



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 12:03 PM EDT

PDB ID : 6TIV  
Title : Crystal structure of the SVS\_A2 protein (205-DREMH-209 /205-AQDLE-209 mutant) from ancestral sequence reconstruction at 2.38 Å resolution  
Authors : Rudraraju, R.; Schnell, R.; Schneider, G.  
Deposited on : 2019-11-22  
Resolution : 2.38 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

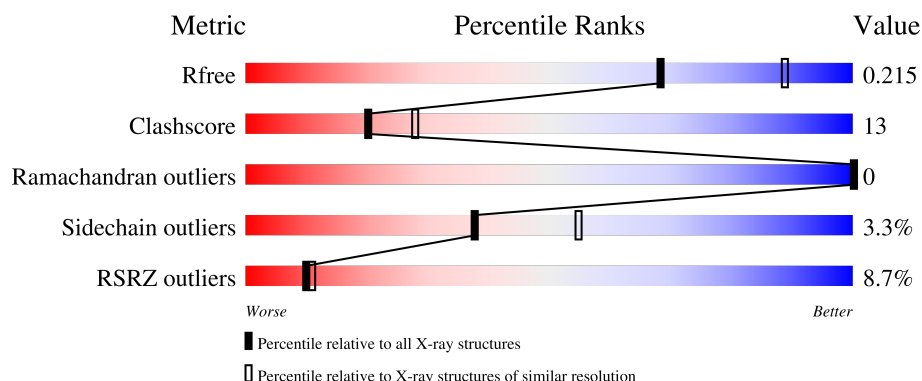
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	<div> <div>9%</div> <div>78%</div> <div>12%</div> <div>8%</div> </div>
1	B	361	<div> <div>7%</div> <div>75%</div> <div>13%</div> <div>11%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	402	-	-	X	X
3	PEG	A	405	-	-	X	-
3	PEG	B	602	-	-	X	-
3	PEG	B	603	-	-	X	-
3	PEG	B	604	-	-	X	-
3	PEG	B	605	-	-	X	-
3	PEG	B	606	-	-	X	-
4	EDO	A	403	-	-	X	-

## 2 Entry composition [i](#)

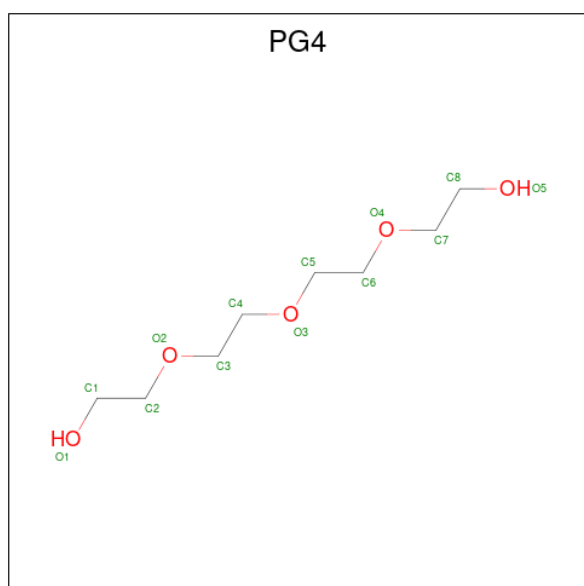
There are 5 unique types of molecules in this entry. The entry contains 5545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SVS variant AT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2608	1640	481	476	11			
1	B	323	Total	C	N	O	S	0	0	0
			2551	1609	470	461	11			

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

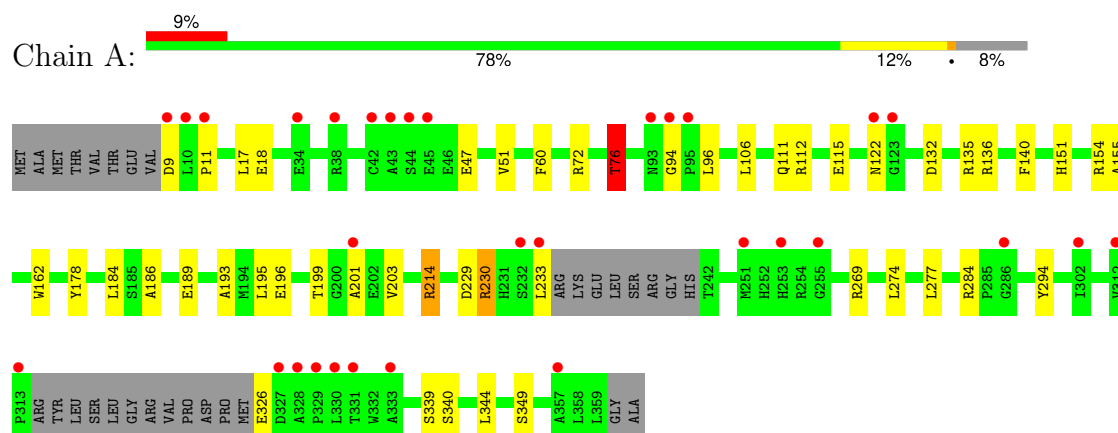
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total	O	0	0
			160	160		
5	B	132	Total	O	0	0
			132	132		

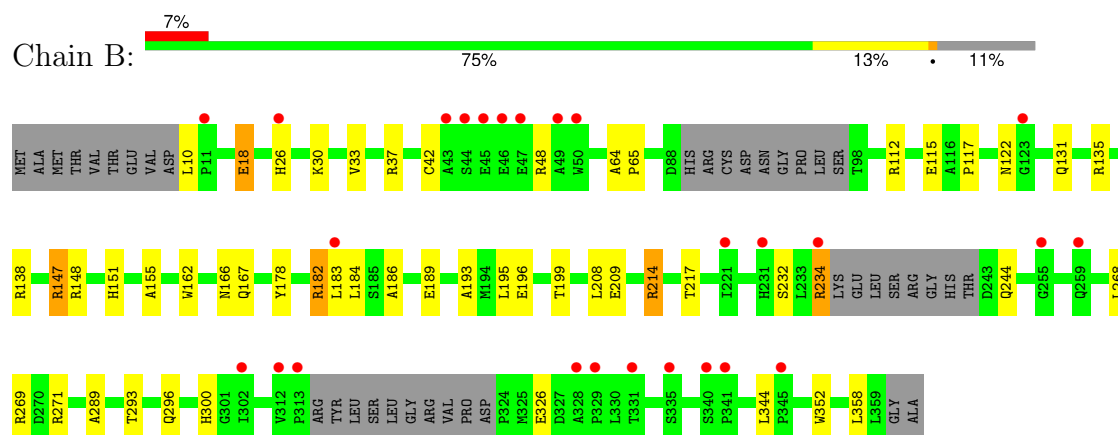
### 3 Residue-property plots

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 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: SVS variant AT2



#### • Molecule 1: SVS variant AT2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.08Å 104.25Å 108.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.38 29.66 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.00-2.38) 99.7 (29.66-2.38)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.186 , 0.210 0.194 , 0.215	Depositor DCC
$R_{free}$ test set	1752 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, EDO, PEG

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	0.75	0/2678	0.93	5/3645 (0.1%)
1	B	0.75	0/2619	0.91	3/3561 (0.1%)
All	All	0.75	0/5297	0.92	8/7206 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	214	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	214	ARG	CG-CD-NE	-6.52	98.12	111.80
1	A	214	ARG	CG-CD-NE	-6.23	98.71	111.80
1	B	147	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	136	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	76	THR	N-CA-CB	-5.02	100.77	110.30
1	A	140	PHE	CB-CA-C	-5.00	100.39	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	A	2608	0	2513	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2551	0	2470	70	0
2	A	13	0	18	0	0
3	A	28	0	40	21	0
3	B	49	0	70	52	0
4	A	4	0	6	7	0
5	A	160	0	0	12	0
5	B	132	0	0	10	0
All	All	5545	0	5117	130	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 13.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLY:HA3	5:A:572:HOH:O	1.07	1.23
1:A:201:ALA:HA	5:A:525:HOH:O	1.36	1.23
1:A:154:ARG:NH1	5:A:501:HOH:O	1.83	1.10
1:B:195:LEU:HB3	3:B:606:PEG:H11	1.34	1.02
1:B:112:ARG:HD3	3:B:604:PEG:H31	1.41	0.99
3:A:402:PEG:H31	1:B:184:LEU:HD11	1.47	0.96
1:B:234:ARG:HD3	1:B:234:ARG:H	1.38	0.89
1:B:193:ALA:HA	3:B:605:PEG:H12	1.56	0.87
1:B:148:ARG:HB3	3:B:605:PEG:H22	1.58	0.85
1:B:208:LEU:HD21	3:B:605:PEG:H21	1.57	0.85
1:B:199:THR:CG2	3:B:606:PEG:H32	2.07	0.84
3:A:402:PEG:H31	1:B:184:LEU:CD1	2.08	0.83
1:B:195:LEU:HB3	3:B:606:PEG:C1	2.09	0.83
1:B:112:ARG:HD3	3:B:604:PEG:C3	2.10	0.81
3:A:405:PEG:H11	1:B:147:ARG:HH22	1.46	0.81
1:A:60:PHE:CD2	1:A:76:THR:HG23	2.18	0.79
1:B:138:ARG:HH11	3:B:602:PEG:C4	1.96	0.78
1:B:186:ALA:HB3	5:B:783:HOH:O	1.83	0.78
1:B:131:GLN:HB3	3:B:602:PEG:H22	1.67	0.76
1:B:209:GLU:OE2	3:B:603:PEG:H32	1.86	0.75
1:A:112:ARG:HB2	3:A:402:PEG:H42	1.68	0.75
1:B:289:ALA:HA	3:B:607:PEG:H42	1.69	0.74
1:B:199:THR:HG21	3:B:606:PEG:H32	1.68	0.74
1:A:151:HIS:CE1	3:A:406:PEG:H41	2.24	0.73
1:A:60:PHE:CE2	1:A:76:THR:HG23	2.26	0.70
1:B:148:ARG:HG2	3:B:603:PEG:H31	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:606:PEG:C4	5:B:770:HOH:O	2.41	0.68
1:A:60:PHE:CD2	1:A:76:THR:CG2	2.77	0.67
1:A:112:ARG:HD3	3:A:402:PEG:O2	1.93	0.67
1:A:151:HIS:HE1	3:A:406:PEG:H41	1.59	0.67
1:B:293:THR:HG22	3:B:606:PEG:H21	1.77	0.67
3:A:405:PEG:H32	1:B:115:GLU:OE2	1.94	0.67
1:A:94:GLY:CA	5:A:572:HOH:O	1.85	0.66
1:B:138:ARG:HH11	3:B:602:PEG:H42	1.61	0.65
1:B:112:ARG:CD	3:B:604:PEG:H31	2.23	0.65
1:A:233:LEU:C	5:A:535:HOH:O	2.36	0.64
1:B:196:GLU:OE2	3:B:605:PEG:O1	2.16	0.64
1:B:268:LEU:HG	1:B:344:LEU:HD13	1.80	0.63
1:B:138:ARG:HH11	3:B:602:PEG:H41	1.64	0.62
1:B:234:ARG:HD3	1:B:234:ARG:N	2.13	0.61
1:B:193:ALA:HA	3:B:605:PEG:C1	2.29	0.61
3:B:606:PEG:H41	5:B:770:HOH:O	2.01	0.61
1:B:138:ARG:NH1	3:B:602:PEG:H41	2.16	0.60
1:B:271:ARG:HD2	1:B:344:LEU:HD23	1.83	0.60
1:B:65:PRO:HD2	3:B:606:PEG:H42	1.83	0.59
1:A:60:PHE:CE2	1:A:76:THR:CG2	2.86	0.59
1:B:217:THR:HG21	3:B:605:PEG:H42	1.86	0.57
1:A:186:ALA:HB3	5:A:577:HOH:O	2.02	0.57
3:A:405:PEG:C1	1:B:147:ARG:HH22	2.16	0.57
1:A:184:LEU:HD21	3:B:604:PEG:H42	1.85	0.57
1:A:162:TRP:HZ3	3:B:604:PEG:H22	1.69	0.57
1:B:178:TYR:CZ	1:B:182:ARG:HG3	2.41	0.56
1:A:122:ASN:ND2	5:A:509:HOH:O	2.37	0.56
1:A:132:ASP:OD1	1:A:135:ARG:NH2	2.25	0.56
1:A:294:TYR:HB2	4:A:403:EDO:H11	1.88	0.56
1:A:196:GLU:HA	4:A:403:EDO:H21	1.88	0.56
1:B:293:THR:O	3:B:606:PEG:H22	2.05	0.56
3:A:405:PEG:H12	1:B:151:HIS:HE1	1.69	0.55
1:A:214:ARG:NH2	3:A:405:PEG:H31	2.22	0.55
3:A:406:PEG:H22	1:B:189:GLU:OE1	2.06	0.55
1:A:18:GLU:H	1:A:18:GLU:CD	2.09	0.55
1:A:17:LEU:HD21	1:A:277:LEU:HD21	1.89	0.55
1:B:26:HIS:HB3	5:B:821:HOH:O	2.08	0.54
1:B:64:ALA:HA	3:B:606:PEG:C4	2.38	0.54
1:A:94:GLY:C	5:A:572:HOH:O	2.29	0.54
1:A:184:LEU:HD11	3:B:604:PEG:H11	1.88	0.54
1:A:11:PRO:O	1:A:230:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:THR:OG1	4:A:403:EDO:C2	2.57	0.53
3:A:402:PEG:H22	1:B:183:LEU:HD23	1.91	0.52
1:A:72:ARG:O	1:A:76:THR:HB	2.10	0.52
1:B:151:HIS:HD2	3:B:603:PEG:H21	1.74	0.52
3:A:402:PEG:H41	1:B:162:TRP:HZ3	1.75	0.52
1:A:201:ALA:CA	5:A:525:HOH:O	2.17	0.51
1:B:117:PRO:HB3	3:B:602:PEG:H12	1.92	0.51
1:A:189:GLU:OE2	1:A:214:ARG:NH2	2.44	0.50
1:A:162:TRP:HZ3	3:B:604:PEG:C2	2.24	0.50
1:B:189:GLU:OE2	1:B:214:ARG:NH2	2.33	0.50
1:B:352:TRP:HB2	1:B:358:LEU:HD23	1.93	0.50
1:B:18:GLU:H	1:B:18:GLU:CD	2.15	0.50
3:B:606:PEG:H42	5:B:770:HOH:O	2.09	0.50
3:A:405:PEG:H12	1:B:151:HIS:CE1	2.47	0.50
1:B:166:ASN:HD22	1:B:244:GLN:NE2	2.09	0.49
3:B:603:PEG:H11	5:B:765:HOH:O	2.12	0.49
1:A:199:THR:OG1	4:A:403:EDO:H21	2.13	0.49
1:B:151:HIS:CD2	3:B:603:PEG:H21	2.48	0.49
1:B:199:THR:HG23	3:B:606:PEG:H32	1.92	0.49
1:B:148:ARG:HA	3:B:603:PEG:H22	1.94	0.49
1:A:274:LEU:HD12	1:A:339:SER:HA	1.94	0.49
1:A:284:ARG:NH2	5:A:515:HOH:O	2.46	0.48
1:B:131:GLN:HB3	3:B:602:PEG:C2	2.38	0.48
1:A:115:GLU:OE2	1:A:154:ARG:NH2	2.45	0.48
1:B:234:ARG:NH1	1:B:234:ARG:HG2	2.29	0.47
1:B:300:HIS:HD2	5:B:770:HOH:O	1.98	0.47
1:A:199:THR:OG1	4:A:403:EDO:H22	2.15	0.47
1:B:178:TYR:CZ	1:B:182:ARG:CG	2.99	0.46
1:A:214:ARG:HH21	3:A:405:PEG:H31	1.80	0.45
1:B:234:ARG:HG2	1:B:234:ARG:HH11	1.81	0.45
1:A:195:LEU:HB3	4:A:403:EDO:O2	2.16	0.45
3:B:604:PEG:C1	5:B:701:HOH:O	2.64	0.45
1:A:94:GLY:C	1:A:96:LEU:N	2.70	0.44
1:B:131:GLN:CB	3:B:602:PEG:H22	2.43	0.44
1:A:47:GLU:O	1:A:51:VAL:HG23	2.17	0.44
1:B:271:ARG:HD2	1:B:344:LEU:CD2	2.47	0.44
1:A:184:LEU:HD11	3:B:604:PEG:C1	2.48	0.43
3:B:604:PEG:H11	5:B:701:HOH:O	2.18	0.43
1:A:151:HIS:NE2	3:B:603:PEG:H42	2.34	0.43
1:B:33:VAL:O	1:B:37:ARG:HG3	2.18	0.43
3:A:405:PEG:H41	3:B:604:PEG:C4	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HH11	3:A:402:PEG:H12	1.84	0.43
1:A:193:ALA:CB	3:A:404:PEG:H21	2.48	0.43
1:B:293:THR:O	3:B:606:PEG:C2	2.67	0.43
1:A:155:ALA:HB2	3:A:405:PEG:H21	2.01	0.43
3:A:404:PEG:H12	5:A:526:HOH:O	2.18	0.42
1:A:111:GLN:HG2	1:A:154:ARG:NH1	2.35	0.42
1:B:296:GLN:NE2	3:B:607:PEG:O1	2.40	0.42
1:A:196:GLU:HG3	1:A:203:VAL:HG23	2.01	0.42
1:B:234:ARG:HH11	1:B:234:ARG:CG	2.33	0.41
1:B:138:ARG:NH1	3:B:602:PEG:C4	2.69	0.41
1:B:155:ALA:HB1	1:B:184:LEU:HD22	2.02	0.41
1:B:232:SER:HA	1:B:234:ARG:HE	1.84	0.41
3:B:604:PEG:H42	3:B:604:PEG:H11	2.02	0.41
1:A:196:GLU:HB2	5:A:604:HOH:O	2.20	0.41
1:B:217:THR:HG21	3:B:605:PEG:C4	2.50	0.41
1:A:96:LEU:CD2	1:A:106:LEU:HD22	2.51	0.41
1:A:294:TYR:CB	4:A:403:EDO:H11	2.51	0.41
1:B:135:ARG:N	3:B:602:PEG:H31	2.35	0.40
1:B:147:ARG:HG2	5:B:732:HOH:O	2.20	0.40
1:A:178:TYR:OH	1:A:229:ASP:OD2	2.29	0.40
1:B:135:ARG:HB2	3:B:602:PEG:H31	2.02	0.40
1:B:42:CYS:CB	1:B:48:ARG:HG2	2.51	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	325/361 (90%)	317 (98%)	8 (2%)	0	100	100
1	B	315/361 (87%)	310 (98%)	5 (2%)	0	100	100
All	All	640/722 (89%)	627 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	265/290 (91%)	257 (97%)	8 (3%)	41	59
1	B	258/290 (89%)	249 (96%)	9 (4%)	36	52
All	All	523/580 (90%)	506 (97%)	17 (3%)	38	55

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	76	THR
1	A	230	ARG
1	A	269	ARG
1	A	326	GLU
1	A	340	SER
1	A	344	LEU
1	A	349	SER
1	B	10	LEU
1	B	18	GLU
1	B	30	LYS
1	B	122	ASN
1	B	167	GLN
1	B	182	ARG
1	B	234	ARG
1	B	269	ARG
1	B	326	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	HIS
1	B	151	HIS

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Mol	Chain	Res	Type
1	B	163	GLN
1	B	244	GLN
1	B	296	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PEG	A	404	-	6,6,6	1.01	0	5,5,5	0.69	0
3	PEG	A	402	-	6,6,6	0.66	0	5,5,5	0.74	0
3	PEG	A	406	-	6,6,6	0.26	0	5,5,5	0.32	0
3	PEG	B	602	-	6,6,6	0.36	0	5,5,5	0.57	0
3	PEG	B	605	-	6,6,6	0.86	0	5,5,5	0.58	0
3	PEG	B	601	-	6,6,6	0.30	0	5,5,5	0.16	0
3	PEG	B	604	-	6,6,6	0.33	0	5,5,5	0.45	0
3	PEG	A	405	-	6,6,6	0.85	0	5,5,5	0.59	0
3	PEG	B	607	-	6,6,6	0.57	0	5,5,5	0.47	0
3	PEG	B	603	-	6,6,6	0.41	0	5,5,5	0.46	0
2	PG4	A	401	-	12,12,12	0.44	0	11,11,11	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	B	606	-	6,6,6	1.17	0	5,5,5	1.11	0
4	EDO	A	403	-	3,3,3	0.29	0	2,2,2	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	404	-	-	3/4/4/4	-
3	PEG	A	402	-	-	3/4/4/4	-
3	PEG	A	406	-	-	2/4/4/4	-
3	PEG	B	602	-	-	3/4/4/4	-
3	PEG	B	605	-	-	2/4/4/4	-
3	PEG	B	601	-	-	1/4/4/4	-
3	PEG	B	604	-	-	4/4/4/4	-
3	PEG	A	405	-	-	1/4/4/4	-
3	PEG	B	607	-	-	1/4/4/4	-
3	PEG	B	603	-	-	3/4/4/4	-
2	PG4	A	401	-	-	6/10/10/10	-
3	PEG	B	606	-	-	4/4/4/4	-
4	EDO	A	403	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	PEG	C1-C2-O2-C3
3	A	404	PEG	O1-C1-C2-O2
3	A	402	PEG	O1-C1-C2-O2
3	A	406	PEG	O1-C1-C2-O2
3	B	604	PEG	C1-C2-O2-C3
2	A	401	PG4	O4-C7-C8-O5
3	A	402	PEG	O2-C3-C4-O4
3	B	603	PEG	O2-C3-C4-O4
3	B	602	PEG	O2-C3-C4-O4
3	B	604	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	B	607	PEG	O2-C3-C4-O4
4	A	403	EDO	O1-C1-C2-O2
3	B	606	PEG	O1-C1-C2-O2
2	A	401	PG4	C3-C4-O3-C5
3	A	405	PEG	O1-C1-C2-O2
3	B	604	PEG	O1-C1-C2-O2
3	B	605	PEG	O1-C1-C2-O2
3	B	606	PEG	C1-C2-O2-C3
3	B	606	PEG	C4-C3-O2-C2
3	A	402	PEG	C4-C3-O2-C2
3	B	602	PEG	O1-C1-C2-O2
3	B	601	PEG	O2-C3-C4-O4
3	A	404	PEG	C4-C3-O2-C2
2	A	401	PG4	C4-C3-O2-C2
3	B	603	PEG	C4-C3-O2-C2
3	B	605	PEG	C4-C3-O2-C2
3	B	603	PEG	C1-C2-O2-C3
2	A	401	PG4	C8-C7-O4-C6
3	A	404	PEG	C1-C2-O2-C3
2	A	401	PG4	C6-C5-O3-C4
3	B	606	PEG	O2-C3-C4-O4
3	A	406	PEG	C1-C2-O2-C3
3	B	604	PEG	C4-C3-O2-C2
2	A	401	PG4	O2-C3-C4-O3

There are no ring outliers.

11 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	PEG	2	0
3	A	402	PEG	7	0
3	A	406	PEG	3	0
3	B	602	PEG	11	0
3	B	605	PEG	7	0
3	B	604	PEG	12	0
3	A	405	PEG	9	0
3	B	607	PEG	2	0
3	B	603	PEG	7	0
3	B	606	PEG	13	0
4	A	403	EDO	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/361 (91%)	0.60	31 (9%) <b>8</b> <b>9</b>	16, 26, 56, 79	0
1	B	323/361 (89%)	0.59	26 (8%) <b>12</b> <b>13</b>	17, 28, 61, 93	0
All	All	654/722 (90%)	0.60	57 (8%) <b>10</b> <b>11</b>	16, 27, 59, 93	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	GLY	6.4
1	A	123	GLY	5.7
1	A	201	ALA	5.7
1	B	234	ARG	5.6
1	B	313	PRO	4.9
1	A	328	ALA	4.9
1	A	327	ASP	4.2
1	A	11	PRO	4.2
1	B	45	GLU	4.1
1	A	313	PRO	3.9
1	A	9	ASP	3.8
1	B	49	ALA	3.6
1	B	50	TRP	3.6
1	B	44	SER	3.6
1	A	45	GLU	3.5
1	A	122	ASN	3.4
1	A	232	SER	3.3
1	B	43	ALA	3.3
1	A	44	SER	3.3
1	A	329	PRO	3.3
1	B	46	GLU	3.1
1	B	340	SER	3.0
1	A	312	VAL	3.0
1	A	255	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	2.8
1	A	330	LEU	2.8
1	B	231	HIS	2.8
1	B	312	VAL	2.8
1	B	11	PRO	2.8
1	B	341	PRO	2.8
1	B	302	ILE	2.8
1	B	329	PRO	2.7
1	B	255	GLY	2.7
1	A	302	ILE	2.7
1	A	42	CYS	2.7
1	A	95	PRO	2.6
1	B	47	GLU	2.6
1	A	93	ASN	2.5
1	A	286	GLY	2.5
1	B	331	THR	2.5
1	A	34	GLU	2.5
1	B	345	PRO	2.4
1	B	328	ALA	2.4
1	A	38	ARG	2.4
1	A	251	MET	2.4
1	A	10	LEU	2.4
1	B	183	LEU	2.4
1	A	43	ALA	2.4
1	B	26	HIS	2.3
1	A	357	ALA	2.2
1	B	221	ILE	2.1
1	A	253	HIS	2.1
1	A	233	LEU	2.1
1	A	331	THR	2.1
1	B	335	SER	2.1
1	A	333	ALA	2.0
1	B	123	GLY	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PEG	A	402	7/7	0.60	0.49	34,47,52,54	0
3	PEG	A	404	7/7	0.70	0.38	25,37,46,50	0
3	PEG	B	601	7/7	0.71	0.35	46,48,59,59	0
3	PEG	A	405	7/7	0.73	0.39	37,50,60,61	0
3	PEG	B	607	7/7	0.74	0.28	46,52,58,62	0
3	PEG	B	605	7/7	0.79	0.26	29,31,35,36	0
2	PG4	A	401	13/13	0.80	0.29	33,41,47,47	0
3	PEG	B	606	7/7	0.82	0.27	34,37,44,47	0
3	PEG	B	603	7/7	0.83	0.26	40,55,61,61	0
3	PEG	A	406	7/7	0.89	0.29	37,55,60,60	0
3	PEG	B	602	7/7	0.91	0.22	35,39,44,45	0
3	PEG	B	604	7/7	0.92	0.23	32,35,38,43	0
4	EDO	A	403	4/4	0.95	0.14	32,38,43,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.