



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:22 PM UTC

PDB ID : 9QTF / pdb_00009qtf
Title : Simkania negevensis CE-clan virulence factor SnCE1 C256A catalytically inactive mutant
Authors : Schmoeker, O.; Girbardt, B.; Palm, G.J.; Hoppen, J.; Schulze, S.; Lammers, M.
Deposited on : 2025-04-08
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

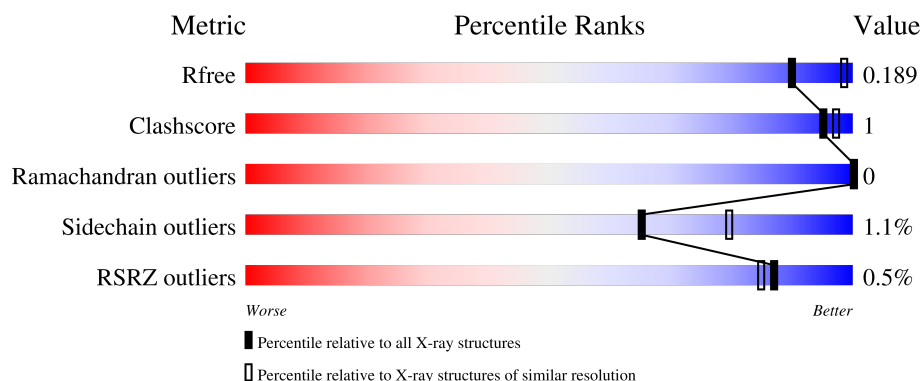
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	242	
1	B	242	
1	C	242	
1	D	242	
1	E	242	

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Mol	Chain	Length	Quality of chain
1	F	242	 77%5%18%
1	G	242	 79%•17%
1	H	242	 78%••18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27774 atoms, of which 13285 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 Deubiquitinase and deneddylase ChlaDub2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	200	Total	C	H	N	O	S	35	0	0
			3351	1112	1654	280	304	1			
1	B	199	Total	C	H	N	O	S	35	0	0
			3329	1106	1641	278	303	1			
1	C	200	Total	C	H	N	O	S	35	0	0
			3351	1112	1654	280	304	1			
1	D	197	Total	C	H	N	O	S	35	1	0
			3321	1104	1640	275	300	2			
1	E	199	Total	C	H	N	O	S	35	1	0
			3342	1110	1649	278	303	2			
1	F	199	Total	C	H	N	O	S	35	1	0
			3346	1111	1650	279	304	2			
1	G	200	Total	C	H	N	O	S	35	0	0
			3351	1112	1654	280	304	1			
1	H	199	Total	C	H	N	O	S	35	0	0
			3329	1106	1641	278	303	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP F8L4W9
A	-3	PRO	-	expression tag	UNP F8L4W9
A	-2	LEU	-	expression tag	UNP F8L4W9
A	-1	GLY	-	expression tag	UNP F8L4W9
A	0	SER	-	expression tag	UNP F8L4W9
A	183	ALA	CYS	engineered mutation	UNP F8L4W9
B	-4	GLY	-	expression tag	UNP F8L4W9
B	-3	PRO	-	expression tag	UNP F8L4W9
B	-2	LEU	-	expression tag	UNP F8L4W9
B	-1	GLY	-	expression tag	UNP F8L4W9
B	0	SER	-	expression tag	UNP F8L4W9
B	183	ALA	CYS	engineered mutation	UNP F8L4W9
C	-4	GLY	-	expression tag	UNP F8L4W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	PRO	-	expression tag	UNP F8L4W9
C	-2	LEU	-	expression tag	UNP F8L4W9
C	-1	GLY	-	expression tag	UNP F8L4W9
C	0	SER	-	expression tag	UNP F8L4W9
C	183	ALA	CYS	engineered mutation	UNP F8L4W9
D	-4	GLY	-	expression tag	UNP F8L4W9
D	-3	PRO	-	expression tag	UNP F8L4W9
D	-2	LEU	-	expression tag	UNP F8L4W9
D	-1	GLY	-	expression tag	UNP F8L4W9
D	0	SER	-	expression tag	UNP F8L4W9
D	183	ALA	CYS	engineered mutation	UNP F8L4W9
E	-4	GLY	-	expression tag	UNP F8L4W9
E	-3	PRO	-	expression tag	UNP F8L4W9
E	-2	LEU	-	expression tag	UNP F8L4W9
E	-1	GLY	-	expression tag	UNP F8L4W9
E	0	SER	-	expression tag	UNP F8L4W9
E	183	ALA	CYS	engineered mutation	UNP F8L4W9
F	-4	GLY	-	expression tag	UNP F8L4W9
F	-3	PRO	-	expression tag	UNP F8L4W9
F	-2	LEU	-	expression tag	UNP F8L4W9
F	-1	GLY	-	expression tag	UNP F8L4W9
F	0	SER	-	expression tag	UNP F8L4W9
F	183	ALA	CYS	engineered mutation	UNP F8L4W9
G	-4	GLY	-	expression tag	UNP F8L4W9
G	-3	PRO	-	expression tag	UNP F8L4W9
G	-2	LEU	-	expression tag	UNP F8L4W9
G	-1	GLY	-	expression tag	UNP F8L4W9
G	0	SER	-	expression tag	UNP F8L4W9
G	183	ALA	CYS	engineered mutation	UNP F8L4W9
H	-4	GLY	-	expression tag	UNP F8L4W9
H	-3	PRO	-	expression tag	UNP F8L4W9
H	-2	LEU	-	expression tag	UNP F8L4W9
H	-1	GLY	-	expression tag	UNP F8L4W9
H	0	SER	-	expression tag	UNP F8L4W9
H	183	ALA	CYS	engineered mutation	UNP F8L4W9

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	2	0
			20	4	12	1	3		
2	B	1	Total	C	H	N	O	2	0
			20	4	12	1	3		
2	C	1	Total	C	H	N	O	2	0
			20	4	12	1	3		
2	D	1	Total	C	H	N	O	2	0
			20	4	12	1	3		
2	E	1	Total	C	H	N	O	2	0
			20	4	12	1	3		
2	E	1	Total	C	H	N	O	2	0
			20	4	12	1	3		
2	G	1	Total	C	H	N	O	2	0
			20	4	12	1	3		
2	H	1	Total	C	H	N	O	2	0
			20	4	12	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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


- Molecule 5 is water.

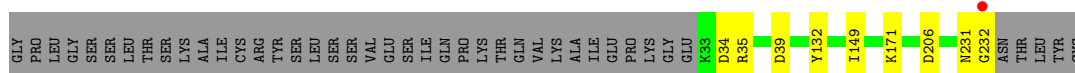
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	109	Total	O	0	0
			109	109		
5	C	102	Total	O	0	0
			102	102		
5	D	136	Total	O	0	0
			136	136		
5	E	129	Total	O	0	0
			129	129		
5	F	103	Total	O	0	0
			103	103		
5	G	98	Total	O	0	0
			98	98		
5	H	96	Total	O	0	0
			96	96		

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.

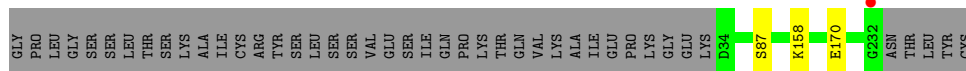
- Molecule 1: Deubiquitinase and deneddylase ChlaDub2

Chain A:  79% 17%




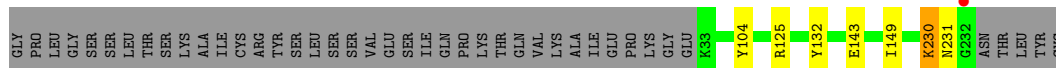
- Molecule 1: Deubiquitinase and deneddylase ChlaDub2

Chain B:  81% 18%




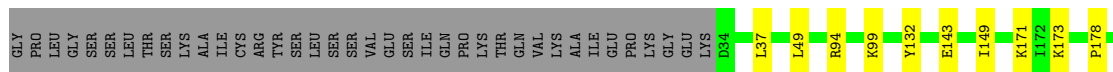
- Molecule 1: Deubiquitinase and deneddylase ChlaDub2

Chain C:  80% 17%




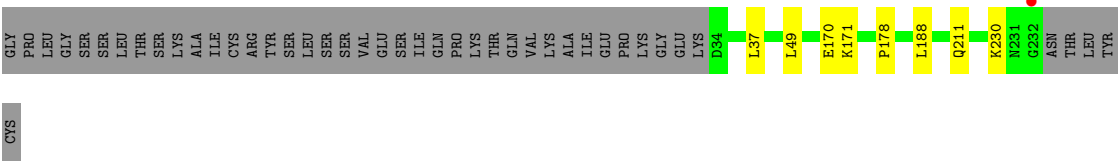
- Molecule 1: Deubiquitinase and deneddylase ChlaDub2

Chain D:  76% 19%

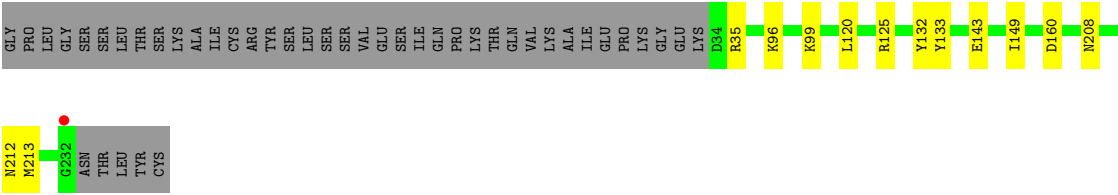


- Molecule 1: Deubiquitinase and deneddylase ChlaDub2

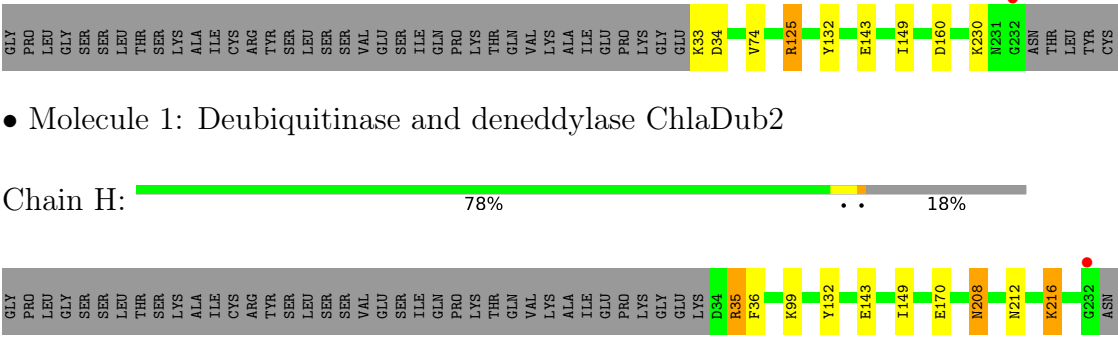
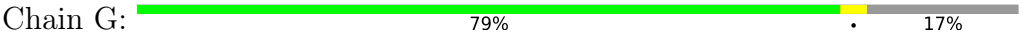
Chain E:  79% 18%



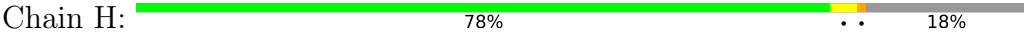
● Molecule 1: Deubiquitinase and deneddylase ChlaDub2



● Molecule 1: Deubiquitinase and deneddylase ChlaDub2



● Molecule 1: Deubiquitinase and deneddylase ChlaDub2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.63Å 151.17Å 80.78Å 90.00° 105.07° 90.00°	Depositor
Resolution (Å)	48.55 – 2.21 48.55 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.55-2.21) 95.7 (48.55-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.155 , 0.191 0.154 , 0.189	Depositor DCC
R_{free} test set	4203 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	27774	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.03	0/1748	1.30	4/2359 (0.2%)
1	B	1.02	1/1739 (0.1%)	1.28	0/2348
1	C	0.99	0/1748	1.28	0/2359
1	D	0.99	0/1735	1.31	2/2342 (0.1%)
1	E	1.02	0/1747	1.26	0/2358
1	F	0.98	0/1747	1.29	3/2358 (0.1%)
1	G	1.00	0/1748	1.30	2/2359 (0.1%)
1	H	0.98	0/1739	1.30	2/2348 (0.1%)
All	All	1.00	1/13951 (0.0%)	1.29	13/18831 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	SER	C-O	-5.08	1.16	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	LYS	CA-C-O	7.51	133.58	120.80
1	A	232	GLY	CA-C-O	-6.96	106.19	120.80
1	G	125	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	F	96	LYS	CB-CG-CD	6.23	125.63	111.30
1	H	212	ASN	CA-CB-CG	-6.06	106.54	112.60
1	G	34	ASP	N-CA-C	-6.00	105.26	113.30
1	F	208	ASN	CA-CB-CG	5.92	118.53	112.60
1	A	34	ASP	N-CA-C	-5.65	105.73	113.30
1	H	216	LYS	CB-CG-CD	5.64	124.28	111.30
1	A	206	ASP	CA-CB-CG	5.61	118.21	112.60
1	F	212	ASN	CA-CB-CG	-5.47	107.13	112.60
1	D	94	ARG	CG-CD-NE	-5.14	100.70	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ASP	CA-CB-CG	5.13	117.73	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	1654	1649	2	0
1	B	1688	1641	1636	1	0
1	C	1697	1654	1649	4	0
1	D	1681	1640	1636	6	0
1	E	1693	1649	1645	6	0
1	F	1696	1650	1644	5	0
1	G	1697	1654	1649	3	0
1	H	1688	1641	1636	6	0
2	A	8	12	12	0	0
2	B	8	12	12	1	0
2	C	8	12	12	0	0
2	D	8	12	12	0	0
2	E	16	24	24	0	0
2	G	8	12	12	0	0
2	H	8	12	12	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	E	4	6	6	0	0
5	A	108	0	0	1	0
5	B	109	0	0	2	0
5	C	102	0	0	0	0
5	D	136	0	0	2	0
5	E	129	0	0	3	0
5	F	103	0	0	0	0
5	G	98	0	0	0	0
5	H	96	0	0	1	0
All	All	14489	13285	13246	33	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 1.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:PRO:HG2	1:E:178:PRO:HB2	1.87	0.57
1:H:208:ASN:HD22	1:H:208:ASN:H	1.53	0.55
1:H:170:GLU:HG2	5:H:446:HOH:O	2.10	0.51
1:C:230:LYS:C	1:C:231:ASN:HD22	2.20	0.50
1:D:171:LYS:HE3	5:D:429:HOH:O	2.15	0.46
1:G:143:GLU:H	1:G:143:GLU:CD	2.24	0.45
1:E:170:GLU:HG2	5:E:446:HOH:O	2.16	0.45
1:E:211:GLN:HB2	5:E:453:HOH:O	2.17	0.45
1:G:125:ARG:HH11	1:G:160:ASP:CG	2.24	0.45
1:A:171:LYS:HE3	5:A:468:HOH:O	2.16	0.45
1:D:143:GLU:H	1:D:143:GLU:CD	2.26	0.44
1:C:143:GLU:H	1:C:143:GLU:CD	2.25	0.44
1:D:173:LYS:HE3	5:D:518:HOH:O	2.16	0.44
1:E:230:LYS:HG2	1:E:230:LYS:O	2.19	0.43
1:H:35:ARG:HD3	1:H:36:PHE:CE2	2.53	0.43
2:B:301:TRS:O1	5:B:401:HOH:O	2.21	0.43
1:H:132:TYR:HB2	1:H:149:ILE:HG21	2.00	0.43
1:B:170:GLU:HG2	5:B:433:HOH:O	2.19	0.43
1:D:132:TYR:HB2	1:D:149:ILE:HG21	2.01	0.42
1:H:143:GLU:H	1:H:143:GLU:CD	2.28	0.42
1:C:104:TYR:O	1:C:125:ARG:HD3	2.19	0.42
1:F:125:ARG:HH11	1:F:160:ASP:CG	2.28	0.42
1:G:132:TYR:HB2	1:G:149:ILE:HG21	2.02	0.42
1:D:49:LEU:HD22	1:D:188:LEU:HG	2.02	0.42
1:C:132:TYR:HB2	1:C:149:ILE:HG21	2.02	0.41
1:F:120:LEU:HB3	1:F:133:TYR:HB2	2.02	0.41
1:F:213[B]:MET:HE2	1:F:213[B]:MET:HB3	1.96	0.41
1:F:143:GLU:H	1:F:143:GLU:CD	2.29	0.41
1:H:208:ASN:HD22	1:H:208:ASN:N	2.17	0.41
1:E:171:LYS:HE3	5:E:476:HOH:O	2.20	0.40
1:F:132:TYR:HB2	1:F:149:ILE:HG21	2.02	0.40
1:A:132:TYR:HB2	1:A:149:ILE:HG21	2.04	0.40
1:E:49:LEU:HD22	1:E:188:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/242 (82%)	193 (98%)	5 (2%)	0	100	100
1	B	197/242 (81%)	190 (96%)	7 (4%)	0	100	100
1	C	198/242 (82%)	193 (98%)	5 (2%)	0	100	100
1	D	196/242 (81%)	190 (97%)	6 (3%)	0	100	100
1	E	198/242 (82%)	192 (97%)	6 (3%)	0	100	100
1	F	198/242 (82%)	194 (98%)	4 (2%)	0	100	100
1	G	198/242 (82%)	193 (98%)	5 (2%)	0	100	100
1	H	197/242 (81%)	191 (97%)	6 (3%)	0	100	100
All	All	1580/1936 (82%)	1536 (97%)	44 (3%)	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	177/214 (83%)	175 (99%)	2 (1%)	65	79
1	B	176/214 (82%)	175 (99%)	1 (1%)	78	89
1	C	177/214 (83%)	176 (99%)	1 (1%)	78	89
1	D	176/214 (82%)	174 (99%)	2 (1%)	65	79
1	E	177/214 (83%)	176 (99%)	1 (1%)	78	89
1	F	177/214 (83%)	175 (99%)	2 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	177/214 (83%)	174 (98%)	3 (2%)	53	69
1	H	176/214 (82%)	172 (98%)	4 (2%)	44	59
All	All	1413/1712 (82%)	1397 (99%)	16 (1%)	65	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	231	ASN
1	B	158	LYS
1	C	230	LYS
1	D	37	LEU
1	D	99	LYS
1	E	37	LEU
1	F	35	ARG
1	F	99	LYS
1	G	33	LYS
1	G	74	VAL
1	G	230	LYS
1	H	35	ARG
1	H	99	LYS
1	H	208	ASN
1	H	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	212	ASN
1	A	229	GLN
1	B	89	HIS
1	B	212	ASN
1	B	229	GLN
1	C	89	HIS
1	C	229	GLN
1	C	231	ASN
1	D	89	HIS
1	F	89	HIS
1	G	89	HIS
1	G	204	GLN

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Mol	Chain	Res	Type
1	G	212	ASN
1	H	204	GLN
1	H	208	ASN
1	H	231	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRS	A	301	-	7,7,7	0.30	0	9,9,9	0.41	0
4	EDO	E	301	-	3,3,3	0.25	0	2,2,2	0.37	0
2	TRS	D	301	-	7,7,7	0.35	0	9,9,9	0.62	0
2	TRS	E	302	-	7,7,7	0.34	0	9,9,9	0.71	0
2	TRS	B	301	-	7,7,7	0.39	0	9,9,9	0.52	0
2	TRS	H	301	-	7,7,7	0.31	0	9,9,9	0.49	0
2	TRS	G	301	-	7,7,7	0.48	0	9,9,9	0.59	0
2	TRS	C	301	-	7,7,7	0.39	0	9,9,9	0.70	0
2	TRS	E	303	-	7,7,7	0.31	0	9,9,9	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	A	301	-	-	2/9/9/9	-
4	EDO	E	301	-	-	0/1/1/1	-
2	TRS	D	301	-	-	3/9/9/9	-
2	TRS	E	302	-	-	0/9/9/9	-
2	TRS	B	301	-	-	0/9/9/9	-
2	TRS	H	301	-	-	3/9/9/9	-
2	TRS	G	301	-	-	2/9/9/9	-
2	TRS	C	301	-	-	0/9/9/9	-
2	TRS	E	303	-	-	4/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	303	TRS	N-C-C2-O2
2	G	301	TRS	N-C-C2-O2
2	H	301	TRS	C2-C-C3-O3
2	D	301	TRS	N-C-C1-O1
2	E	303	TRS	C3-C-C2-O2
2	E	303	TRS	N-C-C3-O3
2	H	301	TRS	N-C-C3-O3
2	D	301	TRS	C2-C-C1-O1
2	D	301	TRS	C3-C-C1-O1
2	H	301	TRS	C1-C-C3-O3
2	A	301	TRS	C1-C-C3-O3
2	E	303	TRS	C1-C-C2-O2
2	G	301	TRS	C1-C-C2-O2
2	A	301	TRS	N-C-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	TRS	1	0

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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	200/242 (82%)	-0.63	1 (0%) 87 85	33, 48, 79, 134	0
1	B	199/242 (82%)	-0.66	1 (0%) 87 85	34, 48, 79, 127	0
1	C	200/242 (82%)	-0.63	1 (0%) 87 85	33, 49, 83, 118	0
1	D	197/242 (81%)	-0.67	1 (0%) 87 85	30, 45, 81, 110	1 (0%)
1	E	199/242 (82%)	-0.63	1 (0%) 87 85	33, 47, 81, 128	1 (0%)
1	F	199/242 (82%)	-0.60	1 (0%) 87 85	31, 48, 83, 116	1 (0%)
1	G	200/242 (82%)	-0.56	1 (0%) 87 85	34, 51, 82, 123	0
1	H	199/242 (82%)	-0.53	1 (0%) 87 85	33, 51, 87, 118	0
All	All	1593/1936 (82%)	-0.61	8 (0%) 87 85	30, 48, 82, 134	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	232	GLY	4.6
1	C	232	GLY	3.9
1	A	232	GLY	3.5
1	G	232	GLY	3.3
1	B	232	GLY	3.2
1	F	232	GLY	3.0
1	H	232	GLY	3.0
1	D	230	LYS	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	E	301	4/4	0.88	0.12	20,73,76,77	1
2	TRS	C	301	8/8	0.89	0.10	20,65,67,67	2
3	NA	D	302	1/1	0.90	0.10	69,69,69,69	0
2	TRS	G	301	8/8	0.91	0.10	20,64,73,75	2
2	TRS	H	301	8/8	0.94	0.07	20,56,58,58	2
3	NA	B	302	1/1	0.94	0.15	62,62,62,62	0
2	TRS	E	302	8/8	0.94	0.08	20,66,69,70	2
2	TRS	B	301	8/8	0.94	0.08	20,59,64,64	2
2	TRS	A	301	8/8	0.95	0.08	20,66,75,76	2
2	TRS	E	303	8/8	0.96	0.07	20,63,66,66	2
3	NA	E	304	1/1	0.96	0.10	61,61,61,61	0
2	TRS	D	301	8/8	0.96	0.07	20,56,60,60	2

6.5 Other polymers [i](#)

There are no such residues in this entry.