Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 09:12 am BST

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)

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 (i) symbol.

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

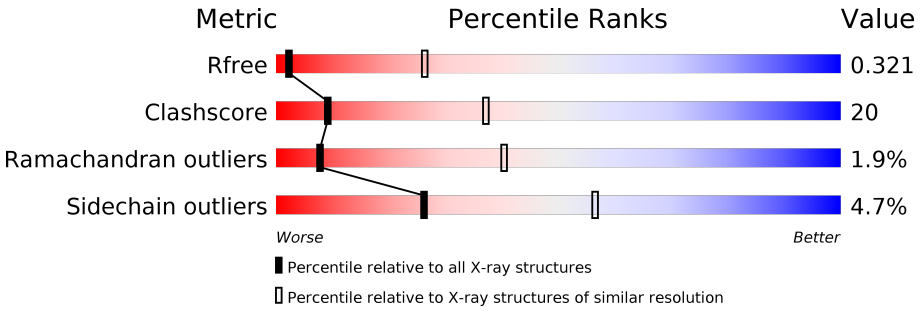
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)

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 on 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	60% 25% • • 11%
2	Y	424	49% 35% • • 10%
3	E	70	56% 23% • 20%
4	V	131	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 criteria:

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	C	N	O	S	0	0	0
			5876	3677	1030	1135	34			

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	C	N	O	S	0	0	0
			2936	1951	478	495	12			

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
3	E	56	Total	C	N	O	0	0	0
			460	306	78	76			

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

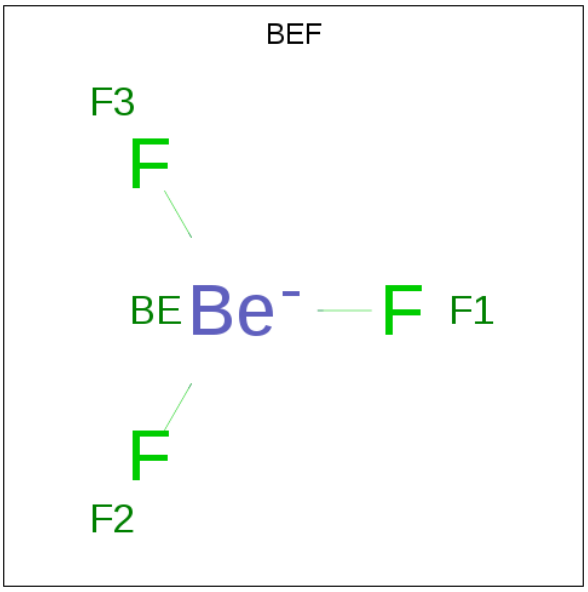
- Molecule 4 is a protein called AYC08.

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

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

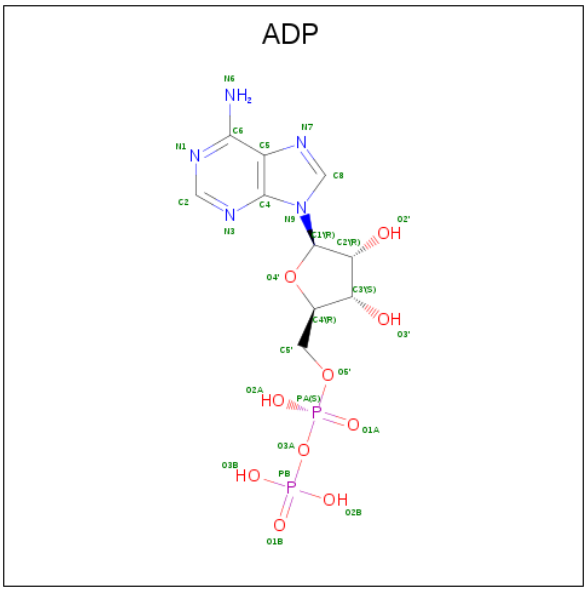
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

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



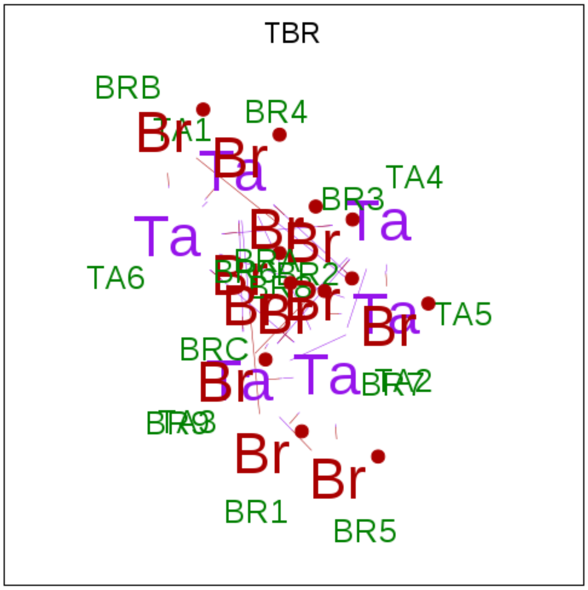
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Be	F			
6	A	1	4	1	3		0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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 Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0
8	A	1	Total Br Ta 18 12 6	0	0

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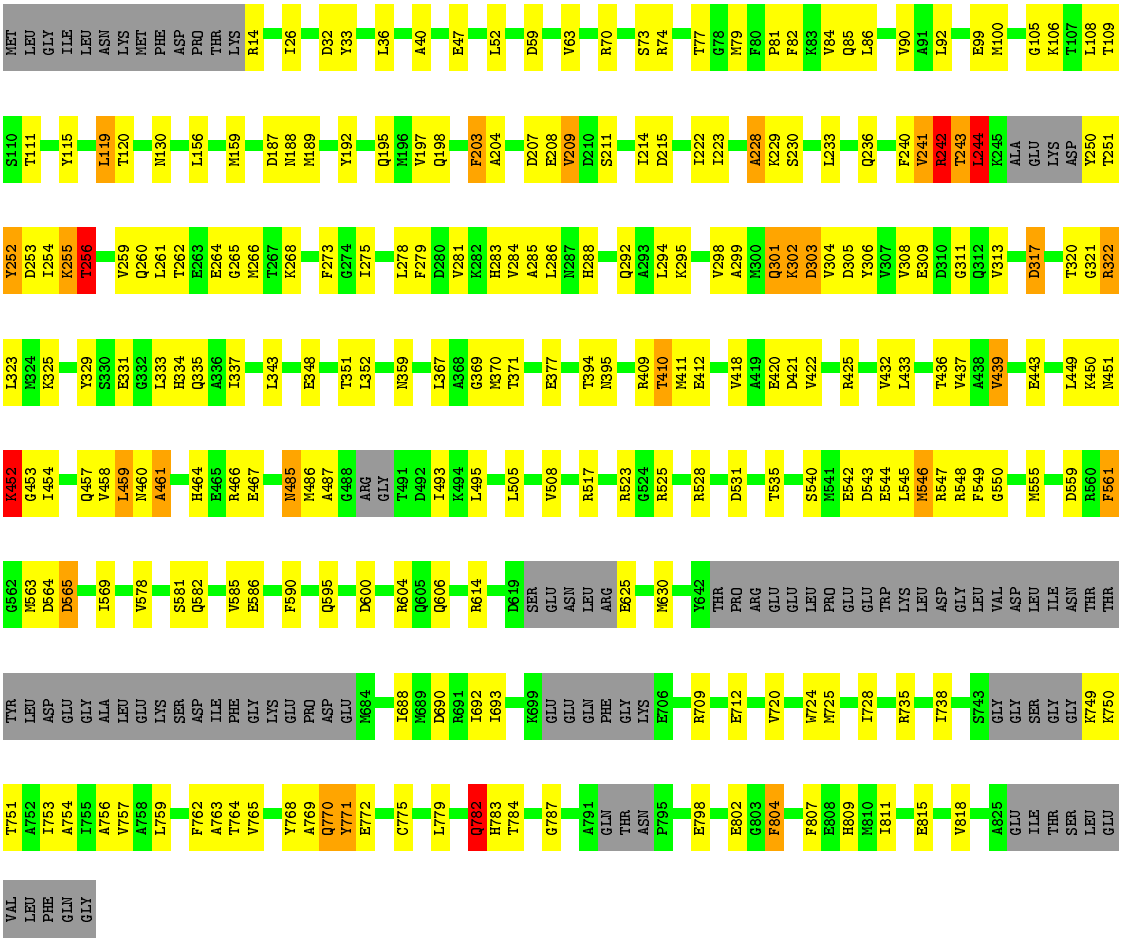
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Br Ta 18 12 6	0	0
8	Y	1	Total Br Ta 18 12 6	0	0
8	Y	1	Total Br Ta 18 12 6	0	0
8	Y	1	Total Br Ta 18 12 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

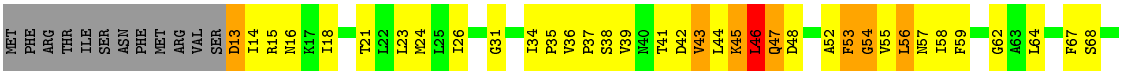
- Molecule 1: Protein translocase subunit SecA, Insertion Peptide Chimera

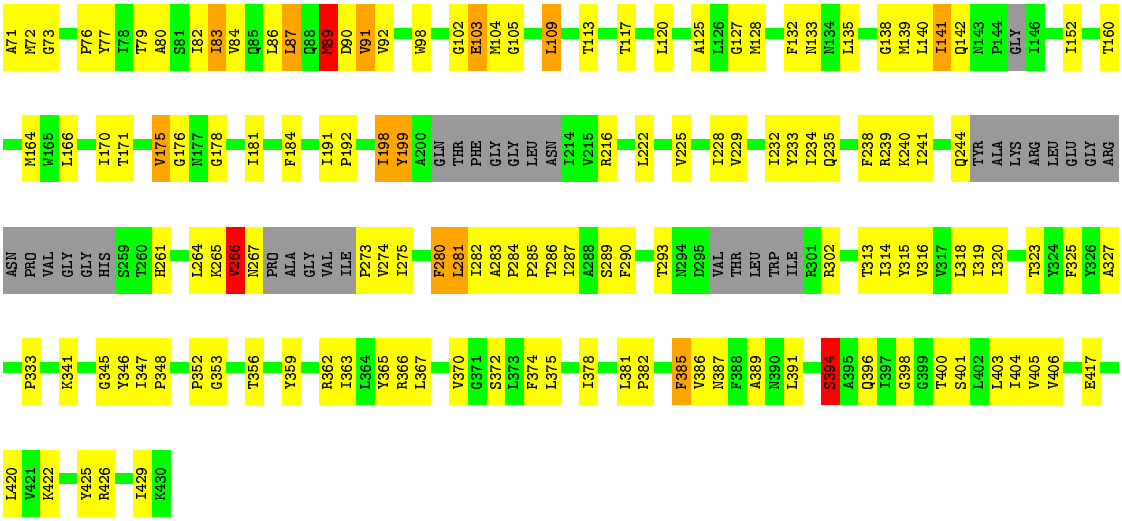
Chain A:



- Molecule 2: Protein translocase subunit SecY

Chain Y:



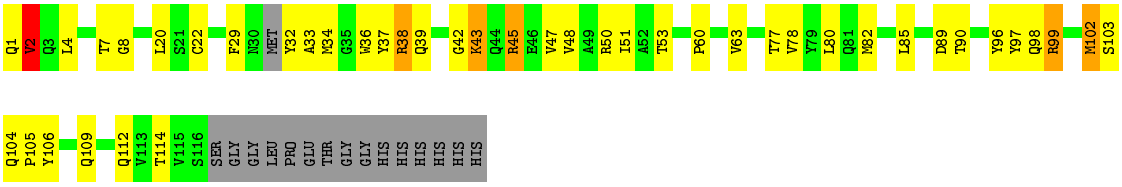


- Molecule 3: Preprotein translocase SecE subunit

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 – 3.70 110.68 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.85-3.70) 99.9 (110.68-3.70)	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 0.298 , 0.321	Depositor DCC
R_{free} test set	1513 reflections (5.06%)	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)	0.32 , 176.0	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	0.66	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.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TBR, BEF, 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(^{o})	Ideal(^{o})
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 (i)

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:461:ALA:HA	1:A:464:HIS:HB3	1.71	0.71
1:A:254:ILE:HA	1:A:548:ARG:HB3	1.72	0.71
1:A:782:GLN:O	1:A:784:THR:N	2.20	0.71
1:A:261:LEU:HD22	2:Y:341:LYS:HZ3	1.56	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:281:LEU:HD21	2:Y:315:TYR:CZ	2.30	0.67
2:Y:43:VAL:HB	2:Y:140:LEU:HD12	1.75	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
4:V:32:TYR:HA	4:V:99:ARG:HA	1.80	0.62
2:Y:86:LEU:HD21	2:Y:280:PHE:CZ	2.35	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:595:GLN:HB2	8:A:1004:TBR:BR2	2.57	0.59
1:A:228:ALA:HB1	1:A:230:SER:HB3	1.85	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:450:LYS:HD3	8:A:1015:TBR:BRA	2.62	0.55
1:A:236:GLN:HB3	1:A:273:PHE:HE1	1.71	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: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:41:THR:HG22	2:Y:45:LYS:NZ	2.23	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:273:PRO:HB3	2:Y:327:ALA:CB	2.39	0.52
2:Y:45:LYS:HZ1	2:Y:55:VAL:HG23	1.74	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:693:ILE:HG23	8:A:1010:TBR:BR7	2.65	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
2:Y:16:ASN:HD22	2:Y:16:ASN:N	2.09	0.51
1:A:192:TYR:HB2	1:A:195:GLN:HG2	1.93	0.51
1:A:348:GLU:OE2	8:A:1013:TBR:BR2	2.84	0.50
1:A:14:ARG:NH1	8:A:1018:TBR:BR1	2.99	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
3:E:15:LEU:O	3:E:18:VAL:HB	2.12	0.50
2:Y:36:VAL:CG1	2:Y:152:ILE:HG13	2.42	0.50
2:Y:283:ALA:HB3	2:Y:284:PRO:HD3	1.94	0.50
2:Y:267:ASN:HA	2:Y:367:LEU:HD11	1.94	0.50
2:Y:91:VAL:HG23	2:Y:92:VAL:N	2.19	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
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:38:SER:CB	2:Y:152:ILE:HG12	2.42	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:H	4:V:109:GLN:CD	2.15	0.49
2:Y:13:ASP:N	2:Y:13:ASP:OD2	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
4:V:34:MET:HE2	4:V:78:VAL:HG11	1.95	0.49
2:Y:43:VAL:HB	2:Y:140:LEU:CD1	2.42	0.49
2:Y:244:GLN:O	2:Y:345:GLY:HA3	2.13	0.49
2:Y:54:GLY:HA3	2:Y:57:ASN:HB2	1.93	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
3:E:25:GLU:HG2	3:E:29:TYR:CD2	2.50	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
1:A:244:LEU:HA	1:A:244:LEU:HD23	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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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:259:VAL:HG22	1:A:260:GLN:H	1.80	0.46
1:A:242:ARG:HH12	1:A:268:LYS:CE	2.29	0.46
1:A:84:VAL:HG11	1:A:395:ASN:HB2	1.98	0.46
2:Y:240:LYS:HD2	2:Y:261:HIS:CE1	2.51	0.46
2:Y:91:VAL:HG23	2:Y:92:VAL:HG12	1.98	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:382:PRO:HD3	2:Y:398:GLY:O	2.15	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
8:A:1012:TBR:BR5	2:Y:289:SER:OG	2.84	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
1:A:73:SER:OG	1:A:108:LEU:HD21	2.16	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
4:V:82:MET:HB3	4:V:85:LEU:HD11	1.98	0.45
2:Y:417:GLU:OE1	8:Y:502:TBR:BR9	2.89	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
4:V:29:PHE:CE1	4:V:34:MET:SD	3.10	0.45
4:V:29:PHE:HE1	4:V:34:MET:SD	2.39	0.45
2:Y:375:LEU:O	2:Y:378:ILE:HG22	2.16	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:242:ARG:HG2	1:A:243:THR:N	2.32	0.44
1:A:86:LEU:O	1:A:90:VAL:HG23	2.18	0.44
2:Y:238:PHE:O	3:E:18:VAL:HG13	2.17	0.44
2:Y:133:ASN:HD21	2:Y:141:ILE:HG12	1.82	0.44
1:A:625:GLU:HG3	8:A:1010:TBR:BR9	2.72	0.44
1:A:26:ILE:HG12	1:A:63:VAL:HA	1.98	0.44
1:A:753:ILE:HG13	2:Y:89:MET:SD	2.56	0.44
4:V:109:GLN:H	4:V:109:GLN:NE2	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:46:LEU:HD23	4:V:105:PRO:HG3	1.99	0.44
2:Y:14:ILE:O	2:Y:18:ILE:N	2.49	0.44
2:Y:239:ARG:HB3	2:Y:264:LEU:CB	2.47	0.44
2:Y:54:GLY:HA3	2:Y:57:ASN:CB	2.48	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:313:THR:HA	2:Y:316:VAL:HG12	1.99	0.43
2:Y:45:LYS:HE2	2:Y:45:LYS:HB2	1.89	0.43
2:Y:45:LYS:NZ	2:Y:56:LEU:H	2.16	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
2:Y:275:ILE:HG12	2:Y:404:ILE:HD11	2.00	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
3:E:22:ASN:HB3	3:E:25:GLU:HB3	2.00	0.43
2:Y:184:PHE:HD1	2:Y:405:VAL:HA	1.84	0.43
1:A:214:ILE:HG21	1:A:377:GLU:OE1	2.19	0.43
4:V:38:ARG:NH2	4:V:89:ASP:HA	2.34	0.43
2:Y:103:GLU:HA	2:Y:103:GLU:OE1	2.18	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
1:A:256:THR:HB	1:A:548:ARG:NH2	2.33	0.43
2:Y:387:ASN:C	2:Y:389:ALA:N	2.72	0.43
2:Y:140:LEU:HA	2:Y:140:LEU:HD23	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
2:Y:79:THR:HG23	2:Y:120:LEU:HD13	2.00	0.42
1:A:771:TYR:HE1	2:Y:135:LEU:HD22	1.84	0.42
4:V:7:THR:OG1	4:V:8:GLY:N	2.52	0.42
2:Y:84:VAL:HA	2:Y:87:LEU:HB2	2.00	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:229:VAL:HB	3:E:26:LEU:HD11	2.00	0.42
2:Y:128:MET:O	2:Y:132:PHE:HB2	2.20	0.42
2:Y:76:PRO:HA	2:Y:79:THR:HG22	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:410:THR:OG1	1:A:542:GLU:HB2	2.20	0.41
1:A:77:THR:HG23	1:A:79:MET:H	1.84	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:313:VAL:HG23	1:A:334:HIS:NE2	2.35	0.41
1:A:303:ASP:HB3	1:A:439:VAL:CG2	2.51	0.41
6:A:1002:BEF:F2	7:A:1003:ADP:O1B	2.28	0.41
1:A:693:ILE:HD13	8:A:1010:TBR:BRB	2.76	0.41
2:Y:73:GLY:O	2:Y:76:PRO:HD2	2.21	0.41
1:A:458:VAL:HG11	8:A:1015:TBR:BR4	2.76	0.41
1:A:47:GLU:HA	8:A:1008:TBR:BR8	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:16:LYS:O	3:E:16:LYS:HD2	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: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
2:Y:36:VAL:HG12	2:Y:38:SER:H	1.86	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:458:VAL:HG11	8:A:1015:TBR:BRC	2.77	0.40
1:A:211:SER:HA	1:A:215:ASP:HB2	2.03	0.40
1:A:725:MET:HB3	1:A:725:MET:HE3	1.91	0.40
1:A:775:CYS:HB2	2:Y:135:LEU:HD13	2.02	0.40
4:V:36:TRP:CG	4:V:80:LEU:HD22	2.55	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
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 (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	730/836 (87%)	676 (93%)	42 (6%)	12 (2%)	9 43
2	Y	368/424 (87%)	335 (91%)	24 (6%)	9 (2%)	6 35
3	E	54/70 (77%)	49 (91%)	4 (7%)	1 (2%)	8 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	V	111/131 (85%)	99 (89%)	10 (9%)	2 (2%)	8 41
All	All	1263/1461 (86%)	1159 (92%)	80 (6%)	24 (2%)	8 40

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 (i)

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%)	32	60
2	Y	313/354 (88%)	293 (94%)	20 (6%)	17	48
3	E	50/63 (79%)	48 (96%)	2 (4%)	31	60
4	V	93/108 (86%)	88 (95%)	5 (5%)	22	54
All	All	1078/1231 (88%)	1027 (95%)	51 (5%)	26	56

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

Some 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 carbohydrates 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	$\#\|Z\| > 2$
8	TBR	Y	502	-	0,36,36	0.00	-	-		
8	TBR	A	1006	-	0,36,36	0.00	-	-		
8	TBR	A	1012	-	0,36,36	0.00	-	-		
8	TBR	A	1014	-	0,36,36	0.00	-	-		
8	TBR	A	1004	-	0,36,36	0.00	-	-		
8	TBR	A	1005	-	0,36,36	0.00	-	-		
6	BEF	A	1002	7	0,3,3	0.00	-	-		
8	TBR	A	1008	-	0,36,36	0.00	-	-		
8	TBR	A	1016	-	0,36,36	0.00	-	-		
8	TBR	Y	501	-	0,36,36	0.00	-	-		
8	TBR	A	1018	-	0,36,36	0.00	-	-		
8	TBR	A	1015	-	0,36,36	0.00	-	-		
8	TBR	A	1013	-	0,36,36	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	TBR	Y	503	-	0,36,36	0.00	-	-		
8	TBR	A	1010	-	0,36,36	0.00	-	-		
8	TBR	A	1017	-	0,36,36	0.00	-	-		
8	TBR	A	1007	-	0,36,36	0.00	-	-		
7	ADP	A	1003	1,5,6	24,29,29	0.95	1 (4%)	29,45,45	1.35	4 (13%)
8	TBR	A	1009	-	0,36,36	0.00	-	-		
8	TBR	A	1011	-	0,36,36	0.00	-	-		

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	1,5,6	-	4/12/32/32	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	C5-C4	2.49	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1003	ADP	N3-C2-N1	-3.18	123.71	128.68
7	A	1003	ADP	C4-C5-N7	-2.70	106.58	109.40
7	A	1003	ADP	C3'-C2'-C1'	2.40	104.59	100.98
7	A	1003	ADP	PA-O3A-PB	-2.11	125.59	132.83

There are no chirality outliers.

All (4) 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	C5'-O5'-PA-O3A
7	A	1003	ADP	C3'-C4'-C5'-O5'

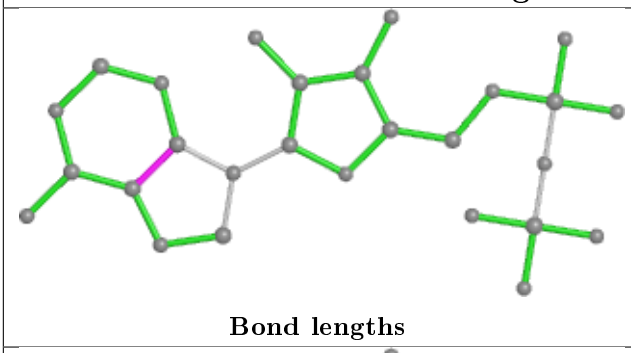
There are no ring outliers.

18 monomers are involved in 31 short contacts:

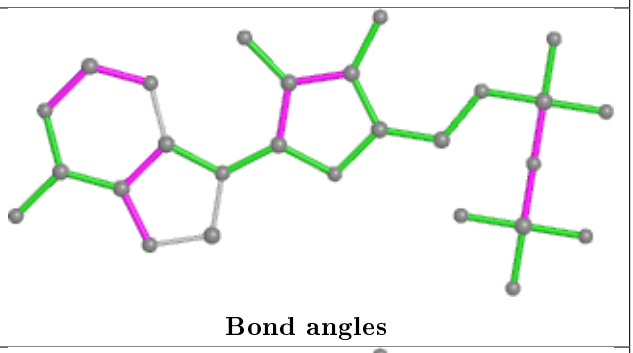
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Y	502	TBR	2	0
8	A	1006	TBR	2	0
8	A	1012	TBR	2	0
8	A	1014	TBR	5	0
8	A	1004	TBR	1	0
8	A	1005	TBR	1	0
6	A	1002	BEF	1	0
8	A	1008	TBR	1	0
8	A	1016	TBR	1	0
8	A	1018	TBR	1	0
8	A	1015	TBR	3	0
8	A	1013	TBR	2	0
8	A	1010	TBR	3	0
8	A	1017	TBR	2	0
8	A	1007	TBR	2	0
7	A	1003	ADP	1	0
8	A	1009	TBR	1	0
8	A	1011	TBR	1	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.

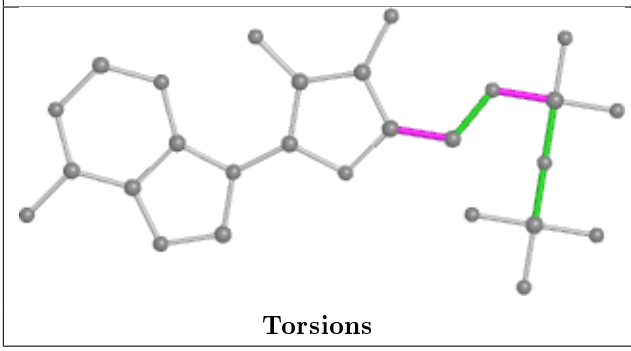
Ligand ADP A 1003



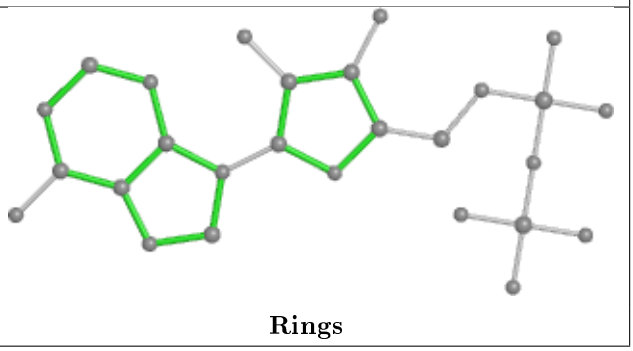
Bond lengths



Bond angles



Torsions



Rings

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

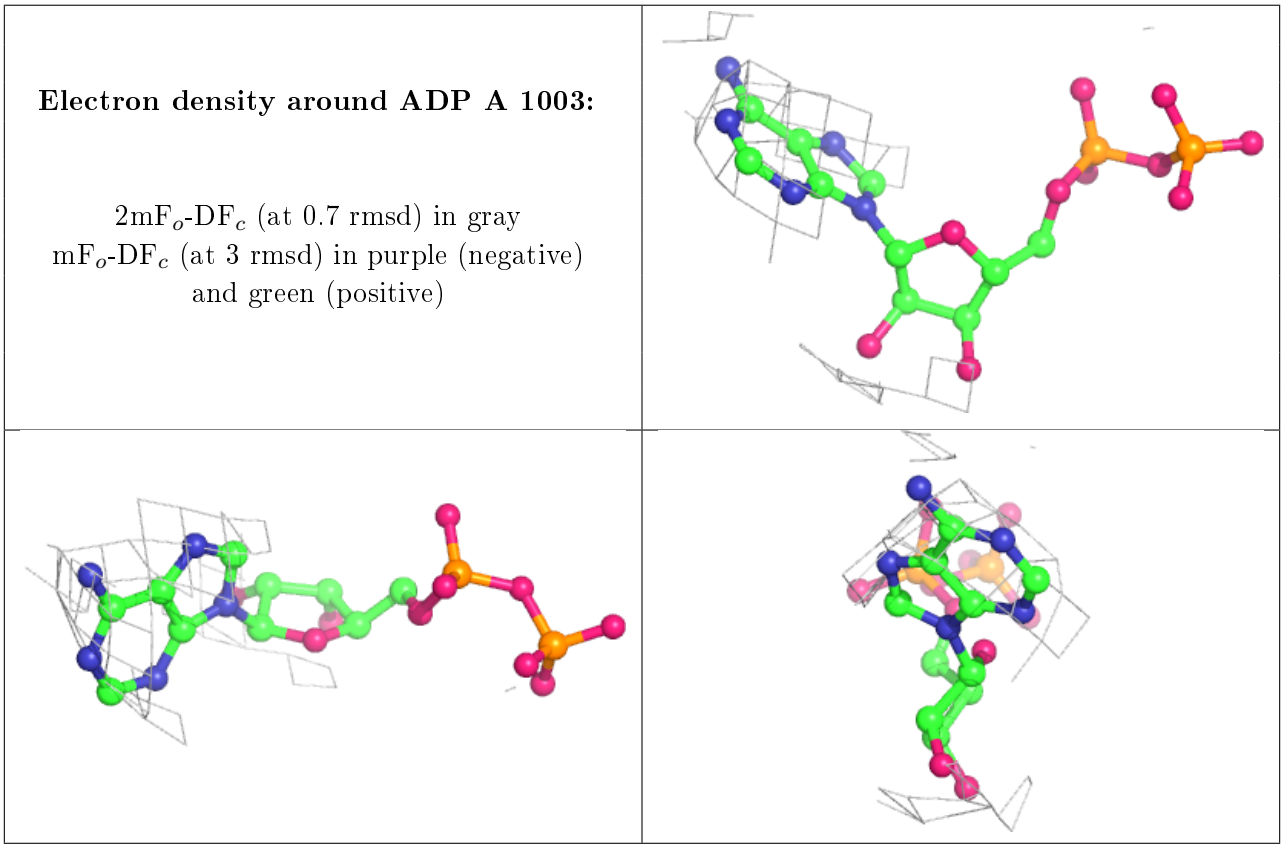
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.