

Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 - 03:27 AM EDT

PDB ID	:	6X3J
Title	:	Crystal structure of streptogramin A acetyltransferase VatA from Staphylo-
		coccus aureus in complex with streptogram analog $F0224$ (46)
Authors	:	Chaires, H.A.; Fraser, J.S.
Deposited on	:	2020-05-21
Resolution	:	2.70 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.70 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.



Motria	Whole archive	Similar resolution
	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
			2%		
1	A	209	86%	12%	•
			4%		
1	В	209	81%	17%	•
			3%		
1	С	209	89%	11%)
			3%		_
1	D	209	86%	13%	•
			4%		_
1	E	209	84%	15%	•



Mol	Chain	Length	Quality of chain		
			5%		
1	F	209	77%	20%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SXA	А	403	Х	-	-	-
4	SXA	В	405	Х	-	-	-
4	SXA	D	302	Х	-	-	-
4	SXA	Е	407	Х	-	-	-
4	SXA	F	405	Х	-	-	-
4	SXA	F	406	Х	-	-	Х



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20998 atoms, of which 10359 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.

Mol	Chain	Residues			Atoms	8			ZeroOcc	AltConf	Trace
1	Λ	206	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
1		200	3295	1066	1646	277	298	8	0	0	
1	В	206	Total	С	Η	Ν	0	S	0	0	0
1	D	200	3295	1066	1646	277	298	8	0	0	0
1	С	200	Total	С	Η	Ν	0	S	0	0	0
1	U	209	3359	1084	1682	284	301	8	0		
1	Л	207	Total	С	Η	Ν	0	S	0	0	0
1	D	201	3315	1072	1655	281	299	8	0	0	0
1	F	207	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0
1		201	3319	1072	1659	281	299	8	0	0	0
1	1 E	201	Total	С	Η	Ν	Ο	S	0	0	0
	T,	204	3248	1054	1619	271	296	8		0	0

• Molecule 1 is a protein called Virginiamycin A acetyltransferase, VatA.

• Molecule 2 is (2R)-2-[(3S,4R,5E,10E,12E,14S,16R,26aR)-16-fluoro-14-hydroxy-4,12-dim ethyl-1,7,22-trioxo-4,7,8,9,14,15,16,17,24,25,26,26a-dodecahydro-1H,3H,22H-21,18-(aze no)pyrrolo[2,1-c][1,8,4,19]dioxadiazacyclotetracosin-3-yl]propyl isoquinolin-3-ylcarbam ate (three-letter code: O7V) (formula: $C_{38}H_{44}FN_5O_8$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Δ	1	Total C F H N O	Ο	0
2	Л	T	96 38 1 44 5 8	0	0
2	В	1	Total C F H N O	9	0
	2 В	L	96 38 1 44 5 8	2	0
9	В	1	Total C F H N O	Ο	0
	Z D	1	96 38 1 44 5 8	0	0
9	С	1	Total C F H N O	0	1
	U	T	192 76 2 88 10 16	0	
2	F	1	Total C F H N O	0	0
	1	96 38 1 44 5 8	0	0	
9	F	1	Total C F H N O	0	0
	Ľ		96 38 1 44 5 8	0	0

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is THIOACETIC ACID S-{2-[3-(2-HYDROXY-3,3-DIMETHYL-4-PHOSPHO NOOXY-BUTYRYLAMINO)-PROPIONYLAMINO]-ETHYL} ESTER (three-letter code: SXA) (formula: C₁₃H₂₅N₂O₈PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	А	1	Total 44	C 13	Н 24	N 2	0 4	S 1	0	0
								\overline{Co}	ntinued on r	next page



Mol	Chain	Residues		A	tom	IS			ZeroOcc	AltConf
4		1	Total	С	Η	Ν	0	S	2	0
4 D	L	44	13	24	2	4	1	2	0	
4	Л	1	Total	С	Η	Ν	0	\mathbf{S}	2	0
4 D	L	44	13	24	2	4	1	2	0	
4	F	E 1	Total	С	Η	Ν	0	\mathbf{S}	2	0
	Ľ		44	13	24	2	4	1		0
4	F	1	Total	С	Η	Ν	0	\mathbf{S}	2	0
4 Г	1	44	13	24	2	4	1	2	U	
4		1	Total	С	Η	Ν	0	\mathbf{S}	1	0
	T,	1	44	13	24	2	4	1	L	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	2	Total Cl 2 2	0	0
5	С	2	Total Cl 2 2	0	0
5	Е	4	Total Cl 4 4	0	0
5	F	3	Total Cl 3 3	0	0

• Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	36	Total O 36 36	0	0
7	В	45	Total O 45 45	0	0
7	С	32	$\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
7	D	28	$\begin{array}{ccc} \text{Total} & \text{O} \\ 28 & 28 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Е	31	Total O 31 31	0	0
7	F	36	Total O 36 36	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Virginiamycin A acetyltransferase,VatA



•

20%



• Molecule 1: Virginiamycin A acetyltransferase,VatA

Chain F:



77%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	104.80Å 109.22Å 173.03Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	86.51 - 2.70	Depositor
Resolution (A)	89.64 - 2.70	EDS
% Data completeness	100.0 (86.51-2.70)	Depositor
(in resolution range)	$100.0 \ (89.64-2.70)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.24 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
P. P.	0.234 , 0.271	Depositor
Λ, Λ_{free}	0.235 , 0.272	DCC
R_{free} test set	2796 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	53.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 52.4	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20998	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: O7V, CL, MG, PO4, SXA $\,$

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).

Mal	Chain	Bond lengths		Bond angles	
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.32	0/1691	0.51	1/2289~(0.0%)
1	В	0.42	1/1691~(0.1%)	0.60	3/2289~(0.1%)
1	С	0.31	0/1719	0.50	1/2325~(0.0%)
1	D	0.34	0/1702	0.52	1/2303~(0.0%)
1	Е	0.32	0/1702	0.51	1/2303~(0.0%)
1	F	0.33	0/1671	0.56	2/2264~(0.1%)
All	All	0.34	1/10176~(0.0%)	0.53	9/13773~(0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	В	196	GLU	CB-CG	-5.95	1.40	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	100	ARG	CB-CA-C	5.73	121.87	110.40
1	В	100	ARG	CB-CA-C	5.68	121.75	110.40
1	В	196	GLU	CG-CD-OE1	-5.57	107.17	118.30
1	F	100	ARG	CB-CA-C	5.48	121.36	110.40
1	Е	100	ARG	CB-CA-C	5.32	121.04	110.40
1	С	100	ARG	CB-CA-C	5.14	120.67	110.40
1	В	196	GLU	CG-CD-OE2	5.12	128.53	118.30
1	F	34	ASN	N-CA-CB	5.06	119.72	110.60
1	А	100	ARG	CB-CA-C	5.04	120.47	110.40

There are no chirality outliers.

There are no planarity outliers.



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	А	1649	1646	1645	14	5
1	В	1649	1646	1645	28	2
1	С	1677	1682	1682	13	5
1	D	1660	1655	1658	18	2
1	Е	1660	1659	1658	27	0
1	F	1629	1619	1619	29	0
2	А	52	44	0	3	0
2	В	104	88	0	1	0
2	С	104	88	0	3	0
2	Е	52	44	0	3	0
2	F	52	44	0	0	0
3	А	5	0	0	0	0
3	Е	5	0	0	1	0
4	А	20	24	21	0	0
4	В	20	24	21	3	0
4	D	20	24	21	0	0
4	Е	20	24	21	2	0
4	F	40	48	42	4	0
5	В	2	0	0	1	0
5	С	2	0	0	0	0
5	Е	4	0	0	2	0
5	F	3	0	0	2	0
6	С	1	0	0	0	0
6	D	1	0	0	0	0
7	А	36	0	0	1	0
7	В	45	0	0	1	0
7	С	32	0	0	1	0
7	D	28	0	0	0	0
7	Е	31	0	0	0	0
7	F	36	0	0	2	0
All	All	10639	$10\overline{359}$	10033	131	7

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

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:82:MET:CE	1:B:119:ILE:HD12	1.87	1.04
1:B:82:MET:HE1	1:B:119:ILE:HD12	1.38	1.00
1:E:87:HIS:NE2	4:F:405:SXA:O1	2.16	0.78
1:B:155:VAL:HG12	1:B:159:SER:OG	1.83	0.77
5:F:402:CL:CL	7:F:523:HOH:O	2.40	0.76
1:F:127:ILE:HG12	1:F:145:ILE:HD12	1.68	0.76
1:B:82:MET:HE2	1:B:119:ILE:HD12	1.69	0.74
1:E:61:VAL:HG11	2:E:401:O7V:C26	2.18	0.74
1:D:199:PRO:O	1:D:203:ASN:ND2	2.24	0.71
1:B:155:VAL:CG1	1:B:159:SER:OG	2.41	0.69
5:B:403:CL:CL	7:B:528:HOH:O	2.49	0.67
1:E:132:THR:HG22	1:E:134:MET:CE	2.24	0.67
1:B:126:TRP:HE1	4:B:405:SXA:H2A	1.64	0.63
1:D:48:GLY:O	1:F:21:ARG:NH2	2.33	0.62
1:D:21:ARG:HG2	1:D:21:ARG:O	2.00	0.61
1:F:193:ILE:O	1:F:197:ASN:ND2	2.35	0.60
1:F:79:THR:OG1	1:F:132:THR:HG23	2.02	0.60
1:F:21:ARG:O	1:F:21:ARG:HG2	2.02	0.59
1:F:86:ASN:HB3	1:F:114:PRO:HG2	1.85	0.59
1:A:11:PRO:HG3	1:A:40:TYR:CZ	2.39	0.58
1:D:48:GLY:O	1:F:21:ARG:CZ	2.52	0.58
1:B:110:LEU:HB3	1:B:115:LEU:HD11	1.85	0.57
1:F:83:ASN:HB3	1:F:115:LEU:CD2	2.34	0.57
1:E:132:THR:HG22	1:E:134:MET:HE3	1.87	0.57
1:C:197:ASN:HB3	1:C:209:LEU:HD21	1.87	0.56
1:E:86:ASN:HB3	1:E:114:PRO:HG2	1.86	0.56
1:F:83:ASN:HB3	1:F:115:LEU:HD22	1.88	0.56
1:F:14:ILE:HG22	1:F:15:LEU:HG	1.87	0.56
1:B:155:VAL:HG12	1:B:159:SER:HG	1.71	0.55
1:C:161:VAL:HG23	1:C:166:LEU:HD11	1.89	0.55
1:E:121:ILE:HD13	1:E:127:ILE:HD11	1.89	0.55
1:F:137:VAL:HG11	1:F:151:VAL:HG12	1.89	0.54
1:C:133:ILE:HG23	1:C:137:VAL:HG21	1.89	0.54
1:E:126:TRP:NE1	4:E:407:SXA:S1	2.75	0.54
1:D:121:ILE:HD13	1:D:127:ILE:HD11	1.88	0.54
1:D:207:GLU:HA	1:D:210:LYS:HB2	1.89	0.54
1:B:86:ASN:HB3	1:B:114:PRO:HG2	1.90	0.54
1:E:98:LEU:HB3	1:F:17:ILE:HD11	1.90	0.53
1:D:133:ILE:HG23	1:D:137:VAL:HG21	1.90	0.53
1:E:32:ASN:HB3	1:E:35:ILE:HD12	1.91	0.52
1:E:163:GLY:N	5:E:405:CL:CL	2.77	0.52
1:B:126:TRP:NE1	4:B:405:SXA:H2A	2.25	0.52



	A L O	Interatomic Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:108:PRO:CG	2:E:401:O7V:O52	2.57	0.52
1:E:26:ILE:HB	1:E:37:VAL:HG11	1.92	0.52
1:F:24:GLN:NE2	1:F:45:SER:HB3	2.25	0.52
1:B:44:ASP:O	1:B:76:PRO:HB3	2.10	0.51
1:C:185:GLN:NE2	7:C:501:HOH:O	2.40	0.51
1:D:61:VAL:HG23	1:D:62:ILE:HG13	1.91	0.51
1:D:15:LEU:HD22	1:D:21:ARG:HA	1.93	0.51
1:E:137:VAL:HG11	1:E:151:VAL:HG12	1.92	0.51
1:E:74:ILE:CD1	1:E:127:ILE:HD12	2.41	0.50
1:A:97:HIS:NE2	2:A:401:O7V:O52	2.45	0.49
1:F:132:THR:HG22	1:F:134:MET:HE2	1.95	0.49
1:D:184:LEU:HD21	1:D:209:LEU:HD13	1.94	0.48
1:E:151:VAL:HG13	1:E:166:LEU:HD22	1.95	0.48
1:D:82:MET:SD	1:D:119:ILE:HD12	2.53	0.48
1:F:82:MET:SD	1:F:119:ILE:HD12	2.53	0.48
1:B:44:ASP:HB3	1:B:76:PRO:HD3	1.96	0.48
1:F:97:HIS:HA	1:F:103:TRP:O	2.14	0.48
1:B:78:THR:HA	1:B:131:VAL:O	2.14	0.47
1:B:147:ALA:N	4:B:405:SXA:O40	2.43	0.47
1:B:34:ASN:O	1:B:65:LYS:HA	2.14	0.47
1:E:137:VAL:HG11	1:E:151:VAL:CG1	2.44	0.47
1:E:98:LEU:HB3	1:F:17:ILE:CD1	2.45	0.47
1:A:61:VAL:HG11	2:A:401:O7V:C31	2.44	0.47
1:C:167:LYS:HE3	7:F:522:HOH:O	2.14	0.47
1:B:21:ARG:HH11	1:E:21:ARG:HH22	1.62	0.47
1:A:121:ILE:HD13	1:A:127:ILE:HD11	1.96	0.46
1:C:147:ALA:HB2	4:F:406:SXA:C42	2.45	0.46
1:B:121:ILE:HG12	1:B:139:ILE:HD12	1.98	0.46
1:B:181:TRP:CD2	1:B:206:ILE:HD13	2.51	0.46
1:C:61:VAL:HG22	1:C:61:VAL:O	2.16	0.46
1:D:191:MET:O	1:D:191:MET:HG3	2.15	0.46
1:D:197:ASN:HB3	1:D:209:LEU:HD21	1.96	0.46
1:C:190:ASP:OD2	1:C:191:MET:N	2.49	0.46
1:A:190:ASP:OD1	1:A:192:LYS:HD3	2.16	0.45
1:A:39:GLU:O	1:A:40:TYR:HB2	2.16	0.45
2:A:401:O7V:C47	2:A:401:O7V:N07	2.79	0.45
1:C:121:ILE:HD13	1:C:127:ILE:HD11	1.98	0.45
1:E:14:ILE:N	3:E:406:PO4:O4	2.29	0.45
1:F:90:ASP:N	5:F:403:CL:CL	2.87	0.45
1:A:132:THR:HG22	1:A:134:MET:CE	2.47	0.45
1:F:27:LYS:HD2	1:F:39:GLU:HG2	1.98	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:83:ASN:ND2	1:E:117:GLY:O	2.50	0.44
1:B:34:ASN:HB3	1:B:65:LYS:HG2	2.00	0.44
1:B:191:MET:O	1:B:195:ASN:ND2	2.50	0.43
1:D:133:ILE:HG23	1:D:137:VAL:CG2	2.48	0.43
1:B:79:THR:OG1	1:B:132:THR:HG23	2.18	0.43
2:C:401[A]:O7V:C47	2:C:401[A]:O7V:N07	2.81	0.43
1:D:86:ASN:HB3	1:D:114:PRO:HG2	2.00	0.43
1:B:82:MET:HE2	1:B:119:ILE:CD1	2.43	0.43
1:C:82:MET:SD	1:C:119:ILE:HD12	2.59	0.43
1:C:133:ILE:HG23	1:C:137:VAL:CG2	2.48	0.43
1:B:35:ILE:HG13	1:B:58:HIS:HE1	1.83	0.43
1:F:78:THR:HA	1:F:131:VAL:O	2.19	0.43
1:F:128:GLY:HA2	4:F:405:SXA:C42	2.49	0.42
1:F:144:ILE:HB	1:F:160:ILE:HG12	2.00	0.42
1:A:192:LYS:N	1:A:192:LYS:HD2	2.34	0.42
1:F:39:GLU:O	1:F:40:TYR:HB2	2.20	0.42
1:C:161:VAL:CG2	1:C:166:LEU:HD11	2.49	0.42
1:F:129:ARG:H	4:F:405:SXA:H42A	1.84	0.42
1:A:24:GLN:NE2	7:A:502:HOH:O	2.52	0.42
2:C:401[A]:O7V:O01	1:E:42:TYR:OH	2.31	0.42
1:F:11:PRO:HB2	1:F:39:GLU:HB3	2.02	0.42
1:A:26:ILE:HB	1:A:37:VAL:HG11	2.02	0.42
1:B:137:VAL:HG11	1:B:151:VAL:HG12	2.02	0.42
1:F:42:TYR:CZ	1:F:73:SER:HB2	2.55	0.42
2:B:402:O7V:N07	2:B:402:O7V:C47	2.83	0.41
1:E:7:HIS:O	1:E:195:ASN:ND2	2.51	0.41
1:E:129:ARG:H	4:E:407:SXA:H42	1.84	0.41
1:A:80:PHE:CE1	1:A:133:ILE:HD12	2.55	0.41
1:A:68:ILE:HD13	1:A:74:ILE:HD11	2.03	0.41
1:C:86:ASN:HB3	1:C:114:PRO:HG2	2.03	0.41
1:B:62:ILE:HG12	1:B:110:LEU:HD21	2.01	0.41
1:B:144:ILE:HB	1:B:160:ILE:HG12	2.03	0.41
1:D:199:PRO:O	1:D:203:ASN:CG	2.59	0.41
1:E:20:ASN:O	5:E:404:CL:CL	2.76	0.41
1:E:21:ARG:O	1:E:21:ARG:HG3	2.21	0.41
1:F:139:ILE:HD13	1:F:145:ILE:HD11	2.03	0.41
1:B:126:TRP:CE3	1:B:144:ILE:HG23	2.56	0.41
2:E:401:O7V:N07	2:E:401:O7V:C47	2.84	0.41
1:F:27:LYS:N	1:F:28:PRO:HD2	2.36	0.41
1:D:168:PHE:HZ	1:D:171:LYS:HG3	1.86	0.40
1:E:160:ILE:HG22	1:E:169:ILE:HD12	2.03	0.40



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:H	1:B:154:ASN:ND2	2.19	0.40
1:A:192:LYS:O	1:A:196:GLU:HG3	2.21	0.40
1:F:161:VAL:HG23	1:F:166:LEU:HD11	2.04	0.40
1:A:193:ILE:O	1:A:197:ASN:ND2	2.55	0.40
1:E:26:ILE:HG21	1:E:37:VAL:HG21	2.03	0.40
2:C:401[B]:O7V:N07	2:C:401[B]:O7V:C47	2.85	0.40
1:D:191:MET:SD	1:D:194:ILE:HB	2.62	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:SER:OG	$1:C:205:ASP:OD1[4_545]$	1.03	1.17
1:B:196:GLU:OE1	1:D:174:SER:HG[3_644]	1.05	0.55
1:A:109:SER:HG	$1:C:205:ASP:OD1[4_545]$	1.11	0.49
1:B:196:GLU:OE1	1:D:174:SER:OG[3_644]	1.86	0.34
1:A:109:SER:OG	$1:C:205:ASP:CG[4_545]$	2.01	0.19
1:A:205:ASP:OD2	1:C:109:SER:OG[3_554]	2.01	0.19
1:A:109:SER:HG	$1:C:205:ASP:CG[4_545]$	1.58	0.02

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	А	204/209~(98%)	197~(97%)	5(2%)	2(1%)	15 37
1	В	204/209~(98%)	201 (98%)	3~(2%)	0	100 100
1	С	207/209~(99%)	199 (96%)	7 (3%)	1 (0%)	29 54
1	D	205/209~(98%)	199 (97%)	6 (3%)	0	100 100
1	Е	205/209~(98%)	200 (98%)	5 (2%)	0	100 100
1	F	202/209~(97%)	197 (98%)	4 (2%)	1 (0%)	29 54



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1227/1254~(98%)	1193~(97%)	30~(2%)	4 (0%)	41 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	34	ASN
1	А	91	GLY
1	С	91	GLY
1	А	95	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	Perce	\mathbf{ntiles}
1	А	178/181~(98%)	178 (100%)	0	100	100
1	В	178/181~(98%)	177 (99%)	1 (1%)	86	95
1	С	181/181~(100%)	181 (100%)	0	100	100
1	D	179/181~(99%)	178 (99%)	1 (1%)	86	95
1	Ε	179/181~(99%)	179~(100%)	0	100	100
1	F	176/181~(97%)	175 (99%)	1 (1%)	86	95
All	All	1071/1086~(99%)	1068 (100%)	3 (0%)	92	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	32	ASN
1	D	87	HIS
1	F	123	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:



Mol	Chain	Res	Type
1	В	58	HIS
1	В	154	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 13 are monoatomic - leaving 15 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).

Mal	Trune	Chain	Dec	Timle	Bo	ond leng	ths	Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	O7V	С	401[A]	-	$51,\!56,\!56$	1.14	2 (3%)	63,77,77	1.31	7 (11%)
2	O7V	С	401[B]	-	$51,\!56,\!56$	1.14	3 (5%)	63,77,77	1.29	7 (11%)
4	SXA	В	405	-	18,19,24	1.39	1 (5%)	$23,\!25,\!33$	1.22	3 (13%)
4	SXA	А	403	-	18,19,24	1.41	1 (5%)	23,25,33	0.75	0
3	PO4	Е	406	-	4,4,4	0.92	0	$6,\!6,\!6$	0.43	0
4	SXA	F	405	-	18,19,24	1.72	1 (5%)	$23,\!25,\!33$	1.23	1 (4%)
3	PO4	А	402	-	4,4,4	0.91	0	$6,\!6,\!6$	0.46	0
2	O7V	F	401	-	$51,\!56,\!56$	1.20	2 (3%)	$63,\!77,\!77$	1.15	3 (4%)
2	O7V	Е	401	-	$51,\!56,\!56$	1.21	4 (7%)	$63,\!77,\!77$	1.70	13 (20%)
4	SXA	F	406	-	18,19,24	1.47	1 (5%)	23,25,33	1.05	2 (8%)
2	O7V	В	401	-	$51,\!56,\!56$	1.19	3 (5%)	63,77,77	1.22	6 (9%)



Mal	ol Type Chain Bes	Dec	Dec	Dec	Dec	Dec	Dec	Dec	Dog	in Res	Tinle	Bo	ond leng	$_{\rm ths}$	E	Bond ang	gles
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2							
4	SXA	Е	407	-	18,19,24	1.35	1 (5%)	23,25,33	1.05	1 (4%)							
4	SXA	D	302	-	18,19,24	1.81	1 (5%)	23,25,33	1.29	3 (13%)							
2	O7V	В	402	-	$51,\!56,\!56$	1.15	2 (3%)	63,77,77	1.12	<mark>6 (9%)</mark>							
2	O7V	А	401	-	51,56,56	1.22	3 (5%)	63,77,77	1.35	7 (11%)							

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	O7V	С	401[A]	-	-	11/51/67/67	0/4/5/5
4	SXA	В	405	-	1/1/7/8	6/23/23/30	-
2	O7V	С	401[B]	-	-	13/51/67/67	0/4/5/5
4	SXA	А	403	-	1/1/7/8	6/23/23/30	-
4	SXA	F	405	-	1/1/7/8	11/23/23/30	-
4	SXA	F	406	-	1/1/7/8	5/23/23/30	-
2	O7V	Е	401	-	-	12/51/67/67	0/4/5/5
2	O7V	F	401	-	-	9/51/67/67	0/4/5/5
2	O7V	В	401	-	-	12/51/67/67	0/4/5/5
4	SXA	Е	407	-	1/1/7/8	8/23/23/30	-
2	O7V	А	401	-	-	10/51/67/67	0/4/5/5
2	O7V	В	402	-	-	9/51/67/67	0/4/5/5
4	SXA	D	302	-	1/1/7/8	13/23/23/30	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
4	D	302	SXA	C29-C32	6.82	1.59	1.55
4	F	405	SXA	C29-C32	6.51	1.59	1.55
4	F	406	SXA	C29-C32	5.23	1.58	1.55
4	А	403	SXA	C29-C32	5.00	1.58	1.55
4	В	405	SXA	C29-C32	4.88	1.58	1.55
4	Е	407	SXA	C29-C32	4.83	1.58	1.55
2	F	401	O7V	C55-C06	4.27	1.52	1.49
2	А	401	O7V	C55-C06	3.70	1.51	1.49
2	В	401	O7V	C55-C06	3.62	1.51	1.49
2	Е	401	O7V	C08-C49	-3.60	1.44	1.50



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	401[B]	O7V	C55-C06	3.52	1.51	1.49
2	В	402	O7V	C55-C06	3.45	1.51	1.49
2	С	401[A]	O7V	C55-C06	3.28	1.51	1.49
2	А	401	O7V	C08-C49	-3.16	1.45	1.50
2	Ε	401	O7V	C55-C06	3.12	1.51	1.49
2	С	401[A]	O7V	C08-C49	-3.08	1.45	1.50
2	В	401	O7V	C08-C49	-3.06	1.45	1.50
2	В	402	O7V	C08-C49	-2.84	1.45	1.50
2	С	401[B]	O7V	C08-C49	-2.76	1.46	1.50
2	F	401	O7V	C08-C49	-2.63	1.46	1.50
2	С	401[B]	O7V	C20-C19	-2.48	1.43	1.48
2	А	401	O7V	C02-C12	2.30	1.53	1.50
2	Ε	401	O7V	O42-C24	-2.08	1.41	1.44
2	В	401	O7V	C20-C19	-2.04	1.44	1.48
2	E	401	O7V	C02-C12	2.02	1.53	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	Е	401	O7V	C17-N18-C19	6.66	132.79	122.03
2	А	401	O7V	C27-O28-C29	5.92	128.04	116.06
2	С	401[A]	O7V	C27-O28-C29	4.85	125.88	116.06
2	С	401[B]	O7V	O28-C27-C25	4.53	115.95	108.38
2	В	401	O7V	C27-O28-C29	4.40	124.96	116.06
2	F	401	O7V	C27-O28-C29	4.38	124.93	116.06
2	Е	401	O7V	O42-C24-C25	-4.27	102.31	108.22
2	В	402	O7V	C27-O28-C29	4.01	124.18	116.06
2	Е	401	O7V	O28-C27-C25	3.77	114.69	108.38
2	Е	401	O7V	O52-C19-N18	-3.59	116.29	122.23
2	С	401[B]	O7V	C27-O28-C29	3.38	122.91	116.06
2	С	401[A]	O7V	O28-C27-C25	3.37	114.03	108.38
4	В	405	SXA	C38-C37-N36	3.22	118.39	111.90
2	С	401[B]	O7V	C27-C25-C24	3.21	116.25	111.08
2	А	401	O7V	O28-C27-C25	3.18	113.70	108.38
2	Е	401	O7V	C24-O42-C43	3.17	123.23	117.78
2	А	401	O7V	O28-C29-N30	3.12	114.42	109.32
2	Е	401	O7V	C27-O28-C29	3.11	122.34	116.06
4	F	405	SXA	C43-C42-N41	3.10	118.94	112.42
2	В	401	O7V	O28-C27-C25	3.01	113.42	108.38
2	Е	401	O7V	C23-C22-C24	2.86	116.41	111.11
4	D	302	SXA	C43-C42-N41	2.80	118.29	112.42
2	А	401	O7V	C53-C02-C12	2.76	117.49	111.94



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	302	SXA	C38-C37-N36	2.68	117.31	111.90
2	С	401[A]	O7V	C53-C02-C12	2.66	117.29	111.94
4	F	406	SXA	C37-C38-C39	2.63	116.73	112.36
2	С	401[A]	O7V	O28-C29-N30	2.60	113.57	109.32
2	В	401	O7V	O28-C29-N30	2.58	113.53	109.32
2	Е	401	O7V	C20-C19-N18	2.53	119.73	114.97
2	А	401	O7V	O28-C29-O41	-2.49	119.47	124.25
4	D	302	SXA	C37-C38-C39	2.43	116.41	112.36
2	Е	401	O7V	C27-C25-C24	2.43	115.00	111.08
2	В	401	O7V	C16-C15-C13	-2.40	122.27	125.89
4	В	405	SXA	C43-C42-N41	2.37	117.40	112.42
2	С	401[A]	O7V	C46-C47-N48	2.37	107.41	103.25
2	С	401[B]	O7V	C31-N30-C29	2.36	133.07	127.36
4	F	406	SXA	C38-C37-N36	2.30	116.54	111.90
2	С	401[B]	O7V	O42-C24-C25	2.30	111.39	108.22
2	F	401	O7V	O28-C29-N30	2.29	113.07	109.32
2	С	401[B]	O7V	C46-C47-N48	2.26	107.21	103.25
2	F	401	O7V	O28-C29-O41	-2.25	119.94	124.25
2	А	401	O7V	C46-C47-N48	2.24	107.17	103.25
4	Е	407	SXA	C38-C37-N36	2.22	116.39	111.90
2	С	401[A]	O7V	C24-O42-C43	2.18	121.52	117.78
2	В	401	O7V	C24-O42-C43	2.17	121.51	117.78
4	В	405	SXA	C37-N36-C34	2.17	126.46	122.59
2	В	402	O7V	C24-O42-C43	2.17	121.50	117.78
2	В	402	O7V	C26-C25-C24	2.16	114.69	111.15
2	С	401[B]	O7V	C23-C22-C24	2.15	115.09	111.11
2	В	402	O7V	O28-C29-N30	2.15	112.83	109.32
2	Е	401	O7V	C16-C15-C13	-2.13	122.67	125.89
2	В	402	O7V	C46-C47-N48	2.12	106.97	103.25
2	Е	401	O7V	C47-N48-C44	-2.11	108.65	112.00
2	В	401	O7V	C17-N18-C19	2.11	125.44	122.03
2	С	401[A]	O7V	O28-C29-O41	-2.09	120.24	124.25
2	Е	401	O7V	C53-C02-C12	2.08	116.13	111.94
2	В	402	O7V	C23-C22-C21	2.05	114.95	109.99
2	А	401	O7V	C24-O42-C43	2.04	121.28	117.78
2	Е	401	O7V	C26-C25-C27	2.00	113.94	110.06

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	А	403	SXA	C32
4	В	405	SXA	C32



4

4

F

Continued from previous page... Chain Res Type Mol Atom SXA C32 D 302 4 4 Е 407 SXA C32 F SXA C32

405

406

All (125) torsion outliers are listed below:

SXA

C32

Mol	Chain	Res	Type	Atoms
2	А	401	O7V	C26-C25-C27-O28
2	А	401	O7V	C53-C54-C55-C06
2	А	401	O7V	F19-C54-C55-C06
2	В	401	O7V	C12-C13-C15-C16
2	В	401	O7V	C14-C13-C15-C16
2	В	401	O7V	O42-C24-C25-C26
2	В	402	O7V	C14-C13-C15-C16
2	В	402	O7V	O42-C24-C25-C26
2	В	402	O7V	N30-C29-O28-C27
2	В	402	O7V	O41-C29-O28-C27
2	С	401[A]	O7V	C12-C13-C15-C16
2	С	401[A]	O7V	C14-C13-C15-C16
2	С	401[A]	O7V	C24-C25-C27-O28
2	С	401[A]	O7V	C26-C25-C27-O28
2	С	401[A]	O7V	N30-C29-O28-C27
2	С	401[A]	O7V	O41-C29-O28-C27
2	С	401[A]	O7V	C53-C54-C55-C06
2	С	401[A]	O7V	F19-C54-C55-C06
2	С	401[B]	O7V	C12-C13-C15-C16
2	С	401[B]	O7V	C24-C25-C27-O28
2	С	401[B]	O7V	C26-C25-C27-O28
2	С	401[B]	O7V	N30-C29-O28-C27
2	С	401[B]	O7V	O41-C29-O28-C27
2	С	401[B]	O7V	C53-C54-C55-C06
2	С	401[B]	O7V	F19-C54-C55-C06
2	Е	401	O7V	C14-C13-C15-C16
2	Е	401	O7V	C20-C19-N18-C17
2	Е	401	O7V	O52-C19-N18-C17
2	Е	401	O7V	C24-C25-C27-O28
2	Е	401	O7V	C26-C25-C27-O28
2	F	401	O7V	C14-C13-C15-C16
2	F	401	O7V	O42-C24-C25-C26
2	F	401	O7V	N30-C29-O28-C27
2	F	401	O7V	O41-C29-O28-C27



Mol	Chain	Res	Type	Atoms
4	А	403	SXA	N36-C37-C38-C39
4	А	403	SXA	N41-C42-C43-S1
4	В	405	SXA	N36-C37-C38-C39
4	В	405	SXA	O1-C1-S1-C43
4	В	405	SXA	C2-C1-S1-C43
4	D	302	SXA	C28-C29-C32-O33
4	D	302	SXA	C28-C29-C32-C34
4	D	302	SXA	C30-C29-C32-O33
4	D	302	SXA	C30-C29-C32-C34
4	D	302	SXA	C31-C29-C32-O33
4	D	302	SXA	C31-C29-C32-C34
4	D	302	SXA	N36-C37-C38-C39
4	D	302	SXA	O1-C1-S1-C43
4	D	302	SXA	C2-C1-S1-C43
4	Е	407	SXA	O33-C32-C34-O35
4	Е	407	SXA	N36-C37-C38-C39
4	Е	407	SXA	C42-C43-S1-C1
4	Е	407	SXA	O1-C1-S1-C43
4	Е	407	SXA	C2-C1-S1-C43
4	F	405	SXA	C28-C29-C32-O33
4	F	405	SXA	C28-C29-C32-C34
4	F	405	SXA	C30-C29-C32-O33
4	F	405	SXA	C30-C29-C32-C34
4	F	405	SXA	C31-C29-C32-O33
4	F	405	SXA	C31-C29-C32-C34
4	F	405	SXA	N36-C37-C38-C39
4	F	405	SXA	O1-C1-S1-C43
4	F	405	SXA	C2-C1-S1-C43
4	F	406	SXA	N36-C37-C38-C39
4	F	406	SXA	N41-C42-C43-S1
4	F	406	SXA	C42-C43-S1-C1
2	A	401	O7V	O41-C29-O28-C27
2	В	401	O7V	O41-C29-O28-C27
2	А	401	O7V	N30-C29-O28-C27
2	В	401	O7V	N30-C29-O28-C27
2	Е	401	O7V	O51-C43-C44-C45
2	Е	401	O7V	O42-C43-C44-C45
2	С	401[B]	O7V	O52-C19-C20-C21
2	С	401[B]	O7V	N18-C19-C20-C21
2	C	401[B]	O7V	C14-C13-C15-C16
2	А	401	O7V	C20-C21-C22-C23
2	А	401	O7V	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	С	401[B]	O7V	C20-C21-C22-C23
2	В	401	O7V	N18-C19-C20-C21
2	С	401[B]	O7V	C20-C21-C22-C24
4	А	403	SXA	O1-C1-S1-C43
4	А	403	SXA	C2-C1-S1-C43
2	А	401	O7V	C14-C13-C15-C16
2	С	401[A]	O7V	O42-C24-C25-C26
2	А	401	O7V	O52-C19-C20-C21
2	В	401	O7V	O52-C19-C20-C21
4	А	403	SXA	O33-C32-C34-O35
4	F	405	SXA	O33-C32-C34-O35
4	F	406	SXA	O33-C32-C34-O35
2	В	402	O7V	C12-C13-C15-C16
2	A	401	O7V	N18-C19-C20-C21
2	В	401	O7V	C22-C24-C25-C27
2	В	402	O7V	C22-C24-C25-C27
2	F	401	O7V	C22-C24-C25-C27
4	D	302	SXA	C29-C32-C34-O35
4	В	405	SXA	C29-C32-C34-N36
4	D	302	SXA	C29-C32-C34-N36
4	Е	407	SXA	O33-C32-C34-N36
4	F	405	SXA	O33-C32-C34-N36
4	F	406	SXA	O33-C32-C34-N36
2	С	401[A]	O7V	C20-C21-C22-C23
2	E	401	O7V	C12-C13-C15-C16
2	E	401	O7V	C23-C22-C24-C25
2	E	401	O7V	C23-C22-C24-O42
2	E	401	O7V	C21-C22-C24-C25
2	E	401	O7V	C21-C22-C24-O42
2	В	402	O7V	C15-C16-C17-N18
4	В	405	SXA	O33-C32-C34-O35
2	В	401	O7V	C22-C24-C25-C26
2	В	402	O7V	C22-C24-C25-C26
2	F	401	O7V	C22-C24-C25-C26
4	E	407	SXA	C29-C32-C34-O35
4	E	407	SXA	C29-C32-C34-N36
2	B	402	O7V	C20-C21-C22-C23
4	D	302	SXA	C42-C43-S1-C1
2	В	401	O7V	C15-C16-C17-N18
2	F	401	O7V	C15-C16-C17-N18
2	F	401	O7V	C20-C21-C22-C23
4	A	403	SXA	033-C32-C34-N36

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Mol	Chain	Res	Type	Atoms
4	D	302	SXA	O33-C32-C34-N36
2	С	401[A]	O7V	O51-C43-C44-C45
2	F	401	O7V	C12-C13-C15-C16
2	В	401	O7V	C20-C21-C22-C23
2	С	401[B]	O7V	O42-C43-C44-C45
2	В	401	O7V	C13-C15-C16-C17
4	В	405	SXA	C29-C32-C34-O35

There are no ring outliers.

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	401[A]	O7V	2	0
2	С	401[B]	O7V	1	0
4	В	405	SXA	3	0
3	Е	406	PO4	1	0
4	F	405	SXA	3	0
2	Е	401	O7V	3	0
4	F	406	SXA	1	0
4	Е	407	SXA	2	0
2	В	402	O7V	1	0
2	А	401	O7V	3	0

10 monomers are involved in 20 short contacts:

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 sufficient 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.





























5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	206/209~(98%)	0.51	5 (2%) 59 60	32, 51, 87, 116	0
1	В	206/209~(98%)	0.50	8 (3%) 39 38	34, 50, 80, 126	0
1	С	209/209~(100%)	0.51	6 (2%) 51 52	31, 51, 91, 112	0
1	D	207/209~(99%)	0.54	7 (3%) 45 45	35, 53, 83, 119	0
1	Ε	207/209~(99%)	0.51	9 (4%) 35 33	34, 55, 92, 115	0
1	F	204/209~(97%)	0.59	11 (5%) 25 24	34, 56, 91, 123	0
All	All	1239/1254~(98%)	0.53	46 (3%) 41 41	31, 53, 89, 126	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	7	HIS	3.9
1	F	18	LYS	3.4
1	F	7	HIS	3.4
1	D	207	GLU	3.2
1	Е	21	ARG	3.1
1	Е	207	GLU	3.1
1	F	111	LYS	3.1
1	D	21	ARG	3.0
1	Е	111	LYS	2.8
1	В	193	ILE	2.8
1	А	7	HIS	2.7
1	D	210	LYS	2.7
1	С	208	MET	2.6
1	F	35	ILE	2.6
1	D	191	MET	2.6
1	В	192	LYS	2.6
1	D	18	LYS	2.5
1	А	211	ARG	2.5
1	С	209	LEU	2.4



Mol	Chain	Res Type		RSRZ	
1	С	102	GLY	2.4	
1	D	194	ILE	2.4	
1	Е	18	LYS	2.4	
1	А	111	LYS	2.3	
1	В	33	GLU	2.3	
1	А	17	ILE	2.3	
1	А	184	LEU	2.3	
1	В	107	MET	2.3	
1	Е	192	LYS	2.2	
1	F	119	ILE	2.2	
1	С	192	LYS	2.2	
1	В	210	LYS	2.2	
1	F	33	GLU	2.1	
1	F	200	PHE	2.1	
1	В	32	ASN	2.1	
1	F	71	PHE	2.1	
1	Е	106	TYR	2.1	
1	С	215	LEU	2.1	
1	С	146	ALA	2.1	
1	Е	61	VAL	2.1	
1	D	192	LYS	2.1	
1	В	209	LEU	2.0	
1	F	37	VAL	2.0	
1	F	21	ARG	2.0	
1	F	67	ILE	2.0	
1	Е	105	LYS	2.0	
1	Е	182	LEU	2.0	

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



|--|

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SXA	F	405	20/25	0.68	0.34	$0,\!0,\!85,\!85$	7
4	SXA	F	406	20/25	0.68	0.40	0,0,86,86	9
4	SXA	D	302	20/25	0.72	0.36	$0,\!0,\!82,\!82$	9
4	SXA	В	405	20/25	0.78	0.33	0,0,89,90	7
6	MG	С	404	1/1	0.79	0.06	45,45,45,45	0
2	O7V	Е	401	52/52	0.80	0.33	0,76,79,79	0
4	SXA	А	403	20/25	0.81	0.34	0,0,63,64	11
3	PO4	А	402	5/5	0.82	0.45	71,71,71,71	5
2	O7V	А	401	52/52	0.83	0.28	$0,\!62,\!66,\!66$	0
3	PO4	Е	406	5/5	0.83	0.32	77,77,78,78	5
2	O7V	С	401[A]	52/52	0.84	0.32	$0,\!63,\!68,\!69$	96
2	O7V	С	401[B]	52/52	0.84	0.32	$0,\!63,\!68,\!69$	96
4	SXA	Е	407	20/25	0.84	0.28	0,0,70,71	8
6	MG	D	301	1/1	0.85	0.23	60,60,60,60	0
5	CL	Е	405	1/1	0.86	0.62	91,91,91,91	0
2	O7V	В	402	52/52	0.87	0.27	$0,\!58,\!60,\!60$	0
2	O7V	F	401	52/52	0.88	0.27	$0,\!54,\!58,\!59$	0
5	CL	F	403	1/1	0.88	0.38	87,87,87,87	0
2	O7V	В	401	52/52	0.91	0.24	$0,\!56,\!61,\!61$	23
5	CL	Е	402	1/1	0.91	0.20	73,73,73,73	0
5	CL	С	402	1/1	0.92	0.26	66,66,66,66	0
5	CL	Е	404	1/1	0.93	0.32	90,90,90,90	0
5	CL	F	402	1/1	0.94	0.21	74,74,74,74	0
5	CL	В	403	1/1	0.94	0.15	$65,\!65,\!65,\!65$	0
5	CL	F	404	1/1	0.95	0.56	122,122,122,122	0
5	CL	В	404	1/1	0.96	0.13	$5\overline{7,}57,57,57$	0
5	CL	Е	403	1/1	0.96	0.10	64,64,64,64	0
5	CL	С	403	1/1	0.96	0.10	$85,\!85,\!85,\!85$	0

median, 95^{th} 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.

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.































6.5 Other polymers (i)

There are no such residues in this entry.

