Full wwPDB X-ray Structure Validation Report (i)

Dec 15, 2024 – 11:28 PM EST

PDB ID	:	5EUL
Title	:	Structure of the SecA-SecY complex with a translocating polypeptide substrate
Authors	:	Li, L.; Park, E.; Ling, J.; Ingram, J.; Ploegh, H.; Rapoport, T.A.
Deposited on	:	2015-11-18
Resolution	:	3.70 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

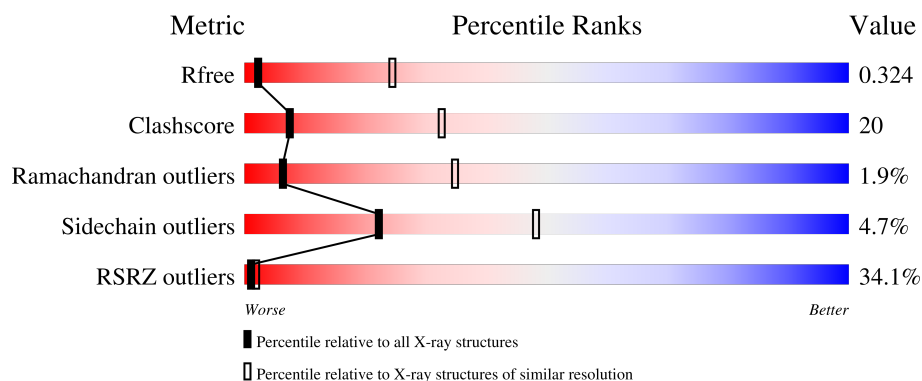|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.70 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	Percentile Ranks	Value
Rfree		0.324
Clashscore		20
Ramachandran outliers		1.9%
Sidechain outliers		4.7%
RSRZ outliers		34.1%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	836	31% 60% 25% · · 11%
2	Y	424	33% 49% 35% · · 10%
3	E	70	19% 56% 23% · 20%
4	V	131	25% 54% 29% · · 12%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	TBR	A	1014	-	-	X	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 10511 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 Protein translocase subunit SecA, Insertion Peptide Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total 5876	C 3677	N 1030	O 1135	S 34	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	828	THR	-	expression tag	UNP P28366
A	829	SER	-	expression tag	UNP P28366
A	830	LEU	-	expression tag	UNP P28366
A	831	GLU	-	expression tag	UNP P28366
A	832	VAL	-	expression tag	UNP P28366
A	833	LEU	-	expression tag	UNP P28366
A	834	PHE	-	expression tag	UNP P28366
A	835	GLN	-	expression tag	UNP P28366
A	836	GLY	-	expression tag	UNP P28366

- Molecule 2 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	380	Total 2936	C 1951	N 478	O 495	S 12	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	60	CYS	GLY	conflict	UNP A4IJK8
Y	208	THR	GLN	conflict	UNP A4IJK8
Y	?	-	GLU	deletion	UNP A4IJK8
Y	?	-	ASN	deletion	UNP A4IJK8
Y	?	-	VAL	deletion	UNP A4IJK8
Y	?	-	GLY	deletion	UNP A4IJK8
Y	?	-	GLU	deletion	UNP A4IJK8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	?	-	ASP	deletion	UNP A4IJK8
Y	210	GLY	LEU	conflict	UNP A4IJK8
Y	211	GLY	PHE	conflict	UNP A4IJK8
Y	213	ASN	ARG	conflict	UNP A4IJK8

- Molecule 3 is a protein called Preprotein translocase SecE subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	56	460	306	78	76	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLY	-	expression tag	UNP A4IJH4
E	62	GLY	-	expression tag	UNP A4IJH4
E	63	HIS	-	expression tag	UNP A4IJH4
E	64	HIS	-	expression tag	UNP A4IJH4
E	65	HIS	-	expression tag	UNP A4IJH4
E	66	HIS	-	expression tag	UNP A4IJH4
E	67	HIS	-	expression tag	UNP A4IJH4
E	68	HIS	-	expression tag	UNP A4IJH4
E	69	HIS	-	expression tag	UNP A4IJH4
E	70	HIS	-	expression tag	UNP A4IJH4

- Molecule 4 is a protein called AYC08.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	V	115	883	553	153	171	6	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

BEF
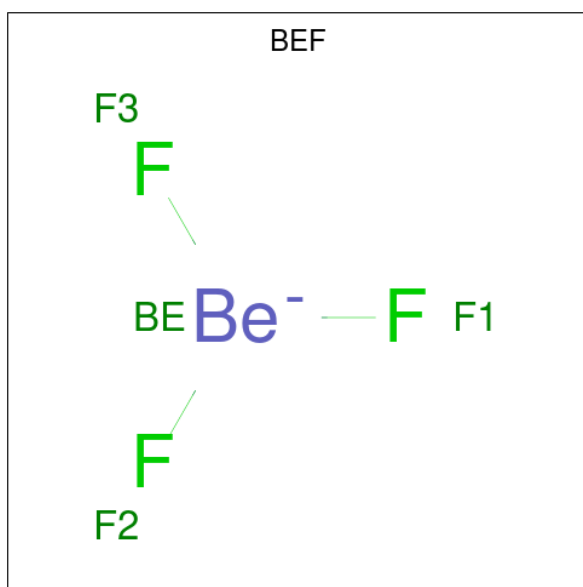
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
6	A	1	4	1	3	0	0

- Molecule 7 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP
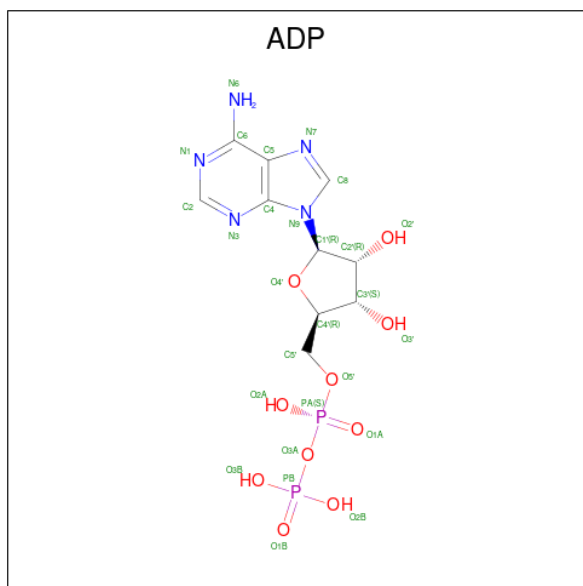
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	27	10	5	10	2	0	0

- Molecule 8 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $Br_{12}Ta_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0
8	A	1	Total 18	Br 12	Ta 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Protein translocase subunit SecA, Insertion Peptide Chimera
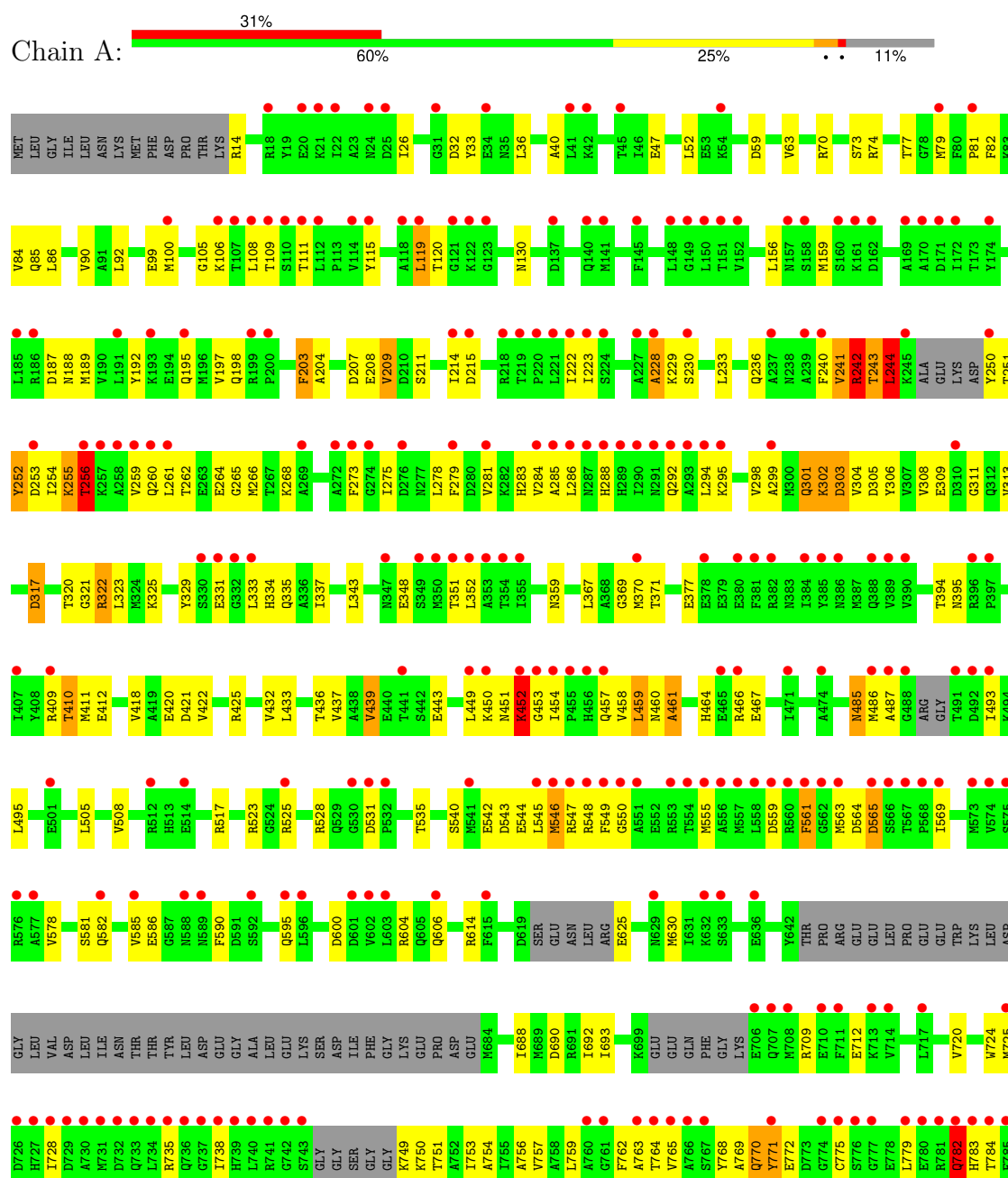
• Molecule 2: Protein translocase subunit SecY

Chain Y:
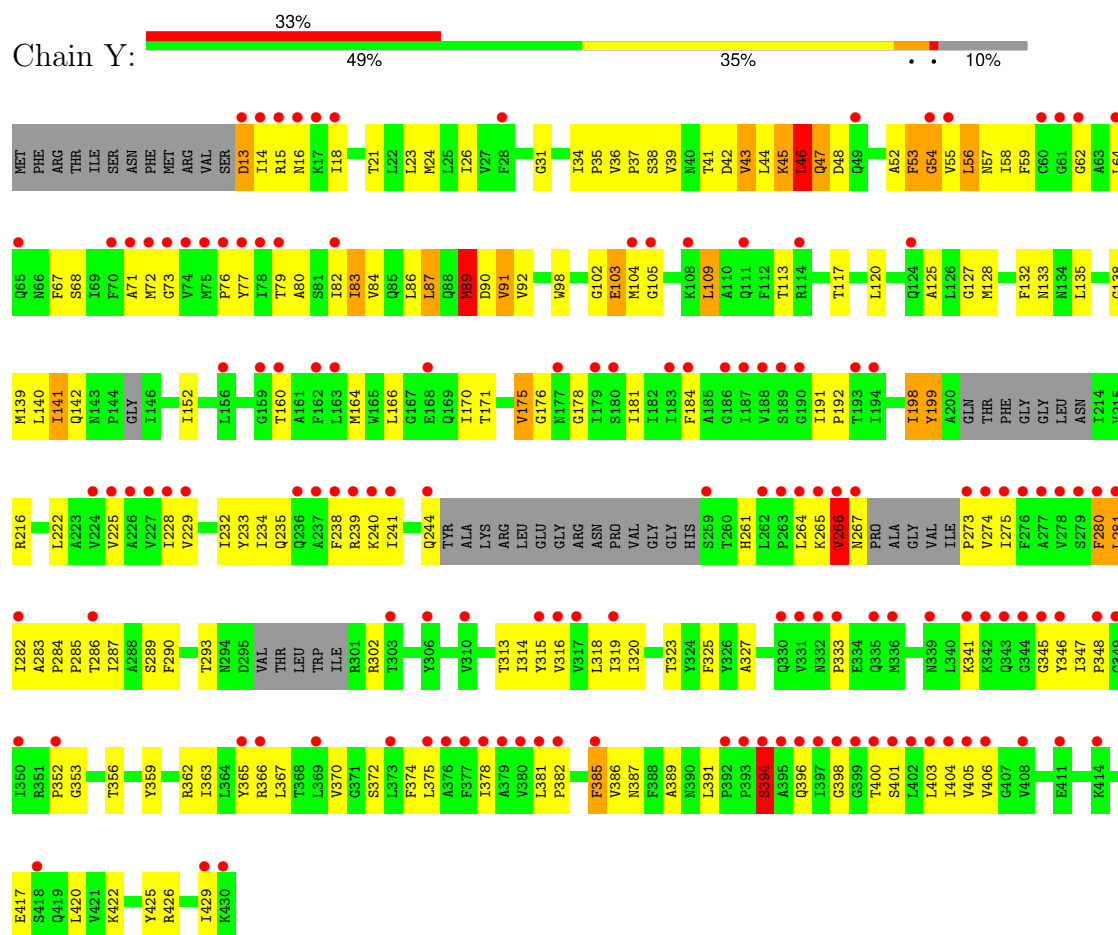
• Molecule 3: Preprotein translocase SecE subunit

Chain E:

• Molecule 4: AYC08

Chain V:

4 Data and refinement statistics (i)

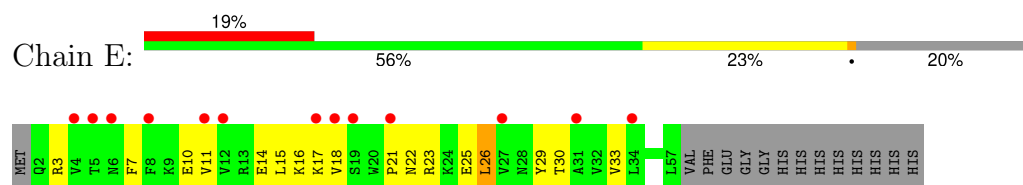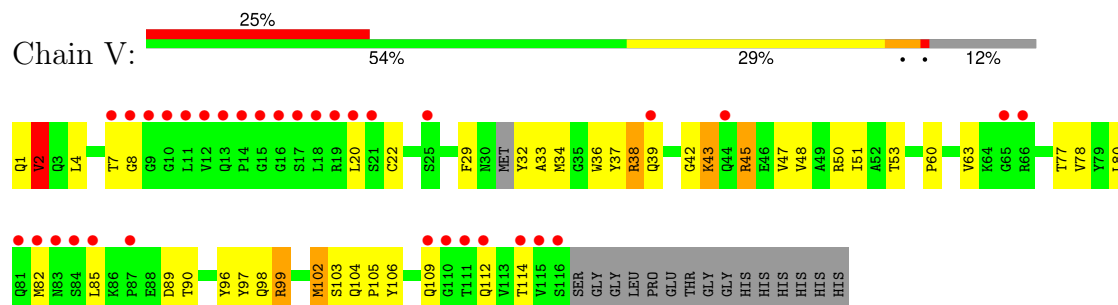| Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	127.80Å 127.80Å 554.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.85 – 3.70 53.85 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.85-3.70) 99.9 (53.85-3.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.295 , 0.315 0.299 , 0.324	Depositor DCC
R_{free} test set	1513 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	191.2	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 96.5	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	10511	wwPDB-VP
Average B, all atoms (Å^2)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BEF, TBR, MG, ADP

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	0.29	1/5950 (0.0%)	0.55	2/7993 (0.0%)
2	Y	0.37	0/2996	0.68	3/4069 (0.1%)
3	E	0.31	0/469	0.52	0/635
4	V	0.29	0/901	0.67	1/1222 (0.1%)
All	All	0.32	1/10316 (0.0%)	0.60	6/13919 (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	14
2	Y	0	8
4	V	0	3
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	804	PHE	CB-CG	-5.07	1.42	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	46	LEU	CA-CB-CG	7.64	132.87	115.30
4	V	43	LYS	N-CA-C	6.37	128.19	111.00
1	A	804	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	A	256	THR	N-CA-C	5.74	126.50	111.00
2	Y	89	MET	C-N-CA	5.55	135.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	109	LEU	CA-CB-CG	5.51	127.97	115.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	ALA	Peptide
1	A	229	LYS	Peptide
1	A	242	ARG	Peptide
1	A	243	THR	Peptide
1	A	244	LEU	Peptide
1	A	255	LYS	Peptide
1	A	410	THR	Peptide
1	A	451	ASN	Peptide
1	A	452	LYS	Peptide
1	A	461	ALA	Peptide
1	A	563	MET	Peptide
1	A	768	TYR	Peptide
1	A	770	GLN	Peptide
1	A	782	GLN	Peptide
4	V	102	MET	Peptide
4	V	42	GLY	Peptide
4	V	43	LYS	Peptide
2	Y	138	GLY	Peptide
2	Y	198	ILE	Peptide
2	Y	266	VAL	Peptide
2	Y	394	SER	Peptide
2	Y	425	TYR	Peptide
2	Y	46	LEU	Peptide
2	Y	54	GLY	Peptide
2	Y	89	MET	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	5876	0	5855	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	2936	0	3075	187	0
3	E	460	0	482	26	0
4	V	883	0	845	38	0
5	A	1	0	0	0	0
6	A	4	0	0	1	0
7	A	27	0	12	1	0
8	A	270	0	0	28	0
8	Y	54	0	0	2	0
All	All	10511	0	10269	416	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 20.

All (416) 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)
2:Y:265:LYS:HG3	2:Y:266:VAL:HG23	1.42	1.00
1:A:242:ARG:HH22	1:A:268:LYS:HB3	1.30	0.94
2:Y:229:VAL:HG12	3:E:30:THR:HG21	1.52	0.92
2:Y:24:MET:HB3	2:Y:166:LEU:HD21	1.51	0.90
2:Y:235:GLN:HG3	2:Y:266:VAL:HG22	1.55	0.88
1:A:242:ARG:CZ	1:A:265:GLY:HA2	2.04	0.88
1:A:241:VAL:HG12	1:A:242:ARG:H	1.40	0.86
2:Y:91:VAL:HG23	2:Y:92:VAL:H	1.41	0.85
2:Y:239:ARG:NH2	3:E:14:GLU:O	2.12	0.83
1:A:188:ASN:O	1:A:614:ARG:NH1	2.11	0.82
1:A:550:GLY:HA2	1:A:581:SER:HB3	1.64	0.80
1:A:240:PHE:HZ	1:A:242:ARG:HH21	1.27	0.79
1:A:120:THR:HG21	8:A:1009:TBR:BR1	2.38	0.78
2:Y:370:VAL:HG21	3:E:15:LEU:HD11	1.66	0.78
4:V:4:LEU:O	4:V:109:GLN:NE2	2.18	0.76
8:A:1012:TBR:BRA	2:Y:289:SER:OG	2.58	0.76
2:Y:346:TYR:HB3	2:Y:352:PRO:HG3	1.69	0.75
2:Y:386:VAL:HA	2:Y:389:ALA:HB2	1.67	0.75
1:A:410:THR:O	1:A:412:GLU:N	2.16	0.75
1:A:422:VAL:HG12	1:A:432:VAL:HG11	1.69	0.74
2:Y:14:ILE:O	2:Y:18:ILE:HG13	1.87	0.74
1:A:753:ILE:HD12	2:Y:86:LEU:HG	1.70	0.74
1:A:302:LYS:O	1:A:304:VAL:N	2.21	0.73
1:A:74:ARG:HD3	8:A:1016:TBR:BR8	2.43	0.72
2:Y:366:ARG:CZ	3:E:10:GLU:HB3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:39:GLN:HB2	4:V:45:ARG:HB3	1.72	0.72
1:A:240:PHE:HZ	1:A:242:ARG:NH2	1.87	0.71
1:A:254:ILE:HA	1:A:548:ARG:HB3	1.72	0.71
1:A:261:LEU:HD22	2:Y:341:LYS:HZ3	1.56	0.71
1:A:461:ALA:HA	1:A:464:HIS:HB3	1.71	0.71
1:A:782:GLN:O	1:A:784:THR:N	2.20	0.71
2:Y:366:ARG:HB3	3:E:11:VAL:HA	1.72	0.71
1:A:459:LEU:HD22	1:A:486:MET:HG3	1.74	0.70
4:V:32:TYR:O	4:V:53:THR:OG1	2.08	0.70
2:Y:362:ARG:HH21	2:Y:366:ARG:HH22	1.39	0.70
2:Y:273:PRO:HB3	2:Y:327:ALA:HB2	1.73	0.70
3:E:3:ARG:HB3	3:E:7:PHE:HE2	1.57	0.69
1:A:459:LEU:HD11	1:A:467:GLU:HG3	1.75	0.69
2:Y:265:LYS:CG	2:Y:266:VAL:HG23	2.22	0.69
1:A:804:PHE:HA	2:Y:426:ARG:HH21	1.59	0.68
1:A:301:GLN:HG3	1:A:302:LYS:H	1.59	0.68
2:Y:43:VAL:HB	2:Y:140:LEU:HD12	1.75	0.67
2:Y:281:LEU:HD21	2:Y:315:TYR:CZ	2.30	0.67
1:A:787:GLY:H	2:Y:275:ILE:HG21	1.60	0.67
2:Y:86:LEU:HD21	2:Y:280:PHE:HZ	1.59	0.66
2:Y:46:LEU:HA	4:V:45:ARG:HH21	1.59	0.66
1:A:81:PRO:HG3	1:A:108:LEU:HD11	1.77	0.66
1:A:92:LEU:HD21	1:A:370:MET:HG2	1.77	0.66
1:A:523:ARG:NH1	1:A:535:THR:OG1	2.28	0.66
1:A:322:ARG:HA	1:A:461:ALA:HB2	1.78	0.66
1:A:540:SER:N	1:A:543:ASP:OD1	2.28	0.65
1:A:804:PHE:HA	2:Y:426:ARG:NH2	2.12	0.65
2:Y:139:MET:HE1	4:V:47:VAL:HB	1.78	0.65
1:A:439:VAL:HG12	1:A:460:ASN:HD21	1.61	0.65
2:Y:378:ILE:HG21	2:Y:403:LEU:HD11	1.78	0.65
1:A:457:GLN:OE1	1:A:466:ARG:NH1	2.30	0.64
4:V:33:ALA:N	4:V:98:GLN:O	2.27	0.64
2:Y:281:LEU:HD22	2:Y:319:ILE:HG12	1.78	0.64
2:Y:80:ALA:HB3	2:Y:117:THR:HG22	1.80	0.64
1:A:542:GLU:HG3	1:A:547:ARG:NE	2.13	0.63
1:A:630:MET:SD	1:A:818:VAL:HG21	2.39	0.63
1:A:555:MET:O	1:A:559:ASP:N	2.29	0.63
2:Y:46:LEU:HA	4:V:45:ARG:NH2	2.13	0.63
1:A:266:MET:HG2	1:A:279:PHE:CZ	2.34	0.63
2:Y:225:VAL:HA	2:Y:228:ILE:HG12	1.81	0.63
1:A:304:VAL:HG23	1:A:305:ASP:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:HG11	1:A:369:GLY:HA3	1.81	0.62
2:Y:86:LEU:HD21	2:Y:280:PHE:CZ	2.35	0.62
4:V:32:TYR:HA	4:V:99:ARG:HA	1.80	0.62
1:A:394:THR:O	1:A:395:ASN:HB3	2.00	0.62
1:A:228:ALA:HB2	1:A:348:GLU:H	1.66	0.61
2:Y:239:ARG:HD3	2:Y:241:ILE:HD11	1.81	0.61
1:A:301:GLN:HG3	1:A:302:LYS:N	2.14	0.61
1:A:606:GLN:HE21	2:Y:426:ARG:NH2	1.99	0.61
4:V:1:GLN:O	4:V:2:VAL:HG13	2.00	0.60
1:A:335:GLN:HE22	1:A:348:GLU:HG2	1.65	0.60
1:A:544:GLU:OE1	8:A:1006:TBR:BRC	2.74	0.60
2:Y:323:THR:HG21	2:Y:372:SER:HA	1.83	0.60
1:A:550:GLY:HA2	1:A:581:SER:CB	2.29	0.60
2:Y:175:VAL:HG12	2:Y:176:GLY:H	1.65	0.60
1:A:802:GLU:HB2	8:A:1005:TBR:BR2	2.57	0.60
2:Y:102:GLY:O	2:Y:104:MET:N	2.35	0.60
2:Y:232:ILE:HG21	3:E:30:THR:HG23	1.84	0.60
2:Y:281:LEU:HD11	2:Y:315:TYR:CD1	2.37	0.60
2:Y:400:THR:HA	2:Y:403:LEU:HD12	1.85	0.59
2:Y:52:ALA:O	2:Y:53:PHE:HB2	2.02	0.59
1:A:228:ALA:HB1	1:A:230:SER:HB3	1.85	0.59
1:A:595:GLN:HB2	8:A:1004:TBR:BR2	2.57	0.59
1:A:264:GLU:O	1:A:268:LYS:HB2	2.02	0.59
1:A:545:LEU:O	1:A:550:GLY:N	2.35	0.58
8:A:1017:TBR:BR7	2:Y:104:MET:SD	3.16	0.58
1:A:359:ASN:ND2	1:A:600:ASP:OD1	2.37	0.58
1:A:770:GLN:HE22	2:Y:293:THR:HG21	1.68	0.58
2:Y:286:THR:HA	2:Y:289:SER:HB3	1.86	0.57
2:Y:37:PRO:O	2:Y:142:GLN:NE2	2.38	0.57
1:A:254:ILE:HA	1:A:548:ARG:CB	2.34	0.57
1:A:759:LEU:HD13	2:Y:284:PRO:HG3	1.87	0.57
2:Y:239:ARG:NH2	3:E:14:GLU:HG3	2.20	0.57
2:Y:239:ARG:HB3	2:Y:264:LEU:HB2	1.86	0.57
2:Y:285:PRO:O	2:Y:289:SER:HB2	2.04	0.57
1:A:309:GLU:HG2	8:A:1014:TBR:BR8	2.60	0.56
1:A:738:ILE:HD11	1:A:798:GLU:HB3	1.86	0.56
2:Y:113:THR:O	2:Y:117:THR:HG23	2.04	0.56
2:Y:235:GLN:HG3	2:Y:266:VAL:CG2	2.34	0.56
1:A:309:GLU:HG3	8:A:1014:TBR:BR7	2.61	0.56
3:E:30:THR:HA	3:E:33:VAL:HG12	1.87	0.56
1:A:439:VAL:HG12	1:A:460:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:GLY:N	2:Y:275:ILE:HG21	2.20	0.56
1:A:421:ASP:OD2	1:A:425:ARG:NE	2.38	0.56
2:Y:44:LEU:HD13	2:Y:56:LEU:HA	1.88	0.56
1:A:156:LEU:HB2	1:A:159:MET:HG3	1.88	0.56
2:Y:72:MET:HE2	2:Y:125:ALA:HB2	1.88	0.55
1:A:453:GLY:O	1:A:454:ILE:HG13	2.06	0.55
2:Y:46:LEU:HD11	4:V:47:VAL:HG22	1.88	0.55
2:Y:198:ILE:HG23	2:Y:199:TYR:H	1.70	0.55
3:E:22:ASN:HB3	3:E:25:GLU:CB	2.36	0.55
1:A:36:LEU:HG	1:A:40:ALA:HB3	1.89	0.55
1:A:82:PHE:HB2	1:A:85:GLN:HG3	1.89	0.55
1:A:236:GLN:HB3	1:A:273:PHE:HE1	1.71	0.55
1:A:450:LYS:HD3	8:A:1015:TBR:BRA	2.62	0.55
1:A:304:VAL:HG23	1:A:305:ASP:N	2.22	0.55
1:A:253:ASP:O	1:A:548:ARG:HG2	2.07	0.55
1:A:590:PHE:CE2	2:Y:103:GLU:HG2	2.41	0.55
2:Y:389:ALA:HB1	2:Y:391:LEU:HB2	1.89	0.55
1:A:433:LEU:HD21	1:A:525:ARG:CZ	2.38	0.54
1:A:544:GLU:OE1	8:A:1006:TBR:BR4	2.81	0.54
1:A:779:LEU:HD11	2:Y:62:GLY:HA3	1.87	0.54
1:A:377:GLU:OE2	1:A:517:ARG:NH1	2.41	0.54
1:A:561:PHE:HZ	1:A:569:ILE:HG21	1.72	0.54
4:V:22:CYS:O	4:V:77:THR:HA	2.08	0.54
1:A:418:VAL:HG23	1:A:508:VAL:HG11	1.90	0.54
2:Y:366:ARG:HB2	3:E:14:GLU:HG2	1.89	0.54
1:A:242:ARG:NH2	1:A:265:GLY:HA2	2.22	0.54
2:Y:68:SER:H	2:Y:71:ALA:HB2	1.73	0.54
2:Y:41:THR:HG22	2:Y:45:LYS:NZ	2.23	0.53
2:Y:385:PHE:O	2:Y:389:ALA:HB2	2.08	0.53
2:Y:417:GLU:HA	2:Y:420:LEU:HB3	1.90	0.53
2:Y:238:PHE:HE1	2:Y:265:LYS:HE2	1.73	0.53
4:V:22:CYS:HB3	4:V:78:VAL:HG22	1.91	0.53
3:E:22:ASN:HB3	3:E:25:GLU:HB2	1.90	0.53
4:V:99:ARG:NH2	4:V:102:MET:O	2.37	0.53
1:A:753:ILE:HD11	2:Y:325:PHE:HZ	1.74	0.52
2:Y:286:THR:O	2:Y:290:PHE:N	2.42	0.52
1:A:222:ILE:HG23	1:A:351:THR:HG23	1.90	0.52
1:A:242:ARG:NH2	1:A:265:GLY:O	2.42	0.52
2:Y:225:VAL:O	2:Y:229:VAL:HG13	2.10	0.52
1:A:187:ASP:OD2	1:A:197:VAL:HG22	2.09	0.52
2:Y:44:LEU:HD11	2:Y:67:PHE:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MET:SD	1:A:352:LEU:HD22	2.50	0.52
2:Y:45:LYS:HZ1	2:Y:55:VAL:HG23	1.74	0.52
2:Y:273:PRO:HB3	2:Y:327:ALA:CB	2.39	0.52
4:V:36:TRP:O	4:V:48:VAL:N	2.33	0.51
1:A:261:LEU:CD2	2:Y:341:LYS:HZ3	2.21	0.51
1:A:203:PHE:HD1	1:A:204:ALA:N	2.08	0.51
1:A:335:GLN:NE2	1:A:348:GLU:HG2	2.25	0.51
1:A:240:PHE:CZ	1:A:242:ARG:NH2	2.73	0.51
2:Y:35:PRO:HB3	2:Y:56:LEU:HD21	1.92	0.51
1:A:317:ASP:HB3	1:A:320:THR:OG1	2.10	0.51
1:A:630:MET:CE	2:Y:429:ILE:HA	2.40	0.51
1:A:693:ILE:HG23	8:A:1010:TBR:BR7	2.65	0.51
2:Y:16:ASN:N	2:Y:16:ASN:HD22	2.09	0.51
1:A:192:TYR:HB2	1:A:195:GLN:HG2	1.93	0.51
1:A:14:ARG:NH1	8:A:1018:TBR:BR1	2.99	0.50
1:A:348:GLU:OE2	8:A:1013:TBR:BR2	2.84	0.50
4:V:20:LEU:HD12	4:V:80:LEU:HD23	1.93	0.50
2:Y:387:ASN:C	2:Y:389:ALA:H	2.14	0.50
1:A:285:ALA:HB1	8:A:1013:TBR:BRA	2.66	0.50
1:A:614:ARG:HG3	1:A:720:VAL:HG11	1.93	0.50
2:Y:315:TYR:O	2:Y:319:ILE:HG13	2.11	0.50
2:Y:353:GLY:O	2:Y:356:THR:OG1	2.25	0.50
2:Y:239:ARG:NH2	3:E:18:VAL:HG23	2.25	0.50
1:A:233:LEU:HB3	1:A:236:GLN:HB2	1.94	0.50
1:A:242:ARG:NH2	1:A:268:LYS:HB3	2.12	0.50
1:A:542:GLU:HG3	1:A:547:ARG:HE	1.77	0.50
1:A:770:GLN:NE2	2:Y:293:THR:HG21	2.25	0.50
2:Y:36:VAL:CG1	2:Y:152:ILE:HG13	2.42	0.50
2:Y:91:VAL:HG23	2:Y:92:VAL:N	2.19	0.50
2:Y:267:ASN:HA	2:Y:367:LEU:HD11	1.94	0.50
2:Y:283:ALA:HB3	2:Y:284:PRO:HD3	1.94	0.50
3:E:15:LEU:O	3:E:18:VAL:HB	2.12	0.50
1:A:807:PHE:CE2	1:A:811:ILE:HD11	2.47	0.49
1:A:261:LEU:HD13	2:Y:341:LYS:NZ	2.28	0.49
1:A:756:ALA:HB1	2:Y:280:PHE:HE2	1.77	0.49
1:A:564:ASP:O	1:A:565:ASP:HB2	2.11	0.49
1:A:724:TRP:CE2	1:A:728:ILE:HD11	2.48	0.49
2:Y:38:SER:CB	2:Y:152:ILE:HG12	2.42	0.49
3:E:3:ARG:HB3	3:E:7:PHE:CE2	2.43	0.49
4:V:48:VAL:HG13	4:V:63:VAL:HG21	1.94	0.49
2:Y:21:THR:HA	2:Y:170:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:GLN:C	1:A:784:THR:H	2.13	0.49
1:A:266:MET:HG2	1:A:279:PHE:HZ	1.78	0.49
1:A:409:ARG:HH21	1:A:564:ASP:H	1.61	0.49
1:A:436:THR:HG22	1:A:437:VAL:H	1.77	0.49
4:V:109:GLN:CD	4:V:109:GLN:H	2.15	0.49
2:Y:13:ASP:OD2	2:Y:13:ASP:N	2.45	0.49
4:V:37:TYR:HD2	4:V:96:TYR:HD2	1.59	0.49
1:A:409:ARG:HG2	1:A:410:THR:H	1.77	0.49
1:A:549:PHE:CD1	1:A:585:VAL:HG22	2.48	0.49
2:Y:43:VAL:HB	2:Y:140:LEU:CD1	2.42	0.49
2:Y:54:GLY:HA3	2:Y:57:ASN:HB2	1.93	0.49
2:Y:244:GLN:O	2:Y:345:GLY:HA3	2.13	0.49
4:V:34:MET:HE2	4:V:78:VAL:HG11	1.95	0.49
1:A:262:THR:C	1:A:265:GLY:H	2.17	0.48
2:Y:362:ARG:HH21	2:Y:366:ARG:NH2	2.10	0.48
1:A:809:HIS:CE1	8:A:1011:TBR:BRB	3.21	0.48
2:Y:98:TRP:CE3	2:Y:109:LEU:HD13	2.48	0.48
2:Y:281:LEU:HD21	2:Y:315:TYR:CE1	2.48	0.48
2:Y:31:GLY:HA2	2:Y:34:ILE:HD13	1.94	0.48
1:A:242:ARG:HH22	1:A:268:LYS:CB	2.13	0.48
4:V:29:PHE:HE1	4:V:34:MET:HG3	1.79	0.48
1:A:242:ARG:HH12	1:A:268:LYS:HE2	1.78	0.48
4:V:34:MET:HB2	4:V:51:ILE:HG23	1.95	0.48
1:A:223:ILE:O	1:A:352:LEU:HB2	2.14	0.48
2:Y:45:LYS:C	2:Y:47:GLN:H	2.17	0.48
1:A:281:VAL:HG13	2:Y:348:PRO:HB3	1.95	0.48
1:A:284:VAL:C	1:A:286:LEU:H	2.17	0.48
2:Y:36:VAL:HB	2:Y:39:VAL:HG13	1.95	0.48
1:A:811:ILE:O	1:A:815:GLU:HG3	2.14	0.47
2:Y:14:ILE:HG13	2:Y:15:ARG:N	2.29	0.47
2:Y:42:ASP:OD2	4:V:50:ARG:NE	2.45	0.47
1:A:302:LYS:HD3	8:A:1007:TBR:BR3	2.69	0.47
1:A:763:ALA:HB2	2:Y:283:ALA:HA	1.96	0.47
2:Y:241:ILE:HG22	2:Y:347:ILE:HD12	1.96	0.47
4:V:48:VAL:O	4:V:60:PRO:HD2	2.15	0.47
2:Y:58:ILE:HD11	2:Y:132:PHE:HZ	1.80	0.47
2:Y:86:LEU:O	2:Y:89:MET:HG2	2.14	0.47
3:E:25:GLU:HG2	3:E:29:TYR:CD2	2.50	0.47
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.68	0.47
1:A:284:VAL:HG12	2:Y:346:TYR:OH	2.15	0.47
1:A:292:GLN:NE2	1:A:331:GLU:O	2.48	0.47

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:235:GLN:HA	2:Y:266:VAL:HG13	1.96	0.47
1:A:709:ARG:O	1:A:712:GLU:HG2	2.15	0.46
2:Y:232:ILE:CD1	3:E:29:TYR:HB3	2.45	0.46
2:Y:320:ILE:HA	2:Y:372:SER:OG	2.14	0.46
1:A:443:GLU:HB2	8:A:1007:TBR:BRC	2.71	0.46
4:V:37:TYR:HA	4:V:48:VAL:HG23	1.96	0.46
1:A:84:VAL:HG11	1:A:395:ASN:HB2	1.98	0.46
1:A:242:ARG:HH12	1:A:268:LYS:CE	2.29	0.46
1:A:259:VAL:HG22	1:A:260:GLN:H	1.80	0.46
2:Y:91:VAL:HG23	2:Y:92:VAL:HG12	1.98	0.46
2:Y:240:LYS:HD2	2:Y:261:HIS:CE1	2.51	0.46
1:A:254:ILE:HA	1:A:548:ARG:CA	2.45	0.46
2:Y:82:ILE:O	2:Y:86:LEU:HD13	2.16	0.46
2:Y:45:LYS:HG3	2:Y:48:ASP:OD1	2.15	0.46
2:Y:56:LEU:HB3	2:Y:67:PHE:O	2.16	0.46
2:Y:382:PRO:HD3	2:Y:398:GLY:O	2.15	0.46
1:A:73:SER:OG	1:A:108:LEU:HD21	2.16	0.46
1:A:301:GLN:CG	1:A:302:LYS:H	2.29	0.46
1:A:630:MET:HE3	2:Y:429:ILE:HA	1.98	0.46
8:A:1012:TBR:BR5	2:Y:289:SER:OG	2.84	0.46
2:Y:386:VAL:CA	2:Y:389:ALA:HB2	2.42	0.46
1:A:115:TYR:CE2	1:A:119:LEU:HD21	2.52	0.45
2:Y:417:GLU:OE1	8:Y:502:TBR:BR9	2.89	0.45
4:V:82:MET:HB3	4:V:85:LEU:HD11	1.98	0.45
1:A:105:GLY:O	1:A:109:THR:HG23	2.16	0.45
1:A:302:LYS:O	1:A:303:ASP:C	2.52	0.45
1:A:304:VAL:CG2	1:A:305:ASP:H	2.27	0.45
2:Y:362:ARG:HE	2:Y:366:ARG:CZ	2.29	0.45
1:A:630:MET:HE3	2:Y:429:ILE:HG23	1.97	0.45
1:A:108:LEU:O	1:A:111:THR:HG22	2.17	0.45
1:A:233:LEU:HD13	1:A:236:GLN:OE1	2.16	0.45
1:A:275:ILE:HB	1:A:283:HIS:CE1	2.52	0.45
1:A:487:ALA:HA	1:A:525:ARG:CZ	2.47	0.45
2:Y:375:LEU:O	2:Y:378:ILE:HG22	2.16	0.45
4:V:29:PHE:HE1	4:V:34:MET:SD	2.39	0.45
4:V:29:PHE:CE1	4:V:34:MET:SD	3.10	0.45
1:A:804:PHE:HE1	8:Y:502:TBR:BR2	2.55	0.45
1:A:100:MET:O	1:A:106:LYS:HE2	2.17	0.45
3:E:22:ASN:CG	3:E:23:ARG:H	2.20	0.45
1:A:464:HIS:NE2	8:A:1014:TBR:BRC	3.04	0.45
2:Y:102:GLY:C	2:Y:105:GLY:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:381:LEU:N	2:Y:382:PRO:HD2	2.32	0.45
2:Y:362:ARG:NH2	2:Y:366:ARG:HH22	2.11	0.45
1:A:329:TYR:HB3	1:A:333:LEU:HB3	1.97	0.44
1:A:561:PHE:HZ	1:A:569:ILE:CG2	2.29	0.44
1:A:769:ALA:HA	2:Y:127:GLY:O	2.17	0.44
2:Y:191:ILE:N	2:Y:192:PRO:HD2	2.32	0.44
1:A:86:LEU:O	1:A:90:VAL:HG23	2.18	0.44
1:A:242:ARG:HG2	1:A:243:THR:N	2.32	0.44
2:Y:133:ASN:HD21	2:Y:141:ILE:HG12	1.82	0.44
2:Y:238:PHE:O	3:E:18:VAL:HG13	2.17	0.44
1:A:26:ILE:HG12	1:A:63:VAL:HA	1.98	0.44
1:A:625:GLU:HG3	8:A:1010:TBR:BR9	2.72	0.44
1:A:753:ILE:HG13	2:Y:89:MET:SD	2.56	0.44
4:V:109:GLN:NE2	4:V:109:GLN:H	2.15	0.44
1:A:242:ARG:HG2	1:A:244:LEU:N	2.32	0.44
1:A:322:ARG:HA	1:A:461:ALA:CB	2.47	0.44
4:V:82:MET:CB	4:V:85:LEU:HD11	2.48	0.44
1:A:311:GLY:O	1:A:343:LEU:HD13	2.17	0.44
1:A:762:PHE:HB2	2:Y:287:ILE:HD11	1.99	0.44
2:Y:14:ILE:O	2:Y:18:ILE:N	2.49	0.44
2:Y:46:LEU:HD23	4:V:105:PRO:HG3	1.99	0.44
2:Y:54:GLY:HA3	2:Y:57:ASN:CB	2.48	0.44
2:Y:239:ARG:HB3	2:Y:264:LEU:CB	2.47	0.44
1:A:313:VAL:HG11	1:A:337:ILE:HG22	2.00	0.44
2:Y:15:ARG:HA	2:Y:18:ILE:HD12	1.99	0.44
2:Y:62:GLY:HA2	2:Y:394:SER:HA	1.99	0.44
2:Y:166:LEU:O	2:Y:170:ILE:HG22	2.17	0.44
1:A:303:ASP:HA	1:A:306:TYR:O	2.17	0.44
1:A:33:TYR:O	1:A:36:LEU:HB2	2.18	0.44
1:A:764:THR:HG23	1:A:765:VAL:HG23	2.00	0.44
1:A:266:MET:HG2	1:A:279:PHE:CE2	2.52	0.43
1:A:302:LYS:HE2	1:A:308:VAL:CG2	2.48	0.43
2:Y:160:THR:O	2:Y:164:MET:N	2.47	0.43
1:A:130:ASN:HB2	1:A:322:ARG:NH1	2.32	0.43
1:A:546:MET:SD	1:A:578:VAL:HG22	2.57	0.43
2:Y:45:LYS:NZ	2:Y:56:LEU:H	2.16	0.43
2:Y:45:LYS:HB2	2:Y:45:LYS:HE2	1.89	0.43
2:Y:313:THR:HA	2:Y:316:VAL:HG12	1.99	0.43
2:Y:275:ILE:HG12	2:Y:404:ILE:HD11	2.00	0.43
4:V:34:MET:O	4:V:50:ARG:HA	2.17	0.43
4:V:90:THR:HG23	4:V:114:THR:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:O	1:A:298:VAL:HG22	2.19	0.43
1:A:590:PHE:HE2	2:Y:103:GLU:HG2	1.82	0.43
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.79	0.43
1:A:242:ARG:HG2	1:A:244:LEU:H	1.83	0.43
1:A:295:LYS:O	1:A:299:ALA:HB3	2.19	0.43
1:A:749:LYS:HG2	1:A:750:LYS:H	1.83	0.43
2:Y:184:PHE:HD1	2:Y:405:VAL:HA	1.84	0.43
3:E:22:ASN:HB3	3:E:25:GLU:HB3	2.00	0.43
1:A:214:ILE:HG21	1:A:377:GLU:OE1	2.19	0.43
2:Y:103:GLU:HA	2:Y:103:GLU:OE1	2.18	0.43
4:V:38:ARG:NH2	4:V:89:ASP:HA	2.34	0.43
1:A:256:THR:HB	1:A:548:ARG:NH2	2.33	0.43
1:A:301:GLN:HA	1:A:301:GLN:HE21	1.83	0.43
1:A:321:GLY:HA3	1:A:485:ASN:HB2	2.01	0.43
2:Y:387:ASN:C	2:Y:389:ALA:N	2.72	0.43
2:Y:79:THR:HG23	2:Y:120:LEU:HD13	2.00	0.42
2:Y:140:LEU:HD23	2:Y:140:LEU:HA	1.72	0.42
2:Y:239:ARG:HA	3:E:18:VAL:HG22	2.01	0.42
2:Y:396:GLN:HG3	2:Y:401:SER:OG	2.19	0.42
1:A:771:TYR:HE1	2:Y:135:LEU:HD22	1.84	0.42
2:Y:84:VAL:HA	2:Y:87:LEU:HB2	2.00	0.42
4:V:7:THR:OG1	4:V:8:GLY:N	2.52	0.42
1:A:197:VAL:HG23	1:A:198:GLN:N	2.35	0.42
1:A:421:ASP:O	1:A:425:ARG:HG3	2.19	0.42
1:A:750:LYS:O	1:A:751:THR:C	2.57	0.42
2:Y:76:PRO:HA	2:Y:79:THR:HG22	2.01	0.42
2:Y:128:MET:O	2:Y:132:PHE:HB2	2.20	0.42
2:Y:229:VAL:HB	3:E:26:LEU:HD11	2.00	0.42
1:A:99:GLU:HA	1:A:371:THR:O	2.18	0.42
1:A:422:VAL:HG21	1:A:449:LEU:HD21	2.00	0.42
1:A:85:GLN:HB3	1:A:109:THR:HG22	2.01	0.42
1:A:241:VAL:HG12	1:A:242:ARG:N	2.22	0.42
1:A:493:ILE:HD12	1:A:505:LEU:HD21	2.01	0.42
1:A:770:GLN:HB3	1:A:772:GLU:HG3	2.00	0.42
3:E:25:GLU:OE2	3:E:29:TYR:HE2	2.02	0.42
4:V:97:TYR:CE2	4:V:106:TYR:HB3	2.54	0.42
1:A:244:LEU:HD13	1:A:250:TYR:N	2.35	0.42
1:A:288:HIS:CE1	1:A:292:GLN:HE21	2.37	0.42
1:A:807:PHE:O	1:A:811:ILE:HG13	2.20	0.42
2:Y:48:ASP:HA	2:Y:58:ILE:HG23	2.02	0.42
2:Y:79:THR:HA	2:Y:82:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:234:ILE:HG13	2:Y:374:PHE:CE1	2.54	0.42
2:Y:386:VAL:HA	2:Y:389:ALA:CB	2.43	0.42
1:A:115:TYR:O	1:A:119:LEU:HD22	2.19	0.42
1:A:302:LYS:HE2	1:A:308:VAL:HG21	2.02	0.42
1:A:581:SER:O	1:A:585:VAL:HG23	2.19	0.42
1:A:582:GLN:HA	1:A:585:VAL:HG23	2.01	0.42
1:A:586:GLU:HB3	8:A:1017:TBR:BR5	2.74	0.42
1:A:757:VAL:HG21	2:Y:87:LEU:HD12	2.02	0.42
1:A:275:ILE:HD12	1:A:278:LEU:HA	2.02	0.42
1:A:751:THR:HG22	1:A:754:ALA:H	1.85	0.42
2:Y:267:ASN:HA	2:Y:367:LEU:CD1	2.49	0.42
2:Y:370:VAL:HG21	3:E:15:LEU:CD1	2.42	0.42
2:Y:422:LYS:O	2:Y:426:ARG:HB2	2.20	0.42
2:Y:170:ILE:HG23	2:Y:178:GLY:HA3	2.02	0.42
2:Y:178:GLY:HA2	2:Y:181:ILE:HG12	2.01	0.42
1:A:77:THR:HG23	1:A:79:MET:H	1.84	0.41
1:A:410:THR:OG1	1:A:542:GLU:HB2	2.20	0.41
2:Y:59:PHE:CE2	2:Y:64:LEU:HD11	2.55	0.41
1:A:52:LEU:HD13	1:A:120:THR:HG23	2.02	0.41
1:A:600:ASP:O	1:A:604:ARG:N	2.46	0.41
1:A:259:VAL:HG11	2:Y:341:LYS:HG2	2.02	0.41
1:A:325:LYS:HE2	8:A:1014:TBR:BR4	2.75	0.41
1:A:688:ILE:O	1:A:692:ILE:HG13	2.19	0.41
2:Y:45:LYS:C	2:Y:47:GLN:N	2.73	0.41
2:Y:83:ILE:HG23	2:Y:87:LEU:HD13	2.03	0.41
1:A:303:ASP:HB3	1:A:439:VAL:CG2	2.51	0.41
1:A:313:VAL:HG23	1:A:334:HIS:NE2	2.35	0.41
1:A:693:ILE:HD13	8:A:1010:TBR:BRB	2.76	0.41
6:A:1002:BEF:F2	7:A:1003:ADP:O1B	2.28	0.41
2:Y:73:GLY:O	2:Y:76:PRO:HD2	2.21	0.41
1:A:47:GLU:HA	8:A:1008:TBR:BR8	2.76	0.41
1:A:458:VAL:HG11	8:A:1015:TBR:BR4	2.76	0.41
1:A:84:VAL:CG1	1:A:395:ASN:HB2	2.50	0.41
2:Y:171:THR:HB	2:Y:178:GLY:H	1.86	0.41
1:A:252:TYR:CG	1:A:255:LYS:HB2	2.56	0.41
1:A:630:MET:HG3	1:A:815:GLU:HG2	2.03	0.41
1:A:690:ASP:HA	1:A:693:ILE:HD12	2.02	0.41
2:Y:41:THR:HG22	2:Y:45:LYS:HZ3	1.85	0.41
2:Y:77:TYR:HA	2:Y:117:THR:CG2	2.51	0.41
2:Y:314:ILE:O	2:Y:318:LEU:HG	2.20	0.41
2:Y:406:VAL:HG12	3:E:33:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:36:VAL:HG12	2:Y:38:SER:H	1.86	0.41
2:Y:98:TRP:HE3	2:Y:109:LEU:HD13	1.86	0.41
2:Y:139:MET:HE3	2:Y:140:LEU:HG	2.02	0.41
3:E:16:LYS:HD2	3:E:16:LYS:O	2.21	0.41
4:V:38:ARG:H	4:V:38:ARG:HG2	1.67	0.41
4:V:99:ARG:NH2	4:V:103:SER:O	2.54	0.41
2:Y:229:VAL:O	2:Y:232:ILE:HG22	2.21	0.40
2:Y:389:ALA:HB1	2:Y:391:LEU:CB	2.50	0.40
1:A:211:SER:HA	1:A:215:ASP:HB2	2.03	0.40
1:A:458:VAL:HG11	8:A:1015:TBR:BRC	2.77	0.40
1:A:725:MET:HE3	1:A:725:MET:HB3	1.91	0.40
1:A:775:CYS:HB2	2:Y:135:LEU:HD13	2.02	0.40
2:Y:184:PHE:HE1	2:Y:405:VAL:HG13	1.87	0.40
2:Y:282:ILE:O	2:Y:285:PRO:HG2	2.22	0.40
4:V:36:TRP:CG	4:V:80:LEU:HD22	2.55	0.40
1:A:464:HIS:CD2	8:A:1014:TBR:BRC	3.29	0.40
2:Y:198:ILE:CG2	2:Y:199:TYR:H	2.33	0.40
1:A:495:LEU:HD23	1:A:528:ARG:HD2	2.03	0.40
1:A:753:ILE:HA	1:A:756:ALA:HB3	2.03	0.40
2:Y:222:LEU:O	2:Y:225:VAL:HG12	2.21	0.40
2:Y:359:TYR:O	2:Y:363:ILE:HD13	2.22	0.40
1:A:549:PHE:HD1	1:A:585:VAL:HG22	1.83	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	730/836 (87%)	676 (93%)	42 (6%)	12 (2%)	8	37
2	Y	368/424 (87%)	335 (91%)	24 (6%)	9 (2%)	5	30
3	E	54/70 (77%)	49 (91%)	4 (7%)	1 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	V	111/131 (85%)	99 (89%)	10 (9%)	2 (2%)	7	35
All	All	1263/1461 (86%)	1159 (92%)	80 (6%)	24 (2%)	6	35

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	THR
1	A	411	MET
1	A	452	LYS
1	A	782	GLN
1	A	783	HIS
2	Y	266	VAL
1	A	241	VAL
1	A	242	ARG
1	A	303	ASP
2	Y	90	ASP
2	Y	91	VAL
4	V	2	VAL
1	A	244	LEU
1	A	302	LYS
2	Y	103	GLU
1	A	485	ASN
1	A	565	ASP
2	Y	274	VAL
2	Y	46	LEU
2	Y	53	PHE
2	Y	175	VAL
3	E	21	PRO
4	V	104	GLN
2	Y	333	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/706 (88%)	598 (96%)	24 (4%)	27	53
2	Y	313/354 (88%)	293 (94%)	20 (6%)	14	42
3	E	50/63 (79%)	48 (96%)	2 (4%)	27	52
4	V	93/108 (86%)	88 (95%)	5 (5%)	18	46
All	All	1078/1231 (88%)	1027 (95%)	51 (5%)	22	48

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	59	ASP
1	A	70	ARG
1	A	119	LEU
1	A	203	PHE
1	A	207	ASP
1	A	208	GLU
1	A	209	VAL
1	A	251	THR
1	A	252	TYR
1	A	301	GLN
1	A	317	ASP
1	A	322	ARG
1	A	323	LEU
1	A	367	LEU
1	A	420	GLU
1	A	439	VAL
1	A	452	LYS
1	A	459	LEU
1	A	531	ASP
1	A	546	MET
1	A	561	PHE
1	A	735	ARG
1	A	771	TYR
2	Y	13	ASP
2	Y	23	LEU
2	Y	26	ILE
2	Y	43	VAL
2	Y	45	LYS
2	Y	46	LEU
2	Y	47	GLN
2	Y	56	LEU
2	Y	83	ILE

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Mol	Chain	Res	Type
2	Y	87	LEU
2	Y	141	ILE
2	Y	199	TYR
2	Y	216	ARG
2	Y	233	TYR
2	Y	280	PHE
2	Y	281	LEU
2	Y	302	ARG
2	Y	365	TYR
2	Y	385	PHE
2	Y	394	SER
3	E	17	LYS
3	E	26	LEU
4	V	2	VAL
4	V	38	ARG
4	V	45	ARG
4	V	99	ARG
4	V	112	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	125	HIS
1	A	140	GLN
1	A	292	GLN
1	A	301	GLN
1	A	347	ASN
1	A	383	ASN
1	A	598	GLN
1	A	605	GLN
1	A	613	GLN
1	A	629	ASN
1	A	739	HIS
2	Y	16	ASN
2	Y	66	ASN
2	Y	101	GLN
2	Y	124	GLN
2	Y	134	ASN
2	Y	169	GLN
2	Y	308	HIS
2	Y	335	GLN

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Mol	Chain	Res	Type
4	V	13	GLN

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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\#|Z| > 2$
6	BEF	A	1002	7	0,3,3	-	-	-		
8	TBR	Y	502	-	0,36,36	-	-	-		
8	TBR	A	1016	-	0,36,36	-	-	-		
8	TBR	A	1006	-	0,36,36	-	-	-		
8	TBR	A	1009	-	0,36,36	-	-	-		
7	ADP	A	1003	6,5	24,29,29	0.93	1 (4%)	29,45,45	1.28	2 (6%)
8	TBR	A	1007	-	0,36,36	-	-	-		
8	TBR	A	1010	-	0,36,36	-	-	-		
8	TBR	A	1013	-	0,36,36	-	-	-		
8	TBR	A	1008	-	0,36,36	-	-	-		
8	TBR	A	1011	-	0,36,36	-	-	-		
8	TBR	A	1005	-	0,36,36	-	-	-		
8	TBR	A	1018	-	0,36,36	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	TBR	A	1015	-	0,36,36	-	-	-		
8	TBR	A	1004	-	0,36,36	-	-	-		
8	TBR	A	1012	-	0,36,36	-	-	-		
8	TBR	Y	503	-	0,36,36	-	-	-		
8	TBR	Y	501	-	0,36,36	-	-	-		
8	TBR	A	1017	-	0,36,36	-	-	-		
8	TBR	A	1014	-	0,36,36	-	-	-		

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
7	ADP	A	1003	6,5	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1003	ADP	PA-O3A	2.15	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1003	ADP	N3-C2-N1	-3.66	123.71	128.67
7	A	1003	ADP	C4-C5-N7	-2.61	106.58	109.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1003	ADP	C5'-O5'-PA-O1A
7	A	1003	ADP	C5'-O5'-PA-O2A
7	A	1003	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

18 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	BEF	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Y	502	TBR	2	0
8	A	1016	TBR	1	0
8	A	1006	TBR	2	0
8	A	1009	TBR	1	0
7	A	1003	ADP	1	0
8	A	1007	TBR	2	0
8	A	1010	TBR	3	0
8	A	1013	TBR	2	0
8	A	1008	TBR	1	0
8	A	1011	TBR	1	0
8	A	1005	TBR	1	0
8	A	1018	TBR	1	0
8	A	1015	TBR	3	0
8	A	1004	TBR	1	0
8	A	1012	TBR	2	0
8	A	1017	TBR	2	0
8	A	1014	TBR	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 1003
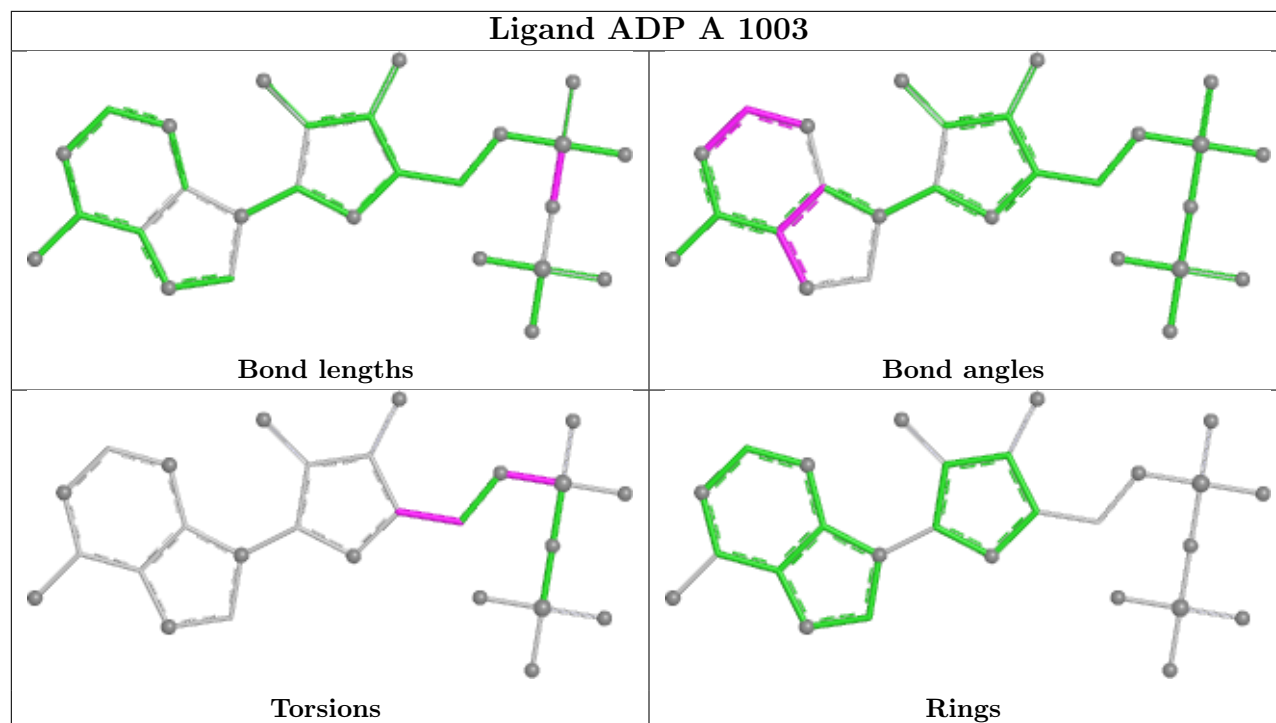
5.7 Other polymers ⓘ

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 ⓘ

Warning: The R factor obtained from EDS is 0.3527, which does not match the depositor's R factor of 0.2952. Please interpret the results in this section carefully.

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	746/836 (89%)	2.32	257 (34%)	1	2	113, 202, 268, 329	0
2	Y	380/424 (89%)	2.53	139 (36%)	1	1	116, 191, 258, 282	0
3	E	56/70 (80%)	1.10	13 (23%)	2	4	155, 220, 261, 265	0
4	V	115/131 (87%)	4.06	33 (28%)	1	2	17, 165, 219, 253	2 (1%)
All	All	1297/1461 (88%)	2.48	442 (34%)	1	2	17, 196, 261, 329	2 (0%)

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	783	HIS	47.7
1	A	784	THR	40.3
1	A	729	ASP	37.4
1	A	331	GLU	33.4
4	V	16	GLY	33.1
1	A	733	GLN	32.5
4	V	15	GLY	32.5
4	V	17	SER	31.9
2	Y	401	SER	31.8
4	V	11	LEU	31.4
2	Y	396	GLN	31.3
1	A	288	HIS	30.6
2	Y	400	THR	28.5
2	Y	344	GLY	28.4
1	A	785	PHE	26.7
4	V	14	PRO	26.6
1	A	732	ASP	26.2
2	Y	399	GLY	26.0
1	A	287	ASN	25.9

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Mol	Chain	Res	Type	RSRZ
1	A	291	ASN	24.5
4	V	10	GLY	23.8
4	V	84	SER	23.1
1	A	285	ALA	23.1
4	V	13	GLN	22.9
1	A	786	ALA	22.5
2	Y	398	GLY	22.4
4	V	19	ARG	22.2
4	V	8	GLY	21.5
4	V	9	GLY	20.8
4	V	83	ASN	20.6
4	V	12	VAL	20.3
1	A	730	ALA	19.3
1	A	284	VAL	18.6
2	Y	187	ILE	18.5
2	Y	397	ILE	17.0
2	Y	244	GLN	16.3
4	V	18	LEU	16.0
2	Y	346	TYR	16.0
2	Y	345	GLY	16.0
1	A	292	GLN	15.6
2	Y	186	GLY	15.6
1	A	554	THR	14.8
2	Y	279	SER	14.5
4	V	116	SER	14.4
1	A	781	ARG	14.2
1	A	736	GLN	14.1
1	A	726	ASP	14.0
2	Y	402	LEU	13.9
1	A	728	ILE	12.9
2	Y	75	MET	12.8
2	Y	341	LYS	12.8
2	Y	404	ILE	12.7
1	A	257	LYS	12.7
1	A	286	LEU	12.5
1	A	289	HIS	12.2
2	Y	74	VAL	12.1
2	Y	275	ILE	11.7
4	V	85	LEU	11.7
1	A	707	GLN	11.6
1	A	541	MET	11.5
1	A	795	PRO	11.4

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Mol	Chain	Res	Type	RSRZ
2	Y	379	ALA	11.3
1	A	780	GLU	11.2
2	Y	378	ILE	10.8
2	Y	343	GLN	10.7
1	A	281	VAL	10.5
2	Y	73	GLY	10.5
1	A	558	LEU	10.4
1	A	764	THR	10.3
2	Y	183	ILE	10.2
1	A	553	ARG	10.2
1	A	219	THR	10.1
1	A	354	THR	10.1
2	Y	278	VAL	10.1
1	A	260	GLN	10.1
4	V	114	THR	10.0
1	A	549	PHE	10.0
1	A	259	VAL	10.0
1	A	397	PRO	9.9
1	A	740	LEU	9.3
1	A	218	ARG	9.2
1	A	767	SER	9.0
1	A	563	MET	8.7
1	A	787	GLY	8.7
1	A	290	ILE	8.7
2	Y	405	VAL	8.6
4	V	110	GLY	8.6
1	A	560	ARG	8.5
3	E	11	VAL	8.4
3	E	8	PHE	8.4
1	A	557	MET	8.3
4	V	65	GLY	8.3
1	A	295	LYS	8.3
2	Y	377	PHE	8.2
4	V	7	THR	8.2
1	A	791	ALA	8.2
1	A	220	PRO	8.0
2	Y	273	PRO	8.0
1	A	258	ALA	7.8
1	A	465	GLU	7.8
1	A	714	VAL	7.8
2	Y	331	VAL	7.7
2	Y	342	LYS	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	706	GLU	7.6
4	V	115	VAL	7.5
1	A	743	SER	7.5
2	Y	380	VAL	7.5
1	A	796	LEU	7.4
1	A	574	VAL	7.3
2	Y	264	LEU	7.3
2	Y	406	VAL	7.3
1	A	555	MET	7.3
2	Y	72	MET	7.2
2	Y	376	ALA	7.2
1	A	742	GLY	7.1
2	Y	316	VAL	7.0
2	Y	369	LEU	7.0
1	A	351	THR	7.0
2	Y	393	PRO	7.0
1	A	782	GLN	6.9
2	Y	403	LEU	6.9
2	Y	190	GLY	6.7
1	A	386	ASN	6.7
2	Y	315	TYR	6.7
2	Y	13	ASP	6.6
1	A	353	ALA	6.6
2	Y	263	PRO	6.6
1	A	332	GLY	6.6
2	Y	262	LEU	6.6
1	A	776	SER	6.5
2	Y	15	ARG	6.5
1	A	453	GLY	6.4
1	A	407	ILE	6.4
1	A	253	ASP	6.3
2	Y	373	LEU	6.3
1	A	272	ALA	6.3
2	Y	282	ILE	6.3
2	Y	265	LYS	6.3
1	A	738	ILE	6.2
1	A	569	ILE	6.2
2	Y	332	ASN	6.1
2	Y	70	PHE	6.1
1	A	171	ASP	6.1
2	Y	319	ILE	6.0
2	Y	189	SER	6.0

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Mol	Chain	Res	Type	RSRZ
4	V	81	GLN	6.0
1	A	789	PRO	6.0
1	A	559	ASP	5.9
2	Y	28	PHE	5.9
1	A	240	PHE	5.9
1	A	760	ALA	5.9
2	Y	188	VAL	5.8
2	Y	259	SER	5.8
2	Y	79	THR	5.8
1	A	330	SER	5.7
2	Y	64	LEU	5.7
1	A	162	ASP	5.7
2	Y	227	VAL	5.7
1	A	797	ARG	5.6
1	A	221	LEU	5.6
2	Y	124	GLN	5.6
1	A	530	GLY	5.6
1	A	222	ILE	5.6
2	Y	16	ASN	5.4
1	A	223	ILE	5.4
1	A	592	SER	5.3
1	A	710	GLU	5.3
2	Y	382	PRO	5.3
1	A	727	HIS	5.2
4	V	66	ARG	5.2
1	A	561	PHE	5.2
1	A	389	VAL	5.2
2	Y	14	ILE	5.2
1	A	185	LEU	5.1
1	A	294	LEU	5.1
4	V	25	SER	5.1
1	A	273	PHE	5.0
2	Y	71	ALA	5.0
1	A	711	PHE	5.0
2	Y	381	LEU	5.0
1	A	388	GLN	5.0
1	A	741	ARG	5.0
2	Y	49	GLN	5.0
3	E	31	ALA	5.0
1	A	731	MET	4.9
1	A	739	HIS	4.9
1	A	798	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	551	ALA	4.9
1	A	279	PHE	4.8
2	Y	160	THR	4.8
2	Y	303	THR	4.8
1	A	725	MET	4.8
1	A	118	ALA	4.8
1	A	556	ALA	4.8
1	A	568	PRO	4.8
1	A	491	THR	4.8
4	V	109	GLN	4.7
1	A	160	SER	4.7
1	A	237	ALA	4.7
2	Y	276	PHE	4.7
2	Y	375	LEU	4.7
1	A	775	CYS	4.7
1	A	790	GLY	4.6
2	Y	392	PRO	4.6
1	A	488	GLY	4.6
1	A	269	ALA	4.6
1	A	396	ARG	4.5
2	Y	317	VAL	4.5
1	A	149	GLY	4.5
1	A	454	ILE	4.4
3	E	4	VAL	4.4
1	A	150	LEU	4.4
1	A	123	GLY	4.4
1	A	110	SER	4.4
2	Y	163	LEU	4.3
1	A	239	ALA	4.3
1	A	737	GLY	4.3
1	A	777	GLY	4.3
1	A	546	MET	4.2
2	Y	352	PRO	4.2
1	A	452	LYS	4.1
1	A	200	PRO	4.1
3	E	19	SER	4.1
2	Y	226	ALA	4.1
1	A	151	THR	4.0
1	A	532	PRO	4.0
1	A	763	ALA	4.0
1	A	121	GLY	4.0
1	A	501	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	Y	60	CYS	3.9
1	A	381	PHE	3.9
4	V	82	MET	3.9
1	A	157	ASN	3.9
2	Y	78	ILE	3.9
2	Y	240	LYS	3.9
4	V	21	SER	3.9
1	A	548	ARG	3.8
1	A	24	ASN	3.8
2	Y	411	GLU	3.8
2	Y	336	MET	3.8
2	Y	366	ARG	3.8
1	A	779	LEU	3.8
1	A	806	MET	3.8
2	Y	168	GLU	3.8
3	E	17	LYS	3.8
1	A	355	ILE	3.8
1	A	550	GLY	3.7
1	A	562	GLY	3.7
1	A	350	MET	3.7
1	A	20	GLU	3.7
1	A	378	GLU	3.7
2	Y	241	ILE	3.7
1	A	250	TYR	3.7
2	Y	162	PHE	3.7
2	Y	330	GLN	3.6
1	A	224	SER	3.6
1	A	466	ARG	3.6
2	Y	77	TYR	3.6
1	A	122	LYS	3.6
1	A	492	ASP	3.6
1	A	215	ASP	3.5
1	A	575	SER	3.5
1	A	45	THR	3.5
1	A	148	LEU	3.5
1	A	774	GLY	3.5
1	A	109	THR	3.5
2	Y	335	GLN	3.5
1	A	172	ILE	3.5
2	Y	281	LEU	3.5
2	Y	306	TYR	3.5
4	V	44	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	158	SER	3.4
1	A	256	THR	3.4
1	A	169	ALA	3.4
1	A	487	ALA	3.4
2	Y	365	TYR	3.4
1	A	299	ALA	3.4
1	A	455	PRO	3.4
2	Y	76	PRO	3.4
2	Y	111	GLN	3.4
1	A	152	VAL	3.3
2	Y	238	PHE	3.3
1	A	195	GLN	3.3
1	A	545	LEU	3.3
4	V	112	GLN	3.3
1	A	115	TYR	3.3
1	A	111	THR	3.3
1	A	547	ARG	3.3
1	A	567	THR	3.3
2	Y	394	SER	3.3
1	A	601	ASP	3.3
2	Y	348	PRO	3.2
3	E	21	PRO	3.2
2	Y	61	GLY	3.2
2	Y	17	LYS	3.2
1	A	713	LYS	3.2
3	E	27	VAL	3.2
3	E	34	LEU	3.1
3	E	5	THR	3.1
1	A	25	ASP	3.1
1	A	565	ASP	3.1
1	A	347	ASN	3.1
1	A	170	ALA	3.0
1	A	514	GLU	3.0
1	A	788	GLY	3.0
2	Y	333	PRO	3.0
1	A	589	ASN	3.0
2	Y	385	PHE	3.0
1	A	107	THR	3.0
1	A	199	ARG	3.0
1	A	333	LEU	3.0
1	A	352	LEU	3.0
1	A	734	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	Y	286	THR	3.0
2	Y	65	GLN	3.0
1	A	41	LEU	2.9
1	A	474	ALA	2.9
1	A	245	LYS	2.9
1	A	385	TYR	2.9
1	A	771	TYR	2.9
1	A	22	ILE	2.9
2	Y	277	ALA	2.9
2	Y	156	LEU	2.9
1	A	596	LEU	2.9
1	A	471	ILE	2.8
1	A	274	GLY	2.8
1	A	382	ARG	2.8
2	Y	236	GLN	2.8
1	A	114	VAL	2.8
2	Y	108	LYS	2.8
1	A	799	TYR	2.8
2	Y	414	LYS	2.8
2	Y	339	ASN	2.8
1	A	766	ALA	2.8
1	A	140	GLN	2.8
4	V	111	THR	2.8
1	A	108	LEU	2.8
2	Y	225	VAL	2.8
2	Y	104	MET	2.8
1	A	228	ALA	2.8
2	Y	55	VAL	2.8
1	A	54	LYS	2.8
1	A	525	ARG	2.7
1	A	119	LEU	2.7
1	A	191	LEU	2.7
1	A	573	MET	2.7
1	A	708	MET	2.7
1	A	595	GLN	2.7
1	A	606	GLN	2.7
2	Y	159	GLY	2.7
3	E	6	ASN	2.7
2	Y	429	ILE	2.7
4	V	20	LEU	2.7
1	A	633	SER	2.7
2	Y	229	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	18	VAL	2.6
2	Y	82	ILE	2.6
1	A	409	ARG	2.6
2	Y	193	THR	2.6
2	Y	274	VAL	2.6
2	Y	179	ILE	2.6
2	Y	280	PHE	2.6
1	A	441	THR	2.6
1	A	486	MET	2.6
1	A	145	PHE	2.6
1	A	615	PHE	2.6
1	A	456	HIS	2.6
1	A	800	GLN	2.5
1	A	230	SER	2.5
2	Y	228	ILE	2.5
2	Y	430	LYS	2.5
1	A	112	LEU	2.5
1	A	214	ILE	2.5
1	A	493	ILE	2.5
1	A	603	LEU	2.5
2	Y	194	ILE	2.5
1	A	227	ALA	2.4
1	A	161	LYS	2.4
2	Y	54	GLY	2.4
1	A	141	MET	2.4
1	A	310	ASP	2.4
1	A	276	ASP	2.4
2	Y	180	SER	2.4
2	Y	267	ASN	2.4
1	A	31	GLY	2.4
2	Y	177	ASN	2.4
1	A	186	ARG	2.4
1	A	735	ARG	2.4
1	A	577	ALA	2.4
1	A	384	ILE	2.4
1	A	761	GLY	2.4
1	A	636	GLU	2.4
1	A	512	ARG	2.3
2	Y	395	ALA	2.3
1	A	602	VAL	2.3
2	Y	418	SER	2.3
1	A	349	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	370	MET	2.3
2	Y	408	VAL	2.3
1	A	18	ARG	2.3
1	A	629	ASN	2.3
1	A	261	LEU	2.2
1	A	293	ALA	2.2
2	Y	237	ALA	2.2
2	Y	239	ARG	2.2
4	V	87	PRO	2.2
1	A	585	VAL	2.2
2	Y	184	PHE	2.2
1	A	380	GLU	2.2
1	A	100	MET	2.2
1	A	449	LEU	2.2
1	A	42	LYS	2.2
1	A	390	VAL	2.2
1	A	137	ASP	2.2
2	Y	224	VAL	2.1
1	A	717	LEU	2.1
1	A	34	GLU	2.1
1	A	174	TYR	2.1
2	Y	105	GLY	2.1
2	Y	18	ILE	2.1
4	V	39	GLN	2.1
2	Y	310	VAL	2.1
1	A	21	LYS	2.1
1	A	457	GLN	2.1
2	Y	62	GLY	2.1
1	A	79	MET	2.1
1	A	566	SER	2.1
1	A	450	LYS	2.1
1	A	588	ASN	2.1
1	A	765	VAL	2.1
2	Y	266	VAL	2.1
3	E	12	VAL	2.1
1	A	531	ASP	2.0
1	A	81	PRO	2.0
1	A	193	LYS	2.0
2	Y	349	GLY	2.0
1	A	582	GLN	2.0
1	A	576	ARG	2.0
2	Y	350	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	106	LYS	2.0
1	A	632	LYS	2.0
2	Y	114	ARG	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 monosaccharides 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.
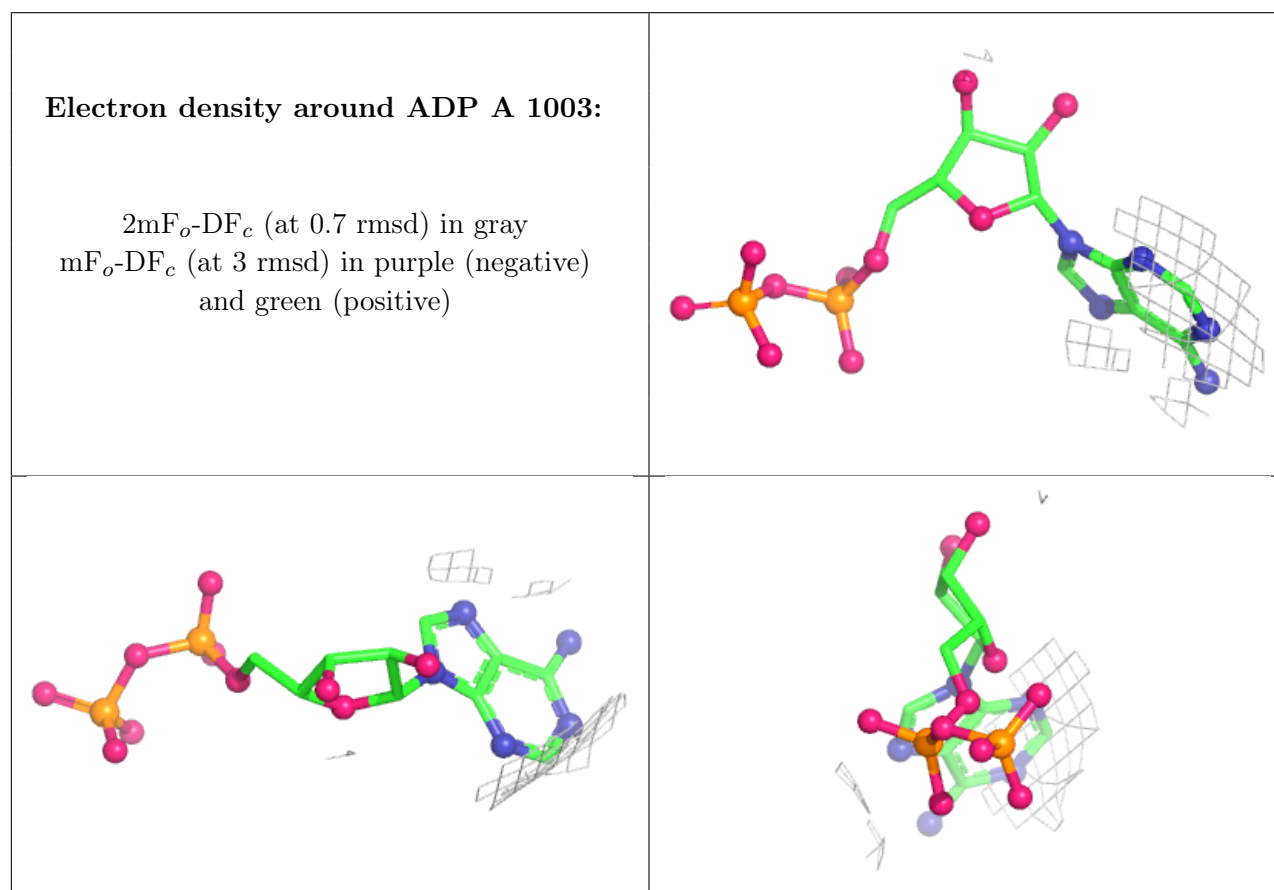
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	1001	1/1	0.55	0.32	156,156,156,156	0
8	TBR	Y	503	18/18	0.62	0.15	222,330,362,376	18
8	TBR	A	1018	18/18	0.64	0.14	249,294,327,336	18
8	TBR	A	1017	18/18	0.65	0.12	239,281,307,310	18
8	TBR	A	1014	18/18	0.66	0.11	256,294,322,323	18
8	TBR	A	1010	18/18	0.70	0.10	320,422,488,488	18
6	BEF	A	1002	4/4	0.71	0.14	248,258,259,292	0
8	TBR	A	1016	18/18	0.74	0.15	205,240,270,278	18
7	ADP	A	1003	27/27	0.76	0.12	217,228,242,264	0
8	TBR	A	1009	18/18	0.78	0.10	315,412,481,486	18
8	TBR	A	1006	18/18	0.79	0.08	261,311,368,380	18
8	TBR	A	1015	18/18	0.83	0.18	150,184,202,207	18
8	TBR	Y	502	18/18	0.84	0.12	214,274,323,365	18
8	TBR	A	1013	18/18	0.88	0.15	212,254,282,284	18
8	TBR	Y	501	18/18	0.88	0.10	247,285,334,358	18
8	TBR	A	1008	18/18	0.89	0.15	216,259,385,416	18
8	TBR	A	1007	18/18	0.90	0.08	204,235,270,286	18
8	TBR	A	1004	18/18	0.92	0.06	267,292,333,345	0
8	TBR	A	1005	18/18	0.92	0.06	296,311,356,389	18
8	TBR	A	1011	18/18	0.94	0.06	249,291,340,349	18

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	TBR	A	1012	18/18	0.95	0.05	262,342,436,479	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 1003:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.