



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:14 AM UTC

PDB ID : 8BAN / pdb_00008ban
Title : Secretagoin (mouse) in complex with its target peptide from SNAP-25
Authors : Schnell, R.; Szodorai, E.
Deposited on : 2022-10-11
Resolution : 2.35 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

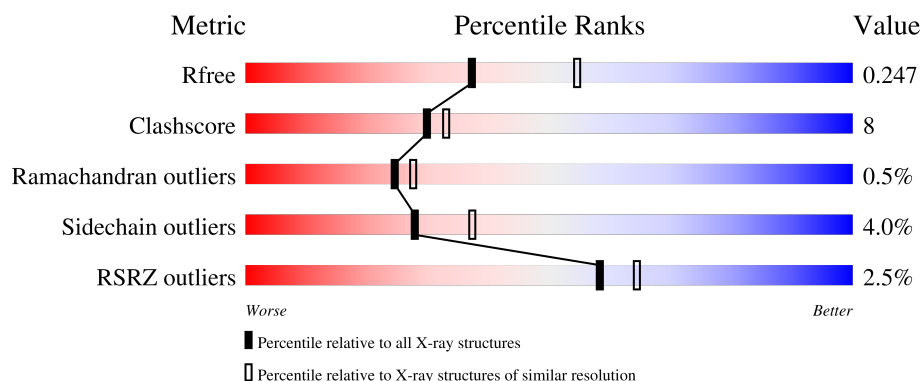
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 ≥ 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	256	4% 76% 18% • •
1	B	256	79% 14% • 5%
2	C	276	4% 76% 13% • • 9%
2	D	276	5% 78% 11% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8380 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 Green fluorescent protein, Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1949	1234	333	373	9			
1	B	244	Total	C	N	O	S	0	1	0
			1948	1233	334	372	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P42212
A	0	MET	-	expression tag	UNP P42212
A	1	ALA	-	expression tag	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	167	THR	ILE	engineered mutation	UNP P42212
A	229	THR	-	linker	UNP P42212
A	230	MET	-	linker	UNP P42212
A	231	ALA	-	linker	UNP P42212
B	-1	SER	-	expression tag	UNP P42212
B	0	MET	-	expression tag	UNP P42212
B	1	ALA	-	expression tag	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	167	THR	ILE	engineered mutation	UNP P42212
B	229	THR	-	linker	UNP P42212
B	230	MET	-	linker	UNP P42212
B	231	ALA	-	linker	UNP P42212

- Molecule 2 is a protein called Secretagoin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	251	Total	C	N	O	S	0	0	0
			2065	1317	344	391	13			
2	D	250	Total	C	N	O	S	0	0	0
			2051	1307	339	392	13			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	4	Total	Ca	0	0
			4	4		
3	D	4	Total	Ca	0	0
			4	4		

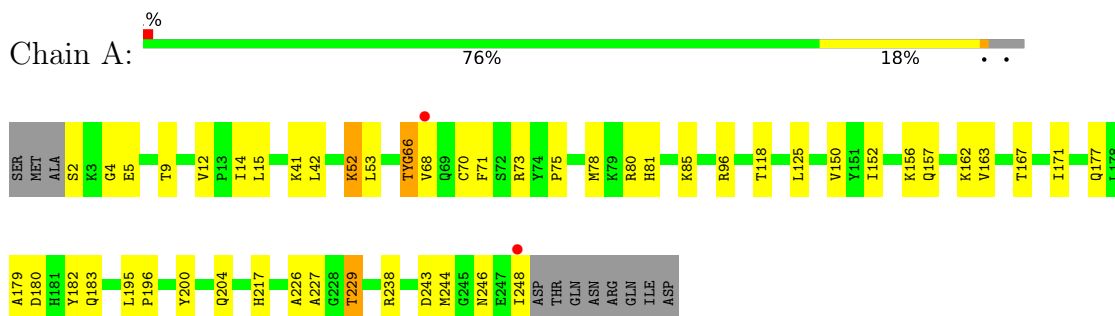
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total	O	0	0
			128	128		
4	B	89	Total	O	0	0
			89	89		
4	C	63	Total	O	0	0
			63	63		
4	D	79	Total	O	0	0
			79	79		

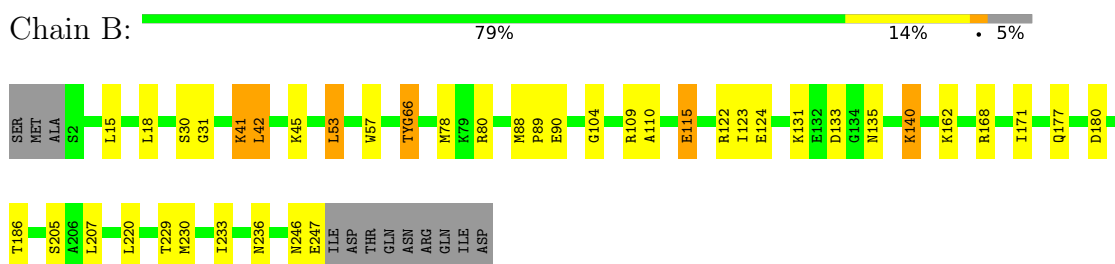
3 Residue-property plots [i](#)

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.

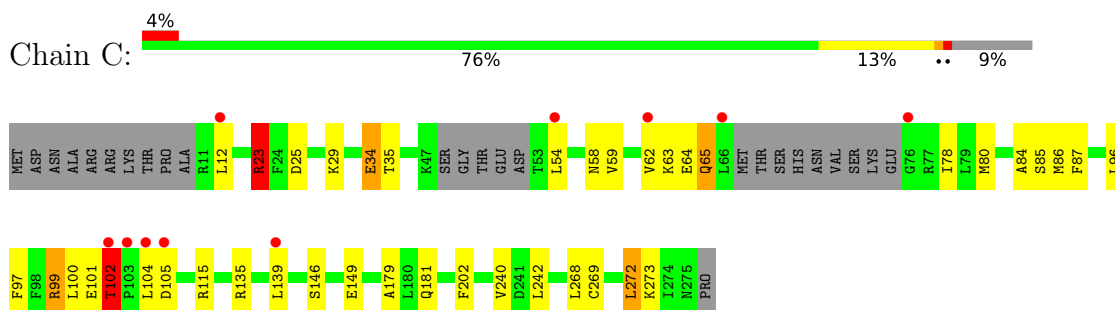
- Molecule 1: Green fluorescent protein,Synaptosomal-associated protein 25



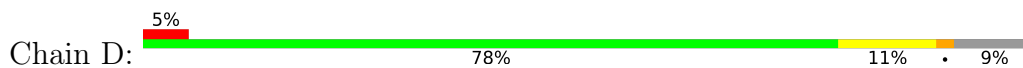
- Molecule 1: Green fluorescent protein,Synaptosomal-associated protein 25

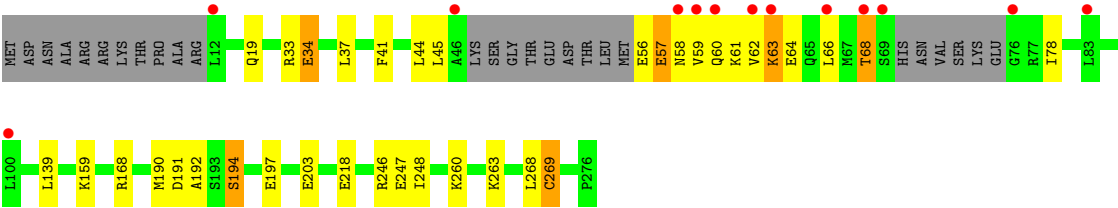


- Molecule 2: Secretagoin



- Molecule 2: Secretagoin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.66Å 121.07Å 126.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.42 – 2.35 87.42 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (87.42-2.35) 99.0 (87.42-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.194 , 0.248 0.198 , 0.247	Depositor DCC
R_{free} test set	2365 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8380	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: CRO, CA

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	1.18	1/1968 (0.1%)	1.04	2/2656 (0.1%)
1	B	1.09	0/1971	1.00	7/2660 (0.3%)
2	C	0.91	0/2099	0.97	6/2809 (0.2%)
2	D	0.86	0/2086	0.89	1/2793 (0.0%)
All	All	1.01	1/8124 (0.0%)	0.98	16/10918 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	ILE	C-O	-6.88	1.17	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	68	THR	N-CA-C	-8.07	102.43	111.71
2	C	35	THR	N-CA-C	-6.89	103.85	111.36
2	C	102	THR	CA-C-N	-6.11	113.39	119.92
2	C	102	THR	C-N-CA	-6.11	113.39	119.92
2	C	54	LEU	N-CA-C	-5.81	104.94	111.28
1	B	41	LYS	N-CA-C	5.45	118.29	109.40
1	B	53	LEU	CA-C-N	-5.29	114.58	120.45
1	B	53	LEU	C-N-CA	-5.29	114.58	120.45
1	A	12	VAL	N-CA-C	5.26	113.86	107.61
1	B	115	GLU	N-CA-C	-5.16	96.92	107.70
2	C	23	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	104	GLY	N-CA-C	5.13	120.47	112.31
2	C	102	THR	N-CA-C	-5.12	98.50	109.81
1	A	217	HIS	N-CA-C	5.10	116.05	108.60
1	B	186	THR	CA-C-N	-5.09	114.71	119.85
1	B	186	THR	C-N-CA	-5.09	114.71	119.85

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	1949	0	1896	39	0
1	B	1948	0	1893	22	0
2	C	2065	0	2041	35	0
2	D	2051	0	2016	45	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	128	0	0	4	0
4	B	89	0	0	2	0
4	C	63	0	0	3	0
4	D	79	0	0	3	0
All	All	8380	0	7846	134	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 8.

All (134) 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:C:58:ASN:O	2:C:62:VAL:HG23	1.38	1.21
2:D:59:VAL:O	2:D:62:VAL:CG1	2.03	1.06
2:D:59:VAL:O	2:D:62:VAL:HG12	1.54	1.06
2:D:59:VAL:C	2:D:62:VAL:HG12	1.93	0.94
2:C:99:ARG:HG3	2:C:179:ALA:HB2	1.54	0.89
2:C:62:VAL:HG22	2:C:86:MET:HG2	1.55	0.87
2:C:269:CYS:HB3	2:D:268:LEU:HD11	1.58	0.85
2:D:33:ARG:O	2:D:34:GLU:HB3	1.77	0.83
2:D:64:GLU:O	2:D:68:THR:OG1	1.97	0.81
2:C:29:LYS:NZ	4:C:401:HOH:O	2.09	0.80
2:D:37:LEU:HD13	2:D:78:ILE:HD13	1.65	0.79
1:B:78:MET:HG2	1:B:229:THR:HG21	1.65	0.77
2:D:59:VAL:O	2:D:62:VAL:HG13	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:CRO:HG11	1:B:220:LEU:HD22	1.67	0.75
1:A:66:CRO:HD1	1:A:66:CRO:N2	2.01	0.73
2:D:247:GLU:OE2	4:D:401:HOH:O	2.08	0.72
2:C:34:GLU:HB2	2:C:78:ILE:HD11	1.70	0.72
2:D:61:LYS:HD3	2:D:64:GLU:OE2	1.91	0.70
2:C:58:ASN:O	2:C:62:VAL:CG2	2.28	0.70
1:A:171:ILE:HD11	1:A:177:GLN:HB2	1.72	0.69
2:D:41:PHE:HB3	2:D:60:GLN:HE21	1.58	0.68
1:A:68:VAL:HG12	1:A:71:PHE:HD2	1.59	0.66
2:C:12:LEU:O	2:C:12:LEU:HG	1.96	0.66
2:D:59:VAL:CA	2:D:62:VAL:HG12	2.26	0.65
1:A:68:VAL:CG1	1:A:71:PHE:HD2	2.10	0.64
2:C:101:GLU:O	2:C:102:THR:OG1	2.12	0.64
2:C:62:VAL:CG2	2:C:86:MET:HG2	2.26	0.63
1:A:163:VAL:HB	1:A:183:GLN:HB3	1.81	0.63
1:A:68:VAL:HG12	1:A:68:VAL:O	1.97	0.63
1:A:75:PRO:HD2	1:A:78:MET:HE3	1.79	0.62
1:B:230:MET:HE2	1:B:236:ASN:HD21	1.63	0.62
2:C:12:LEU:HD21	2:C:87:PHE:HB3	1.79	0.62
2:C:104:LEU:O	2:C:181:GLN:HG2	1.98	0.62
1:B:109:ARG:NE	4:B:301:HOH:O	2.14	0.62
2:C:25:ASP:OD1	2:C:29:LYS:HE2	1.99	0.61
2:D:191:ASP:O	2:D:192:ALA:HB3	2.01	0.61
2:D:33:ARG:O	2:D:34:GLU:CB	2.49	0.61
1:A:246:ASN:C	1:A:248:ILE:H	2.08	0.59
1:A:78:MET:HE1	1:A:227:ALA:HA	1.84	0.59
1:A:73:ARG:NH1	4:A:302:HOH:O	2.30	0.58
1:A:2:SER:N	1:A:5:GLU:OE1	2.36	0.58
2:D:59:VAL:HA	2:D:62:VAL:HG12	1.85	0.58
1:A:75:PRO:HG2	1:A:78:MET:HE3	1.85	0.58
1:A:75:PRO:CD	1:A:78:MET:HE3	2.34	0.58
2:D:62:VAL:HG13	2:D:63:LYS:N	2.19	0.57
2:C:97:PHE:HD1	2:C:100:LEU:CD1	2.17	0.57
2:D:57:GLU:O	2:D:60:GLN:CB	2.53	0.56
1:B:18:LEU:C	1:B:18:LEU:HD23	2.30	0.56
1:A:2:SER:N	4:A:304:HOH:O	2.38	0.56
2:C:268:LEU:HD11	2:D:269:CYS:HB2	1.87	0.56
2:D:45:LEU:HD23	2:D:57:GLU:HB3	1.88	0.56
1:A:78:MET:HE1	1:A:226:ALA:O	2.05	0.55
2:D:57:GLU:HA	2:D:57:GLU:OE1	2.06	0.55
1:B:246:ASN:C	1:B:247:GLU:HG2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:CG1	1:A:71:PHE:CD2	2.90	0.54
1:B:171:ILE:HD11	1:B:177:GLN:HB2	1.89	0.54
1:A:81:HIS:O	1:A:196:PRO:HB3	2.08	0.54
2:C:23:ARG:HH21	2:C:23:ARG:HG2	1.73	0.53
2:D:194:SER:HB3	2:D:197:GLU:OE1	2.09	0.53
2:C:268:LEU:HD11	2:D:269:CYS:CB	2.39	0.52
2:C:62:VAL:O	2:C:65:GLN:HG3	2.09	0.52
1:A:73:ARG:HD2	4:A:302:HOH:O	2.10	0.52
2:C:23:ARG:HH21	2:C:23:ARG:CG	2.22	0.52
1:A:156:LYS:NZ	1:A:195:LEU:HB2	2.25	0.51
2:D:203:GLU:OE2	2:D:263:LYS:NZ	2.23	0.51
2:D:57:GLU:O	2:D:60:GLN:HB3	2.11	0.51
1:B:66:CRO:HG11	1:B:220:LEU:CD2	2.41	0.50
1:B:109:ARG:NH2	4:B:301:HOH:O	2.43	0.49
1:A:75:PRO:CG	1:A:78:MET:HE3	2.42	0.49
2:D:59:VAL:HA	2:D:62:VAL:CG1	2.42	0.49
2:D:45:LEU:CD2	2:D:57:GLU:HB3	2.43	0.49
2:D:56:GLU:O	2:D:58:ASN:N	2.45	0.49
2:D:168:ARG:NH2	4:D:404:HOH:O	2.45	0.49
2:C:63:LYS:O	2:C:65:GLN:N	2.46	0.49
2:D:63:LYS:O	2:D:63:LYS:HD2	2.14	0.48
1:B:133:ASP:OD2	1:B:133:ASP:N	2.44	0.48
1:A:248:ILE:HG13	2:D:248:ILE:HD11	1.96	0.47
1:B:115:GLU:OE1	1:B:122:ARG:NH2	2.47	0.47
1:A:52:LYS:HE3	1:A:53:LEU:O	2.15	0.47
1:A:125:LEU:C	1:A:125:LEU:HD23	2.39	0.47
1:A:238:ARG:NH1	2:D:190:MET:HE3	2.30	0.47
2:C:135:ARG:O	2:C:139:LEU:HG	2.15	0.46
1:A:152:ILE:HG12	1:A:163:VAL:HG22	1.98	0.46
1:B:207:LEU:CD2	1:B:220:LEU:HD12	2.45	0.46
2:D:218:GLU:HB3	2:D:260:LYS:HD2	1.97	0.46
2:C:97:PHE:HD1	2:C:100:LEU:HD11	1.80	0.46
2:D:139:LEU:O	2:D:139:LEU:HD23	2.16	0.46
2:C:146:SER:OG	2:C:149:GLU:HG3	2.15	0.46
2:D:139:LEU:HD23	2:D:139:LEU:C	2.40	0.46
2:D:59:VAL:C	2:D:62:VAL:CG1	2.71	0.46
1:A:246:ASN:C	1:A:248:ILE:N	2.74	0.45
1:B:53:LEU:HD22	1:B:57:TRP:CE2	2.51	0.45
2:D:139:LEU:C	2:D:139:LEU:CD2	2.89	0.45
1:B:115:GLU:CD	1:B:122:ARG:HH21	2.24	0.45
2:D:59:VAL:CA	2:D:62:VAL:CG1	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD12	1:A:118:THR:HG21	1.98	0.44
1:A:41:LYS:HG3	1:A:42:LEU:N	2.33	0.43
1:B:88:MET:HB3	1:B:89:PRO:HA	2.00	0.43
2:C:84:ALA:O	2:C:86:MET:N	2.51	0.43
1:B:31:GLY:HA2	1:B:45:LYS:O	2.18	0.43
1:B:90:GLU:H	1:B:90:GLU:CD	2.26	0.43
1:A:68:VAL:C	1:A:70:CYS:H	2.26	0.43
2:C:99:ARG:HG3	2:C:179:ALA:CB	2.38	0.43
2:C:59:VAL:HG12	2:C:63:LYS:HD3	2.00	0.43
2:D:59:VAL:HG13	2:D:62:VAL:HG11	1.99	0.43
2:D:56:GLU:C	2:D:58:ASN:N	2.77	0.43
1:A:150:VAL:O	1:A:200:TYR:HA	2.18	0.43
1:A:244:MET:HG2	2:D:248:ILE:HG22	2.01	0.43
1:B:110:ALA:HA	1:B:122:ARG:O	2.19	0.42
2:C:63:LYS:C	2:C:65:GLN:N	2.77	0.42
2:D:60:GLN:OE1	2:D:61:LYS:N	2.52	0.42
1:A:4:GLY:HA3	1:A:85:LYS:O	2.19	0.42
2:C:99:ARG:HG2	2:C:100:LEU:N	2.34	0.42
2:D:246:ARG:HD3	4:D:401:HOH:O	2.18	0.42
1:A:167:THR:OG1	1:A:179:ALA:HB3	2.19	0.42
1:A:204:GLN:HG2	4:A:398:HOH:O	2.19	0.42
1:A:96:ARG:HA	1:A:182:TYR:O	2.20	0.42
1:A:68:VAL:C	1:A:70:CYS:N	2.78	0.42
1:B:230:MET:CE	1:B:236:ASN:HD21	2.30	0.41
2:C:80:MET:HE3	2:C:96:LEU:HD13	2.02	0.41
2:C:272:LEU:HD23	4:C:444:HOH:O	2.20	0.41
2:D:62:VAL:CG1	2:D:63:LYS:N	2.84	0.41
1:A:68:VAL:CG1	1:A:68:VAL:O	2.66	0.41
2:C:115:ARG:NH1	4:C:406:HOH:O	2.49	0.41
2:D:44:LEU:HD23	2:D:44:LEU:HA	1.76	0.41
1:B:42:LEU:HD12	1:B:42:LEU:HA	1.85	0.41
1:B:135:ASN:HA	1:B:140:LYS:HD3	2.02	0.41
1:A:246:ASN:O	1:A:248:ILE:N	2.53	0.41
2:C:202:PHE:CG	2:C:272:LEU:HD13	2.56	0.41
1:A:78:MET:HG2	1:A:229:THR:HG21	2.03	0.41
2:C:269:CYS:CB	2:D:268:LEU:HD11	2.38	0.41
1:B:123:ILE:HG22	1:B:124:GLU:N	2.35	0.41
2:C:104:LEU:O	2:C:181:GLN:CG	2.67	0.40
2:C:84:ALA:C	2:C:86:MET:N	2.76	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	240/256 (94%)	235 (98%)	5 (2%)	0	100	100
1	B	240/256 (94%)	233 (97%)	7 (3%)	0	100	100
2	C	245/276 (89%)	237 (97%)	5 (2%)	3 (1%)	10	9
2	D	244/276 (88%)	232 (95%)	10 (4%)	2 (1%)	16	17
All	All	969/1064 (91%)	937 (97%)	27 (3%)	5 (0%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	102	THR
2	C	64	GLU
2	D	34	GLU
2	D	57	GLU
2	C	85	SER

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	211/221 (96%)	203 (96%)	8 (4%)	29	39
1	B	211/221 (96%)	199 (94%)	12 (6%)	18	23
2	C	226/248 (91%)	217 (96%)	9 (4%)	28	37
2	D	225/248 (91%)	219 (97%)	6 (3%)	39	52
All	All	873/938 (93%)	838 (96%)	35 (4%)	28	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	52	LYS
1	A	80	ARG
1	A	157	GLN
1	A	162	LYS
1	A	180	ASP
1	A	229	THR
1	A	243	ASP
1	B	15	LEU
1	B	30	SER
1	B	41	LYS
1	B	42	LEU
1	B	80	ARG
1	B	131	LYS
1	B	140	LYS
1	B	162	LYS
1	B	168	ARG
1	B	180	ASP
1	B	205	SER
1	B	233	ILE
2	C	23	ARG
2	C	34	GLU
2	C	65	GLN
2	C	99	ARG
2	C	105	ASP
2	C	240	VAL
2	C	242	LEU
2	C	272	LEU
2	C	273	LYS
2	D	19	GLN
2	D	63	LYS
2	D	66	LEU
2	D	159	LYS
2	D	194	SER
2	D	269	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	ASN
1	B	170	ASN

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Mol	Chain	Res	Type
1	B	236	ASN
2	C	252	HIS
2	D	172	ASN
2	D	208	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	CRO	A	66	1	22,23,24	3.45	5 (22%)	30,32,34	2.81	10 (33%)
1	CRO	B	66	1	22,23,24	3.49	4 (18%)	30,32,34	2.96	11 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRO	A	66	1	-	3/12/31/32	0/2/2/2
1	CRO	B	66	1	-	5/12/31/32	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	CB2-CA2	14.46	1.49	1.35
1	A	66	CRO	CB2-CA2	13.74	1.48	1.35
1	A	66	CRO	C1-N2	4.96	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	C1-N2	4.40	1.38	1.32
1	B	66	CRO	O2-C2	3.94	1.31	1.23
1	A	66	CRO	CA2-C2	-3.68	1.44	1.48
1	B	66	CRO	C2-N3	-2.88	1.33	1.40
1	A	66	CRO	O2-C2	2.67	1.28	1.23
1	A	66	CRO	CE1-CZ	2.44	1.43	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	O2-C2-CA2	-9.37	125.04	131.02
1	A	66	CRO	O2-C2-CA2	-6.94	126.59	131.02
1	B	66	CRO	CA2-C2-N3	6.67	109.10	103.50
1	A	66	CRO	CG2-CB2-CA2	-6.01	122.72	129.87
1	A	66	CRO	CB2-CA2-C2	5.61	129.16	122.36
1	A	66	CRO	CA2-C2-N3	5.48	108.10	103.50
1	B	66	CRO	OG1-CB1-CA1	5.39	120.49	109.00
1	B	66	CRO	C2-CA2-N2	-4.60	105.65	108.95
1	A	66	CRO	O3-C3-CA3	-3.69	108.88	125.47
1	A	66	CRO	CA1-C1-N3	-3.59	120.44	124.69
1	A	66	CRO	CB2-CA2-N2	-3.45	124.08	128.76
1	B	66	CRO	CA2-N2-C1	3.44	108.49	105.80
1	A	66	CRO	CA1-C1-N2	3.43	128.53	123.88
1	B	66	CRO	CA1-C1-N2	3.35	128.43	123.88
1	A	66	CRO	C2-CA2-N2	-3.05	106.76	108.95
1	B	66	CRO	C1-CA1-N1	-2.96	104.49	109.78
1	B	66	CRO	CB2-CA2-C2	2.85	125.81	122.36
1	B	66	CRO	C2-N3-C1	-2.79	106.77	108.07
1	B	66	CRO	CA1-C1-N3	-2.62	121.59	124.69
1	A	66	CRO	CD2-CE2-CZ	-2.50	117.23	119.88
1	B	66	CRO	C3-CA3-N3	2.14	117.29	112.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	N1-CA1-CB1-CG1
1	B	66	CRO	N1-CA1-CB1-OG1
1	B	66	CRO	C1-CA1-CB1-CG1
1	B	66	CRO	C1-CA1-CB1-OG1
1	A	66	CRO	C3-CA3-N3-C1

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Mol	Chain	Res	Type	Atoms
1	A	66	CRO	N3-C1-CA1-CB1
1	B	66	CRO	N2-C1-CA1-CB1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	1	0
1	B	66	CRO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	244/256 (95%)	-0.38	2 (0%) 82 86	27, 36, 57, 97	0
1	B	243/256 (94%)	-0.19	0 100 100	21, 42, 66, 91	1 (0%)
2	C	251/276 (90%)	0.08	10 (3%) 42 48	29, 48, 96, 118	0
2	D	250/276 (90%)	0.11	13 (5%) 33 38	29, 49, 111, 141	0
All	All	988/1064 (92%)	-0.09	25 (2%) 58 64	21, 43, 84, 141	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	4.3
2	C	66	LEU	3.8
2	D	76	GLY	3.6
2	C	62	VAL	3.4
2	C	102	THR	3.2
2	D	59	VAL	3.1
2	D	62	VAL	2.9
2	D	60	GLN	2.9
2	D	68	THR	2.9
2	C	104	LEU	2.8
2	D	69	SER	2.8
2	D	63	LYS	2.7
2	C	12	LEU	2.6
2	D	12	LEU	2.6
2	D	66	LEU	2.5
2	C	76	GLY	2.5
2	C	105	ASP	2.5
1	A	68	VAL	2.4
2	D	58	ASN	2.2
2	D	46	ALA	2.2
2	C	103	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	139	LEU	2.2
2	C	54	LEU	2.1
2	D	83	LEU	2.1
2	D	100	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CRO	A	66	22/23	0.88	0.11	28,34,40,48	0
1	CRO	B	66	22/23	0.95	0.07	29,37,40,40	0

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
3	CA	D	302	1/1	0.98	0.07	51,51,51,51	0
3	CA	C	303	1/1	0.99	0.09	62,62,62,62	0
3	CA	D	301	1/1	0.99	0.02	33,33,33,33	0
3	CA	C	302	1/1	0.99	0.03	46,46,46,46	0
3	CA	D	303	1/1	0.99	0.08	50,50,50,50	0
3	CA	D	304	1/1	0.99	0.03	45,45,45,45	0
3	CA	C	301	1/1	1.00	0.01	35,35,35,35	0
3	CA	C	304	1/1	1.00	0.02	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.