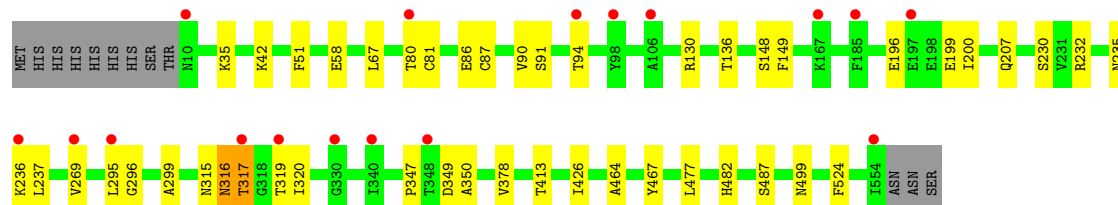
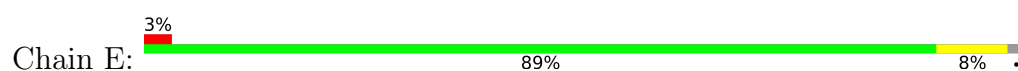
• Molecule 1: Phospholipase D



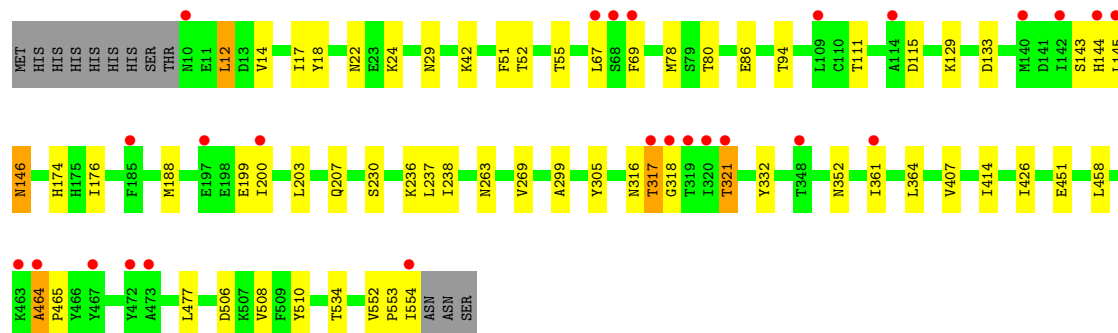
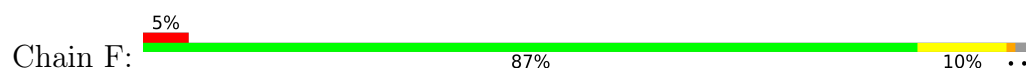
• Molecule 1: Phospholipase D



• Molecule 1: Phospholipase D



• Molecule 1: Phospholipase D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.90Å 216.64Å 277.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.30 19.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.81-2.30) 99.7 (19.81-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.30Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.212 , 0.216 0.213 , 0.217	Depositor DCC
R_{free} test set	2000 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51186	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: NA, 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	0.53	2/4299 (0.0%)	0.60	0/5850
1	B	0.46	0/4328	0.56	0/5889
1	C	0.50	2/4334 (0.0%)	0.60	0/5897
1	D	0.42	0/4328	0.58	3/5889 (0.1%)
1	E	0.40	0/4354	0.52	0/5926
1	F	0.37	0/4354	0.50	0/5926
All	All	0.45	4/25997 (0.0%)	0.56	3/35377 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	4
1	D	0	2
1	E	0	1
1	F	0	1
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	ASN	C-O	9.12	1.28	1.23
1	A	81	CYS	CB-SG	-6.50	1.59	1.81
1	A	185	PHE	C-N	6.17	1.46	1.33
1	C	81	CYS	CB-SG	-5.13	1.64	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	186	THR	C-N-CD	-8.19	102.58	120.60
1	D	186	THR	CA-C-N	8.10	146.43	127.00
1	D	186	THR	C-N-CA	8.10	146.43	127.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	LEU	Peptide
1	A	80	THR	Peptide
1	B	145	LEU	Peptide
1	B	248	LYS	Peptide
1	B	80	THR	Peptide
1	C	185	PHE	Peptide
1	C	191	TYR	Peptide
1	C	463	LYS	Peptide
1	C	80	THR	Peptide
1	D	185	PHE	Peptide
1	D	80	THR	Peptide
1	E	80	THR	Peptide
1	F	80	THR	Peptide

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	4209	4085	4084	33	0
1	B	4238	4113	4113	56	0
1	C	4243	4111	4109	52	0
1	D	4238	4108	4108	63	0
1	E	4262	4133	4132	33	0
1	F	4262	4133	4132	49	0
2	A	8	12	12	3	0
3	A	9	0	0	0	0
3	B	10	0	0	0	0
3	C	11	0	0	0	0
3	D	8	0	0	0	0
3	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	6	0	0	0	0
4	A	256	0	0	5	0
4	B	146	0	0	7	0
4	C	198	0	0	2	1
4	D	144	0	0	6	0
4	E	146	0	0	7	1
4	F	94	0	0	1	0
All	All	26491	24695	24690	281	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (281) 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:100:LYS:NZ	1:D:164:GLN:OE1	1.83	1.11
1:D:186:THR:HG23	1:D:187:PRO:HA	1.35	1.08
1:B:344:TYR:OH	4:B:701:HOH:O	1.85	0.95
1:D:127:SER:OG	4:D:701:HOH:O	1.85	0.93
1:D:186:THR:HG23	1:D:187:PRO:CA	2.00	0.91
1:D:186:THR:HG21	1:D:188:MET:HG2	1.56	0.88
1:C:413:THR:HG22	1:C:415:ASP:H	1.39	0.86
1:B:472:TYR:O	1:B:475:THR:HG22	1.74	0.85
1:E:482:HIS:ND1	4:E:704:HOH:O	2.10	0.84
1:A:227:THR:HG23	1:A:326:THR:HG22	1.61	0.82
1:F:200:ILE:HD11	1:F:321:THR:HG23	1.63	0.81
1:E:315:ASN:O	1:E:317:THR:N	2.14	0.81
1:F:207:GLN:OE1	1:F:230:SER:OG	1.97	0.81
1:F:464:ALA:HB1	1:F:465:PRO:HD2	1.61	0.81
1:F:464:ALA:HB1	1:F:465:PRO:CD	2.13	0.79
1:B:464:ALA:HB1	1:B:465:PRO:CD	2.13	0.78
1:E:317:THR:O	4:E:702:HOH:O	2.02	0.78
1:E:207:GLN:OE1	1:E:230:SER:OG	1.99	0.77
1:A:450:SER:OG	4:A:701:HOH:O	2.03	0.77
1:C:321:THR:N	4:C:702:HOH:O	2.19	0.75
1:D:142:ILE:HD12	1:D:143:SER:N	2.02	0.74
1:C:464:ALA:HB1	1:C:465:PRO:HD2	1.69	0.73
1:B:458:LEU:HD13	1:B:477:LEU:HD12	1.70	0.73
1:A:349:ASP:OD1	1:A:352:ASN:HB2	1.89	0.73
1:C:188:MET:HE3	1:C:188:MET:HA	1.69	0.73
1:C:142:ILE:O	1:C:142:ILE:HG22	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:MET:HE1	1:F:111:THR:HG22	1.71	0.73
1:F:14:VAL:HA	1:F:17:ILE:HD12	1.71	0.73
1:D:263:ASN:O	4:D:702:HOH:O	2.07	0.72
1:D:361:ILE:HD11	1:D:510:TYR:HE2	1.53	0.72
1:B:464:ALA:HB1	1:B:465:PRO:HD2	1.70	0.72
1:E:58:GLU:O	4:E:703:HOH:O	2.06	0.72
1:C:232:ARG:NH1	1:C:321:THR:O	2.22	0.72
1:A:34:SER:OG	4:A:702:HOH:O	2.07	0.72
1:D:406:LYS:NZ	4:D:705:HOH:O	2.23	0.72
1:F:361:ILE:HD11	1:F:510:TYR:HE1	1.55	0.72
1:C:326:THR:HG21	1:C:335:ASP:O	1.91	0.71
1:C:464:ALA:HB1	1:C:465:PRO:CD	2.20	0.71
1:D:361:ILE:HD12	1:D:361:ILE:O	1.90	0.70
1:D:186:THR:OG1	1:D:187:PRO:C	2.35	0.70
1:F:407:VAL:O	4:F:701:HOH:O	2.10	0.69
1:B:142:ILE:HD13	1:B:142:ILE:H	1.57	0.69
1:A:145:LEU:HG	1:A:146:ASN:N	2.08	0.68
1:D:192:ASP:OD1	4:D:703:HOH:O	2.11	0.68
1:A:429:GLY:O	4:A:703:HOH:O	2.11	0.68
1:F:52:THR:O	1:F:55:THR:HG22	1.94	0.67
1:E:524:PHE:O	4:E:705:HOH:O	2.13	0.67
1:D:185:PHE:O	1:D:186:THR:HG22	1.94	0.66
1:C:187:PRO:HB3	1:C:199:GLU:HG3	1.77	0.66
1:F:361:ILE:HD12	1:F:361:ILE:O	1.95	0.66
1:A:199:GLU:OE1	1:A:232:ARG:NH2	2.27	0.66
1:F:317:THR:O	1:F:317:THR:HG23	1.97	0.65
1:F:458:LEU:HD13	1:F:477:LEU:HD12	1.78	0.65
1:C:413:THR:HG22	1:C:415:ASP:N	2.12	0.65
1:A:71:HIS:H	1:A:80:THR:HG22	1.62	0.65
1:F:24:LYS:HE3	1:F:414:ILE:HD12	1.78	0.64
1:C:232:ARG:NH2	1:C:321:THR:O	2.29	0.64
1:B:315:ASN:O	1:B:317:THR:N	2.30	0.64
1:D:185:PHE:O	1:D:188:MET:HE2	1.97	0.64
1:F:188:MET:HE3	1:F:199:GLU:HG3	1.80	0.64
1:F:552:VAL:HG12	1:F:554:ILE:HG12	1.79	0.64
1:E:295:LEU:HD23	1:E:296:GLY:N	2.12	0.64
1:F:78:MET:CE	1:F:111:THR:HG22	2.27	0.64
1:F:361:ILE:HD11	1:F:510:TYR:CE1	2.33	0.63
1:C:142:ILE:O	1:C:144:HIS:N	2.31	0.63
1:D:11:GLU:OE2	1:D:389:LYS:NZ	2.27	0.63
1:C:413:THR:CG2	1:C:415:ASP:H	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ASN:CG	1:E:320:ILE:HD11	2.24	0.62
1:A:70:ASN:HB3	1:A:80:THR:HG22	1.81	0.62
1:C:191:TYR:HA	1:C:192:ASP:CG	2.25	0.62
1:F:12:LEU:HD12	1:F:508:VAL:HG21	1.81	0.62
1:B:240:ASN:OD1	1:B:242:GLY:N	2.32	0.61
1:B:188:MET:HG3	1:B:199:GLU:HG2	1.82	0.61
1:D:361:ILE:HD11	1:D:510:TYR:CE2	2.35	0.60
1:B:236:LYS:O	1:B:237:LEU:HB2	2.02	0.59
1:B:464:ALA:CB	1:B:465:PRO:CD	2.80	0.59
1:D:186:THR:HG22	1:D:232:ARG:NH2	2.16	0.59
1:B:198:GLU:OE1	1:B:201:ARG:NH1	2.36	0.59
1:B:239:SER:HA	1:C:191:TYR:HE2	1.67	0.59
1:B:189:LEU:HD11	1:C:406:LYS:HD3	1.83	0.59
1:F:464:ALA:CB	1:F:465:PRO:CD	2.81	0.58
1:C:436:THR:CG2	1:C:437:SER:O	2.51	0.58
1:E:487:SER:O	4:E:707:HOH:O	2.17	0.58
1:B:142:ILE:O	1:B:143:SER:OG	2.13	0.58
1:A:227:THR:CG2	1:A:326:THR:HG22	2.33	0.58
1:B:344:TYR:CE2	4:B:701:HOH:O	2.56	0.57
1:D:172:SER:O	1:D:173:ASP:HB2	2.04	0.57
1:D:426:ILE:HG21	1:D:477:LEU:HD23	1.87	0.57
1:B:344:TYR:CZ	4:B:701:HOH:O	2.52	0.56
1:C:190:GLY:N	4:C:701:HOH:O	2.17	0.56
1:C:232:ARG:NH2	1:C:321:THR:HG22	2.19	0.56
1:C:464:ALA:CB	1:C:465:PRO:HD2	2.35	0.56
1:F:78:MET:HE2	1:F:111:THR:HA	1.86	0.56
1:C:464:ALA:CB	1:C:465:PRO:CD	2.83	0.56
1:F:42:LYS:HE3	1:F:352:ASN:ND2	2.20	0.56
1:C:200:ILE:HD11	1:C:321:THR:O	2.07	0.55
1:B:436:THR:HG21	4:B:773:HOH:O	2.06	0.55
1:B:248:LYS:HB3	1:C:191:TYR:HB2	1.88	0.55
1:C:232:ARG:CZ	1:C:321:THR:O	2.55	0.55
1:B:315:ASN:O	1:B:316:ASN:C	2.50	0.54
1:F:464:ALA:CB	1:F:465:PRO:HD2	2.33	0.54
1:A:326:THR:HG21	1:A:335:ASP:O	2.07	0.54
1:C:436:THR:HG22	1:C:437:SER:O	2.08	0.54
1:B:507:LYS:HD2	1:B:531:LYS:HD3	1.88	0.54
1:D:200:ILE:HD11	1:D:321:THR:HA	1.90	0.54
1:D:172:SER:OG	1:D:173:ASP:N	2.38	0.54
1:D:319:THR:HB	1:D:320:ILE:HD12	1.88	0.54
1:C:190:GLY:O	1:C:191:TYR:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LEU:HD12	1:D:355:ALA:N	2.22	0.54
1:F:426:ILE:HG21	1:F:477:LEU:HD23	1.89	0.54
1:F:188:MET:HE1	1:F:203:LEU:HG	1.89	0.54
1:A:143:SER:O	1:A:144:HIS:O	2.26	0.53
1:B:142:ILE:C	1:B:143:SER:HG	2.11	0.53
1:A:35:LYS:HD3	1:A:36:PRO:HD2	1.90	0.53
1:F:12:LEU:CD1	1:F:508:VAL:HG21	2.39	0.53
1:C:413:THR:HB	1:C:416:GLY:O	2.08	0.53
1:B:144:HIS:CE1	1:B:145:LEU:HD13	2.44	0.53
1:B:436:THR:CG2	1:B:437:SER:O	2.56	0.53
1:C:436:THR:HG23	1:C:446:SER:HB3	1.89	0.53
1:D:265:ASP:O	1:D:267:GLN:HG3	2.08	0.53
1:B:67:LEU:HD22	1:B:67:LEU:H	1.72	0.53
1:B:144:HIS:CG	1:B:145:LEU:H	2.27	0.53
1:E:236:LYS:O	1:E:237:LEU:HB2	2.09	0.52
1:B:142:ILE:O	1:B:142:ILE:HG12	2.10	0.52
1:C:426:ILE:HG21	1:C:477:LEU:HD23	1.91	0.52
1:D:320:ILE:HG22	1:D:321:THR:H	1.75	0.51
1:B:436:THR:HG22	1:B:437:SER:O	2.10	0.51
1:D:320:ILE:HD12	1:D:320:ILE:N	2.25	0.51
1:B:189:LEU:CD1	1:C:406:LYS:HD3	2.39	0.51
1:B:458:LEU:HD13	1:B:477:LEU:CD1	2.40	0.51
1:D:192:ASP:N	4:D:703:HOH:O	2.43	0.51
1:D:100:LYS:HE3	1:D:104:GLY:HA2	1.91	0.51
1:D:186:THR:OG1	1:D:187:PRO:O	2.27	0.51
1:A:426:ILE:HG21	1:A:477:LEU:HD23	1.93	0.51
1:B:247:GLN:OE1	4:B:702:HOH:O	2.19	0.51
1:C:142:ILE:O	1:C:142:ILE:CG2	2.58	0.51
1:D:81:CYS:SG	1:D:87:CYS:SG	3.09	0.51
1:D:186:THR:CG2	1:D:199:GLU:OE2	2.59	0.50
1:C:470:ARG:HG3	1:C:470:ARG:HH11	1.77	0.50
1:A:199:GLU:OE1	1:A:232:ARG:NH1	2.41	0.50
1:D:236:LYS:O	1:D:237:LEU:HB2	2.10	0.50
1:D:232:ARG:NH1	1:D:321:THR:HG21	2.28	0.49
1:E:90:VAL:O	1:E:90:VAL:HG22	2.12	0.49
1:F:451:GLU:OE1	1:F:554:ILE:HG21	2.13	0.49
1:D:205:LEU:HD11	1:F:332:TYR:O	2.13	0.49
1:E:349:ASP:OD1	1:E:349:ASP:O	2.31	0.49
1:C:191:TYR:OH	1:C:194:GLU:HG2	2.12	0.49
1:F:18:TYR:CZ	1:F:22:ASN:ND2	2.81	0.49
1:F:176:ILE:N	1:F:176:ILE:HD12	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:MET:SD	1:C:235:ASN:OD1	2.71	0.48
1:F:145:LEU:O	1:F:146:ASN:C	2.56	0.48
1:B:319:THR:HG23	1:B:320:ILE:H	1.78	0.48
1:E:199:GLU:OE2	1:E:232:ARG:NH1	2.46	0.48
1:E:315:ASN:O	1:E:316:ASN:C	2.57	0.48
1:E:269:VAL:HG21	1:E:299:ALA:HA	1.96	0.48
1:A:543:THR:HB	1:A:544:PRO:HD3	1.94	0.48
1:B:464:ALA:CB	1:B:465:PRO:HD2	2.41	0.48
1:C:185:PHE:CD1	1:C:186:THR:HA	2.50	0.47
1:B:361:ILE:HG13	1:B:376:SER:HA	1.95	0.47
1:B:188:MET:HG3	1:B:199:GLU:OE2	2.15	0.47
1:C:543:THR:HB	1:C:544:PRO:HD3	1.97	0.47
1:F:22:ASN:HD21	1:F:29:ASN:ND2	2.13	0.47
1:C:191:TYR:CD1	1:C:192:ASP:N	2.83	0.47
1:C:195:SER:O	1:C:199:GLU:HG2	2.15	0.47
1:E:464:ALA:HB2	1:E:467:TYR:CZ	2.50	0.47
1:B:426:ILE:HG21	1:B:477:LEU:HD23	1.96	0.47
1:E:347:PRO:HD2	1:E:350:ALA:HB2	1.96	0.47
1:E:42:LYS:HB3	1:E:42:LYS:HE2	1.78	0.46
1:B:143:SER:O	1:B:144:HIS:O	2.33	0.46
1:B:319:THR:HG23	1:B:320:ILE:N	2.31	0.46
1:E:148:SER:HB3	1:E:149:PHE:CD2	2.50	0.46
1:A:506:ASP:C	1:A:534:THR:HG21	2.40	0.46
1:E:237:LEU:HD12	1:F:238:ILE:HG22	1.98	0.46
1:F:317:THR:O	1:F:317:THR:CG2	2.63	0.46
1:D:458:LEU:HD13	1:D:477:LEU:HD12	1.98	0.46
1:E:316:ASN:O	1:E:317:THR:C	2.58	0.46
1:F:67:LEU:HD12	1:F:86:GLU:C	2.41	0.46
1:C:458:LEU:HD23	1:C:470:ARG:CZ	2.46	0.46
1:C:436:THR:HG23	1:C:437:SER:O	2.17	0.45
1:B:543:THR:HB	1:B:544:PRO:HD3	1.98	0.45
1:D:83:ASP:C	1:D:83:ASP:OD1	2.59	0.45
1:D:320:ILE:HG22	1:D:321:THR:N	2.31	0.45
1:A:295:LEU:HD23	1:A:295:LEU:C	2.42	0.45
1:B:232:ARG:NH2	1:B:321:THR:O	2.50	0.45
1:F:305:TYR:CE1	1:F:364:LEU:HD21	2.51	0.45
1:B:317:THR:O	1:B:317:THR:HG22	2.17	0.45
1:B:499:ASN:HA	4:B:719:HOH:O	2.16	0.45
1:E:81:CYS:SG	1:E:87:CYS:SG	3.15	0.45
1:E:378:VAL:HG22	1:E:413:THR:HB	1.97	0.45
1:F:317:THR:HA	1:F:318:GLY:HA2	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ASP:C	1:B:534:THR:HG21	2.41	0.45
1:D:13:ASP:OD2	1:D:15:ASN:HB2	2.17	0.45
1:A:385:LYS:NZ	1:A:415:ASP:O	2.49	0.45
1:D:186:THR:HG23	1:D:187:PRO:N	2.31	0.45
1:E:426:ILE:HG21	1:E:477:LEU:HD23	2.00	0.44
1:B:248:LYS:O	1:B:249:ASP:HB3	2.17	0.44
1:B:436:THR:HG23	1:B:446:SER:HB3	1.99	0.44
1:D:535:ALA:O	4:D:704:HOH:O	2.21	0.44
1:F:553:PRO:O	1:F:554:ILE:C	2.60	0.44
1:A:496:MET:HE1	2:A:601:EDO:H12	1.98	0.44
1:D:543:THR:HB	1:D:544:PRO:HD3	2.00	0.44
2:A:602:EDO:C2	4:A:923:HOH:O	2.64	0.44
1:B:249:ASP:HB3	1:B:406:LYS:NZ	2.33	0.44
1:C:197:GLU:HG2	1:C:198:GLU:H	1.81	0.44
1:F:188:MET:HE3	1:F:199:GLU:CG	2.47	0.44
1:A:385:LYS:HE2	1:A:385:LYS:HB2	1.78	0.44
1:D:133:ASP:HB3	1:D:263:ASN:HB3	1.99	0.44
1:D:186:THR:CG2	1:D:187:PRO:CA	2.84	0.44
1:D:464:ALA:HB2	1:D:467:TYR:CZ	2.52	0.44
1:C:232:ARG:NH1	1:C:322:ASN:HA	2.33	0.44
1:F:67:LEU:HD12	1:F:86:GLU:O	2.17	0.44
1:F:506:ASP:C	1:F:534:THR:HG21	2.43	0.44
1:E:136:THR:OG1	4:E:706:HOH:O	2.16	0.43
1:C:470:ARG:HG3	1:C:470:ARG:NH1	2.31	0.43
1:A:144:HIS:CG	1:A:145:LEU:H	2.36	0.43
1:B:248:LYS:CB	1:C:191:TYR:HB2	2.46	0.43
1:D:269:VAL:HG21	1:D:299:ALA:HA	1.99	0.43
1:A:186:THR:O	1:A:186:THR:HG23	2.17	0.43
1:A:232:ARG:HH11	1:A:235:ASN:ND2	2.17	0.43
1:A:361:ILE:CG1	1:A:376:SER:HA	2.48	0.43
1:D:142:ILE:HD12	1:D:143:SER:HB3	2.00	0.43
1:D:172:SER:HB2	1:D:223:ASN:CG	2.43	0.43
1:C:185:PHE:CE1	1:C:189:LEU:HD22	2.54	0.43
1:D:185:PHE:HD2	1:D:186:THR:HB	1.83	0.43
1:B:203:LEU:O	1:B:207:GLN:HG3	2.18	0.43
1:B:361:ILE:CG1	1:B:376:SER:HA	2.49	0.43
1:C:145:LEU:O	1:C:146:ASN:C	2.60	0.43
1:F:133:ASP:HB3	1:F:263:ASN:HB3	2.00	0.43
1:F:78:MET:HE3	1:F:115:ASP:OD2	2.19	0.43
1:A:232:ARG:NH1	1:A:321:THR:HG21	2.34	0.43
1:D:231:VAL:HA	1:D:322:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:PRO:O	1:B:554:ILE:HB	2.19	0.42
1:D:142:ILE:HD12	1:D:143:SER:CA	2.49	0.42
1:F:236:LYS:O	1:F:237:LEU:HB2	2.19	0.42
2:A:602:EDO:H21	4:A:923:HOH:O	2.18	0.42
1:F:269:VAL:HG21	1:F:299:ALA:HA	2.00	0.42
1:F:129:LYS:O	1:F:174:HIS:HE1	2.03	0.42
1:B:202:GLN:NE2	4:B:705:HOH:O	2.36	0.42
1:E:196:GLU:O	1:E:200:ILE:HD12	2.19	0.42
1:F:69:PHE:CD1	1:F:69:PHE:C	2.98	0.42
1:A:385:LYS:HZ2	1:A:415:ASP:HB3	1.85	0.42
1:C:236:LYS:O	1:C:237:LEU:HB2	2.20	0.42
1:E:87:CYS:HB3	1:E:91:SER:OG	2.19	0.42
1:E:349:ASP:O	1:E:349:ASP:CG	2.61	0.42
1:C:458:LEU:HD13	1:C:477:LEU:HD12	2.02	0.42
1:D:185:PHE:O	1:D:232:ARG:NH2	2.53	0.42
1:B:186:THR:HB	1:B:232:ARG:HD2	2.01	0.42
1:D:130:ARG:HE	1:D:130:ARG:HB3	1.56	0.42
1:D:345:VAL:HG23	1:D:345:VAL:O	2.18	0.42
1:D:493:THR:HG23	1:D:493:THR:O	2.19	0.42
1:E:67:LEU:HD11	1:E:86:GLU:HA	2.02	0.42
1:B:318:GLY:C	1:B:319:THR:HG22	2.45	0.41
1:D:176:ILE:N	1:D:176:ILE:HD12	2.35	0.41
1:A:145:LEU:CG	1:A:146:ASN:N	2.80	0.41
1:D:319:THR:CB	1:D:320:ILE:HD12	2.50	0.41
1:B:67:LEU:HD22	1:B:67:LEU:N	2.34	0.41
1:A:385:LYS:NZ	1:A:415:ASP:HB3	2.35	0.41
1:C:232:ARG:HH12	1:C:322:ASN:HA	1.85	0.41
1:A:145:LEU:HG	1:A:146:ASN:H	1.85	0.41
1:C:199:GLU:N	1:C:199:GLU:OE1	2.54	0.41
1:D:349:ASP:OD2	1:D:352:ASN:ND2	2.48	0.41
1:D:506:ASP:C	1:D:534:THR:HG21	2.46	0.41
1:B:81:CYS:SG	1:B:87:CYS:SG	3.19	0.41
1:D:192:ASP:HB3	1:D:194:GLU:OE1	2.21	0.41
1:F:316:ASN:O	1:F:317:THR:C	2.64	0.41
1:E:130:ARG:HG3	1:E:130:ARG:HH11	1.85	0.41
1:D:127:SER:O	1:D:129:LYS:HE2	2.20	0.40
1:E:295:LEU:HD23	1:E:295:LEU:C	2.46	0.40
1:E:235:ASN:ND2	1:E:320:ILE:HD11	2.36	0.40
1:A:326:THR:CG2	1:A:335:ASP:O	2.70	0.40
1:A:406:LYS:HE3	1:A:408:LEU:HD21	2.03	0.40
1:B:194:GLU:OE2	1:B:195:SER:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:PHE:O	1:D:186:THR:CG2	2.65	0.40
1:D:200:ILE:CD1	1:D:321:THR:HA	2.49	0.40
1:C:94:THR:HG22	1:C:96:PRO:HD3	2.03	0.40
1:C:187:PRO:O	1:C:192:ASP:HA	2.22	0.40
1:E:499:ASN:HA	4:E:749:HOH:O	2.21	0.40
1:F:78:MET:CE	1:F:115:ASP:OD2	2.69	0.40
1:F:145:LEU:O	1:F:145:LEU:HG	2.20	0.40
1:A:40:TYR:CE1	1:A:351:LYS:HA	2.56	0.40
1:D:186:THR:HG21	1:D:188:MET:CG	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:894:HOH:O	4:E:843:HOH:O[3_656]	1.99	0.21

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	534/557 (96%)	501 (94%)	29 (5%)	4 (1%)	18	23
1	B	538/557 (97%)	501 (93%)	34 (6%)	3 (1%)	21	27
1	C	538/557 (97%)	499 (93%)	34 (6%)	5 (1%)	14	17
1	D	538/557 (97%)	506 (94%)	27 (5%)	5 (1%)	14	17
1	E	543/557 (98%)	515 (95%)	26 (5%)	2 (0%)	30	38
1	F	543/557 (98%)	509 (94%)	28 (5%)	6 (1%)	11	13
All	All	3234/3342 (97%)	3031 (94%)	178 (6%)	25 (1%)	16	20

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	146	ASN
1	B	144	HIS
1	B	316	ASN
1	B	464	ALA
1	C	146	ASN
1	C	191	TYR
1	C	464	ALA
1	D	186	THR
1	E	316	ASN
1	E	317	THR
1	F	12	LEU
1	F	144	HIS
1	F	317	THR
1	F	464	ALA
1	C	141	ASP
1	D	365	ASN
1	F	143	SER
1	F	146	ASN
1	C	143	SER
1	D	144	HIS
1	D	146	ASN
1	A	143	SER
1	A	320	ILE
1	D	320	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	475/492 (96%)	471 (99%)	4 (1%)	73	86
1	B	478/492 (97%)	474 (99%)	4 (1%)	73	86
1	C	478/492 (97%)	469 (98%)	9 (2%)	50	69
1	D	478/492 (97%)	473 (99%)	5 (1%)	68	82
1	E	480/492 (98%)	476 (99%)	4 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	480/492 (98%)	477 (99%)	3 (1%)	78	89
All	All	2869/2952 (97%)	2840 (99%)	29 (1%)	68	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	80	THR
1	A	326	THR
1	A	380	ARG
1	B	51	PHE
1	B	142	ILE
1	B	436	THR
1	B	499	ASN
1	C	51	PHE
1	C	94	THR
1	C	199	GLU
1	C	200	ILE
1	C	321	THR
1	C	326	THR
1	C	413	THR
1	C	436	THR
1	C	540	GLN
1	D	51	PHE
1	D	94	THR
1	D	172	SER
1	D	205	LEU
1	D	493	THR
1	E	35	LYS
1	E	51	PHE
1	E	94	THR
1	E	319	THR
1	F	51	PHE
1	F	94	THR
1	F	321	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	A	316	ASN

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Mol	Chain	Res	Type
1	A	523	GLN
1	B	71	HIS
1	B	352	ASN
1	C	223	ASN
1	C	386	ASN
1	C	409	HIS
1	C	482	HIS
1	C	551	HIS
1	D	311	ASN
1	D	316	ASN
1	D	480	ASN
1	D	482	HIS
1	E	70	ASN
1	E	71	HIS
1	E	409	HIS
1	E	480	ASN
1	E	523	GLN
1	F	22	ASN
1	F	71	HIS
1	F	138	GLN
1	F	174	HIS
1	F	315	ASN
1	F	409	HIS
1	F	480	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 47 are monoatomic - leaving 2 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	$\# Z > 2$
2	EDO	A	601	-	3,3,3	0.56	0	2,2,2	0.25	0
2	EDO	A	602	-	3,3,3	0.69	0	2,2,2	0.70	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	A	601	-	-	0/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EDO	1	0
2	A	602	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	538/557 (96%)	0.24	18 (3%)	49	51	53, 69, 102, 154	0
1	B	542/557 (97%)	0.63	33 (6%)	27	29	58, 80, 122, 167	0
1	C	542/557 (97%)	0.66	33 (6%)	27	29	58, 74, 109, 199	0
1	D	542/557 (97%)	0.47	26 (4%)	35	37	58, 84, 126, 165	0
1	E	545/557 (97%)	0.59	17 (3%)	51	53	62, 85, 117, 150	0
1	F	545/557 (97%)	0.59	26 (4%)	35	37	66, 90, 119, 164	0
All	All	3254/3342 (97%)	0.53	153 (4%)	36	38	53, 81, 119, 199	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	LEU	6.8
1	F	145	LEU	6.5
1	A	187	PRO	6.0
1	C	191	TYR	5.9
1	F	69	PHE	5.8
1	D	192	ASP	5.6
1	C	186	THR	5.4
1	C	192	ASP	5.3
1	F	554	ILE	5.3
1	D	186	THR	5.2
1	B	185	PHE	5.2
1	D	145	LEU	5.2
1	B	186	THR	5.2
1	C	317	THR	5.1
1	F	67	LEU	4.8
1	B	145	LEU	4.8
1	C	464	ALA	4.6
1	C	193	ALA	4.5
1	A	186	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	464	ALA	4.4
1	D	185	PHE	4.1
1	D	320	ILE	4.1
1	D	187	PRO	4.1
1	F	185	PHE	4.1
1	F	144	HIS	4.0
1	B	189	LEU	4.0
1	B	192	ASP	3.9
1	C	554	ILE	3.9
1	C	199	GLU	3.8
1	B	316	ASN	3.8
1	E	317	THR	3.8
1	C	146	ASN	3.8
1	B	554	ILE	3.8
1	A	145	LEU	3.8
1	B	317	THR	3.7
1	D	142	ILE	3.7
1	A	320	ILE	3.6
1	D	188	MET	3.6
1	F	317	THR	3.6
1	C	194	GLU	3.6
1	F	319	THR	3.5
1	B	67	LEU	3.5
1	A	554	ILE	3.5
1	C	200	ILE	3.4
1	C	189	LEU	3.4
1	C	316	ASN	3.4
1	C	142	ILE	3.4
1	B	464	ALA	3.4
1	A	142	ILE	3.3
1	D	193	ALA	3.3
1	B	319	THR	3.2
1	E	94	THR	3.2
1	A	144	HIS	3.2
1	B	142	ILE	3.2
1	F	197	GLU	3.2
1	A	317	THR	3.2
1	E	554	ILE	3.1
1	A	321	THR	3.1
1	A	185	PHE	3.0
1	B	146	ASN	3.0
1	E	106	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	320	ILE	2.9
1	F	68	SER	2.9
1	F	318	GLY	2.9
1	C	185	PHE	2.9
1	C	321	THR	2.9
1	A	11	GLU	2.8
1	A	319	THR	2.8
1	F	463	LYS	2.8
1	B	200	ILE	2.8
1	D	194	GLU	2.8
1	A	200	ILE	2.7
1	D	316	ASN	2.7
1	B	194	GLU	2.7
1	D	348	THR	2.7
1	C	190	GLY	2.7
1	A	316	ASN	2.7
1	B	94	THR	2.7
1	E	319	THR	2.7
1	D	144	HIS	2.6
1	F	10	ASN	2.6
1	B	11	GLU	2.6
1	B	196	GLU	2.6
1	C	187	PRO	2.6
1	E	185	PHE	2.6
1	B	320	ILE	2.6
1	B	144	HIS	2.6
1	B	187	PRO	2.6
1	E	348	THR	2.5
1	D	554	ILE	2.5
1	F	140	MET	2.5
1	D	321	THR	2.5
1	D	343	THR	2.5
1	B	143	SER	2.5
1	D	195	SER	2.5
1	B	193	ALA	2.5
1	B	322	ASN	2.5
1	C	173	ASP	2.5
1	D	350	ALA	2.5
1	D	172	SER	2.4
1	E	10	ASN	2.4
1	C	197	GLU	2.4
1	D	319	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	69	PHE	2.4
1	D	197	GLU	2.4
1	A	195	SER	2.4
1	C	322	ASN	2.3
1	B	76	PHE	2.3
1	C	232	ARG	2.3
1	D	268	SER	2.3
1	E	340	ILE	2.3
1	F	200	ILE	2.3
1	E	269	VAL	2.3
1	E	80	THR	2.3
1	D	146	ASN	2.3
1	E	98	TYR	2.3
1	B	68	SER	2.3
1	A	196	GLU	2.2
1	C	348	THR	2.2
1	D	317	THR	2.2
1	F	321	THR	2.2
1	F	472	TYR	2.2
1	F	467	TYR	2.2
1	F	142	ILE	2.2
1	F	361	ILE	2.2
1	D	349	ASP	2.2
1	A	318	GLY	2.2
1	E	330	GLY	2.2
1	F	114	ALA	2.2
1	B	361	ILE	2.2
1	C	188	MET	2.2
1	C	389	LYS	2.2
1	C	144	HIS	2.2
1	F	473	ALA	2.2
1	B	81	CYS	2.1
1	B	188	MET	2.1
1	C	550	ILE	2.1
1	E	197	GLU	2.1
1	B	104	GLY	2.1
1	E	295	LEU	2.1
1	C	356	VAL	2.1
1	B	92	THR	2.1
1	C	81	CYS	2.1
1	C	143	SER	2.1
1	D	318	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	348	THR	2.0
1	A	197	GLU	2.0
1	C	533	ALA	2.0
1	C	468	LEU	2.0
1	F	109	LEU	2.0
1	B	232	ARG	2.0
1	E	236	LYS	2.0
1	E	167	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
2	EDO	A	601	4/4	0.77	0.23	68,79,91,91	0
3	NA	B	605	1/1	0.77	0.42	75,75,75,75	0
3	NA	C	610	1/1	0.79	0.26	83,83,83,83	0
3	NA	C	605	1/1	0.81	0.36	88,88,88,88	0
3	NA	F	606	1/1	0.83	0.20	86,86,86,86	0
3	NA	B	607	1/1	0.86	0.19	80,80,80,80	0
3	NA	D	606	1/1	0.87	0.24	80,80,80,80	0
3	NA	E	601	1/1	0.88	0.25	76,76,76,76	0
3	NA	F	601	1/1	0.88	0.24	74,74,74,74	0
3	NA	F	602	1/1	0.88	0.24	79,79,79,79	0
3	NA	C	604	1/1	0.88	0.28	73,73,73,73	0
3	NA	F	605	1/1	0.89	0.26	73,73,73,73	0
3	NA	C	611	1/1	0.89	0.17	71,71,71,71	0
2	EDO	A	602	4/4	0.90	0.14	60,71,81,82	0
3	NA	C	609	1/1	0.90	0.16	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	606	1/1	0.90	0.17	65,65,65,65	0
3	NA	C	602	1/1	0.90	0.17	59,59,59,59	0
3	NA	A	609	1/1	0.90	0.19	63,63,63,63	0
3	NA	C	606	1/1	0.91	0.17	74,74,74,74	0
3	NA	C	603	1/1	0.91	0.41	72,72,72,72	0
3	NA	D	608	1/1	0.92	0.14	81,81,81,81	0
3	NA	B	602	1/1	0.92	0.33	77,77,77,77	0
3	NA	B	606	1/1	0.92	0.19	58,58,58,58	0
3	NA	C	601	1/1	0.93	0.14	56,56,56,56	0
3	NA	A	604	1/1	0.93	0.18	63,63,63,63	0
3	NA	B	609	1/1	0.93	0.27	69,69,69,69	0
3	NA	B	610	1/1	0.93	0.15	95,95,95,95	0
3	NA	A	607	1/1	0.94	0.16	43,43,43,43	0
3	NA	A	608	1/1	0.94	0.18	58,58,58,58	0
3	NA	A	605	1/1	0.94	0.11	63,63,63,63	0
3	NA	E	602	1/1	0.94	0.20	107,107,107,107	0
3	NA	A	611	1/1	0.94	0.26	65,65,65,65	0
3	NA	B	601	1/1	0.94	0.08	64,64,64,64	0
3	NA	F	604	1/1	0.94	0.16	79,79,79,79	0
3	NA	A	603	1/1	0.94	0.11	57,57,57,57	0
3	NA	B	603	1/1	0.94	0.22	68,68,68,68	0
3	NA	D	603	1/1	0.95	0.17	80,80,80,80	0
3	NA	C	608	1/1	0.95	0.20	68,68,68,68	0
3	NA	F	603	1/1	0.95	0.14	84,84,84,84	0
3	NA	B	608	1/1	0.95	0.19	69,69,69,69	0
3	NA	D	601	1/1	0.95	0.10	78,78,78,78	0
3	NA	D	602	1/1	0.95	0.18	75,75,75,75	0
3	NA	B	604	1/1	0.96	0.17	74,74,74,74	0
3	NA	D	604	1/1	0.96	0.28	61,61,61,61	0
3	NA	D	605	1/1	0.96	0.10	70,70,70,70	0
3	NA	E	603	1/1	0.96	0.13	69,69,69,69	0
3	NA	C	607	1/1	0.96	0.16	47,47,47,47	0
3	NA	D	607	1/1	0.97	0.30	81,81,81,81	0
3	NA	A	610	1/1	0.98	0.11	76,76,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.