Full wwPDB X-ray Structure Validation Report (i)

Mar 25, 2024 – 03:11 pm GMT

PDB ID	:	8BBJ
Title	:	Secretagogin (mouse) in complex with its target peptide from Syntaxin-4
Authors	:	Schnell, R.; Szodorai, E.
Deposited on	:	2022-10-13
Resolution	:	2.65 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:

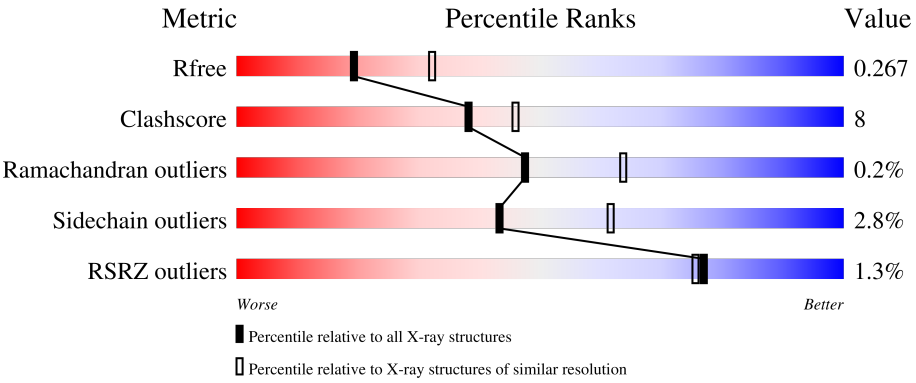
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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
1	A	259	2% 78% 17%
1	B	259	2% 80% 15%
2	C	190	% 70% 25% 5%
2	D	190	77% 15% 7%

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	CAC	C	305	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6925 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,Syntaxin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			2000	1265	345	383	7			
1	B	249	Total	C	N	O	S	4	0	0
			1998	1265	344	382	7			

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 Secretagogin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	181	Total	C	N	O	S	0	0	0
			1467	933	242	284	8			
2	D	177	Total	C	N	O	S	23	0	0
			1435	910	241	275	9			

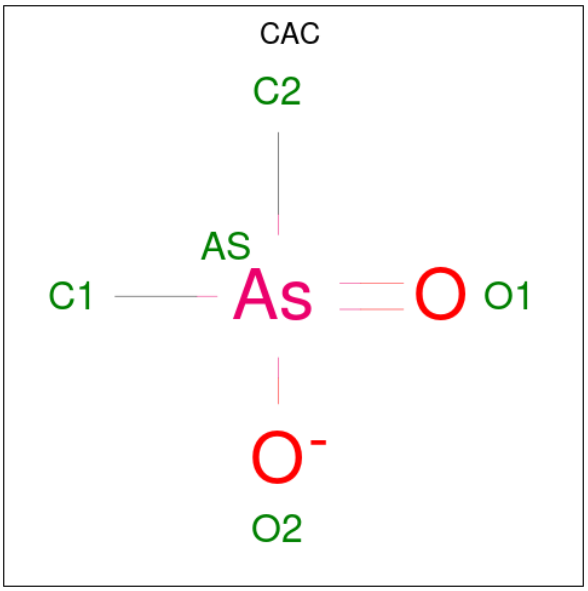
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	87	SER	-	expression tag	UNP Q91WD9
C	88	MET	-	expression tag	UNP Q91WD9
C	89	ALA	-	expression tag	UNP Q91WD9
D	87	SER	-	expression tag	UNP Q91WD9
D	88	MET	-	expression tag	UNP Q91WD9
D	89	ALA	-	expression tag	UNP Q91WD9

- Molecule 3 is CALCIUM ION (three-letter code: 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 CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is water.

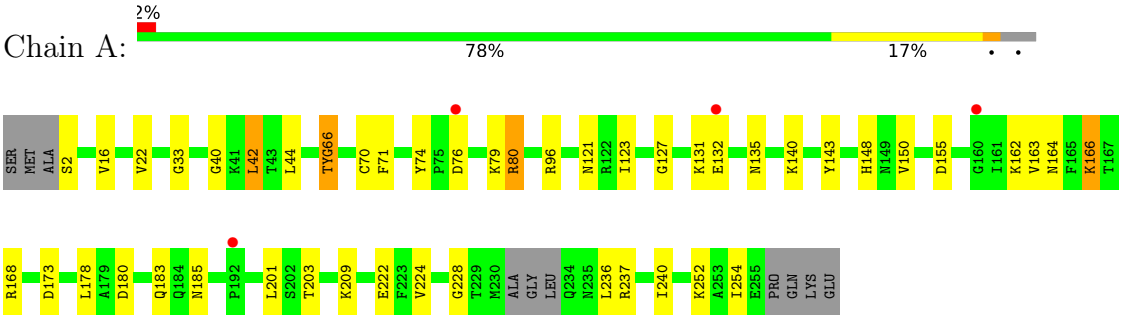
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	2	Total	O	0	0
			2	2		
5	C	2	Total	O	0	0
			2	2		
5	D	7	Total	O	0	0
			7	7		

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.

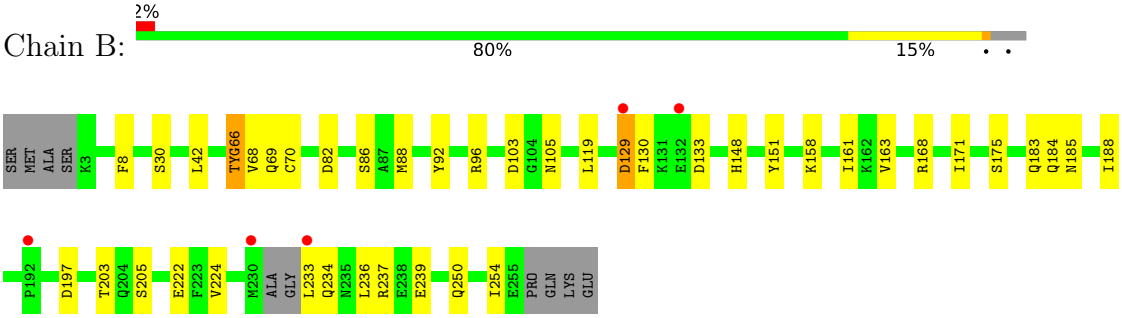
• Molecule 1: Green fluorescent protein,Syntaxin-4

Chain A:



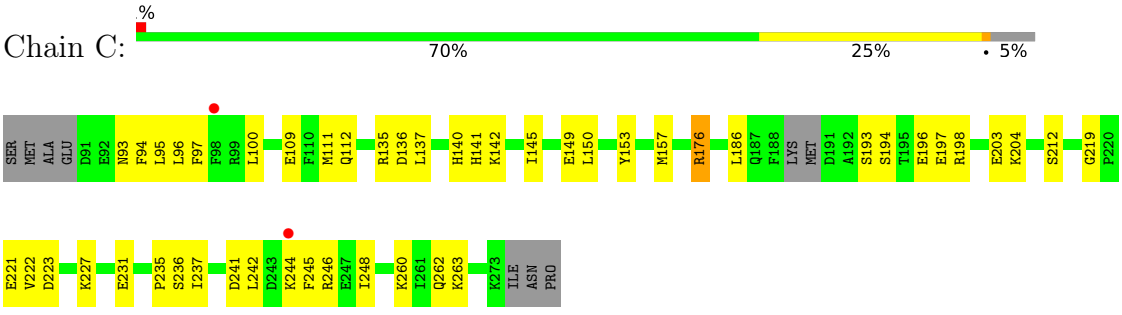
• Molecule 1: Green fluorescent protein,Syntaxin-4

Chain B:



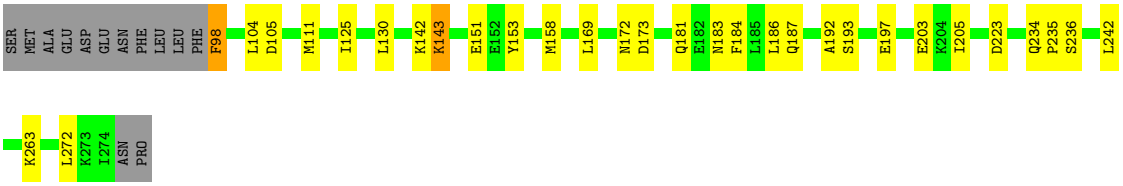
• Molecule 2: Secretagogin

Chain C:



• Molecule 2: Secretagogin

Chain D:


SER
MET
ALA
GLU
ASP
GLU
ASN
PHE
LEU
LEU
PHE
F98
L104
D105
M111
I125
L130
K142
K143
E151
E152
Y153
M158
L169
N172
D173
Q181
E182
N183
F184
L185
L186
Q187
A192
S193
E197
E203
K204
T205
D223
Q234
P235
S236
L242
K263
L272
K273
I274
ASN
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.41Å 103.13Å 121.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.65 48.29 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.29-2.65) 97.4 (48.29-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.213 , 0.269 0.212 , 0.267	Depositor DCC
R_{free} test set	1471 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6925	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8986e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, 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	0.29	0/2017	0.51	0/2718
1	B	0.30	0/2015	0.51	0/2717
2	C	0.29	0/1491	0.47	0/1999
2	D	0.30	0/1458	0.49	0/1953
All	All	0.30	0/6981	0.50	0/9387

There are no bond length outliers.

There are no bond angle outliers.

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	2000	0	1959	32	4
1	B	1998	0	1954	25	4
2	C	1467	0	1435	35	0
2	D	1435	0	1425	19	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	C	5	0	0	4	0
5	A	1	0	0	0	0
5	B	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2	0	0	0	0
5	D	7	0	0	0	0
All	All	6925	0	6773	103	4

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 (103) 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:B:233:LEU:HG	2:D:193:SER:HB2	1.51	0.92
2:C:176:ARG:HH11	4:C:305:CAC:AS	2.22	0.82
2:C:176:ARG:NH2	2:D:173:ASP:OD1	2.12	0.82
2:D:192:ALA:HB1	2:D:197:GLU:HB3	1.61	0.81
1:A:168:ARG:NH2	1:B:197:ASP:OD2	2.15	0.79
2:C:176:ARG:NH1	4:C:305:CAC:AS	2.78	0.77
2:C:237:ILE:HD12	2:C:242:LEU:HD21	1.68	0.76
2:C:176:ARG:NH1	4:C:305:CAC:O2	2.20	0.74
1:A:80:ARG:HD2	1:A:80:ARG:H	1.54	0.71
1:A:135:ASN:HA	1:A:140:LYS:HG3	1.78	0.65
1:B:42:LEU:HB2	1:B:222:GLU:HB2	1.80	0.62
1:B:163:VAL:HB	1:B:183:GLN:HB3	1.82	0.62
2:C:176:ARG:HD2	4:C:305:CAC:O2	2.00	0.62
1:B:203:THR:HG22	1:B:224:VAL:HG13	1.82	0.61
1:B:236:LEU:HD11	2:D:272:LEU:HD11	1.81	0.61
2:C:242:LEU:HD23	2:C:245:PHE:HD1	1.66	0.61
2:D:183:ASN:HB3	2:D:186:LEU:HG	1.84	0.59
1:A:237:ARG:HH21	2:C:186:LEU:HA	1.68	0.58
1:A:76:ASP:OD2	1:A:79:LYS:NZ	2.36	0.58
2:C:194:SER:HB3	2:C:196:GLU:OE2	2.06	0.56
1:B:171:ILE:HB	1:B:175:SER:HB3	1.87	0.56
2:C:194:SER:O	2:C:198:ARG:HG3	2.05	0.55
2:D:234:GLN:HB2	2:D:235:PRO:HD2	1.88	0.55
1:A:236:LEU:HD23	1:A:240:ILE:HG13	1.87	0.54
1:B:66:CRO:HB2	1:B:69:GLN:NE2	2.22	0.54
1:A:76:ASP:O	1:A:80:ARG:NH1	2.40	0.54
2:C:145:ILE:HG23	2:C:149:GLU:HG3	1.89	0.54
1:B:82:ASP:O	1:B:86:SER:OG	2.20	0.54
1:A:163:VAL:HB	1:A:183:GLN:CG	2.38	0.54
1:A:163:VAL:HB	1:A:183:GLN:HG2	1.91	0.53
2:C:203:GLU:OE1	2:C:263:LYS:NZ	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:CRO:HE2	1:B:148:HIS:HE1	1.75	0.51
2:D:142:LYS:C	2:D:143:LYS:HD2	2.30	0.51
1:A:66:CRO:HE2	1:A:148:HIS:CE1	2.46	0.51
1:A:76:ASP:HA	1:A:79:LYS:HG2	1.92	0.51
2:C:222:VAL:HG11	2:C:246:ARG:HG3	1.93	0.51
2:C:93:ASN:O	2:C:94:PHE:HB3	2.10	0.51
1:B:250:GLN:O	1:B:254:ILE:HG12	2.11	0.50
2:C:227:LYS:O	2:C:231:GLU:HG3	2.10	0.50
2:C:241:ASP:HA	2:C:244:LYS:HE2	1.93	0.50
2:D:172:ASN:HD21	2:D:236:SER:HB2	1.77	0.50
1:A:166:LYS:HG3	1:A:180:ASP:OD1	2.12	0.49
1:B:103:ASP:OD1	1:B:130:PHE:HA	2.12	0.49
1:A:66:CRO:HE2	1:A:148:HIS:HE1	1.77	0.49
2:C:109:GLU:OE1	2:C:112:GLN:NE2	2.45	0.49
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.95	0.49
1:B:119:LEU:C	1:B:119:LEU:HD13	2.33	0.49
2:C:111:MET:HE2	2:C:223:ASP:HB3	1.95	0.48
2:C:96:LEU:HD22	2:C:96:LEU:H	1.78	0.48
2:D:111:MET:HE2	2:D:223:ASP:HB3	1.95	0.48
2:C:260:LYS:HG3	2:C:262:GLN:HE22	1.78	0.48
2:C:97:PHE:CD1	2:C:137:LEU:CD2	2.96	0.48
1:A:121:ASN:ND2	1:A:123:ILE:HD11	2.29	0.48
2:C:219:GLY:HA2	2:C:246:ARG:HH12	1.79	0.48
1:B:92:TYR:HA	1:B:188:ILE:HG12	1.96	0.47
1:A:66:CRO:HD1	1:A:66:CRO:N2	2.29	0.47
2:D:104:LEU:O	2:D:181:GLN:HG2	2.15	0.47
2:D:203:GLU:OE1	2:D:263:LYS:NZ	2.32	0.47
1:B:66:CRO:HE2	1:B:148:HIS:CE1	2.49	0.47
1:B:205:SER:OG	1:B:222:GLU:OE2	2.19	0.46
1:A:33:GLY:HA3	1:A:44:LEU:HD23	1.96	0.46
1:B:96:ARG:NH2	1:B:183:GLN:OE1	2.43	0.46
2:D:143:LYS:HD2	2:D:143:LYS:N	2.30	0.46
1:A:143:TYR:CZ	1:A:209:LYS:HE2	2.50	0.46
2:C:145:ILE:CG2	2:C:149:GLU:HG3	2.45	0.46
1:A:183:GLN:NE2	1:A:185:ASN:OD1	2.41	0.46
1:A:155:ASP:HB2	1:A:162:LYS:HG3	1.97	0.45
2:C:212:SER:OG	2:C:221:GLU:OE2	2.35	0.45
1:B:158:LYS:HD2	1:B:184:GLN:OE1	2.17	0.44
2:D:130:LEU:HD22	2:D:158:MET:HE2	1.98	0.44
1:A:164:ASN:HD21	1:A:166:LYS:NZ	2.15	0.44
2:C:136:ASP:O	2:C:140:HIS:ND1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:HB	1:A:224:VAL:HG13	2.00	0.44
2:D:98:PHE:HB3	2:D:153:TYR:OH	2.18	0.43
1:B:236:LEU:HD23	2:D:205:ILE:HD12	2.00	0.43
1:B:8:PHE:HZ	1:B:88:MET:HG3	1.83	0.43
1:A:16:VAL:HG22	1:A:121:ASN:HB3	2.00	0.43
2:C:135:ARG:HB2	2:C:150:LEU:HD21	2.01	0.43
1:A:40:GLY:HA2	1:A:71:PHE:O	2.18	0.42
1:A:164:ASN:HD21	1:A:166:LYS:HZ1	1.67	0.42
1:A:131:LYS:HA	1:A:131:LYS:HD2	1.44	0.42
1:A:150:VAL:HB	1:A:201:LEU:HB2	2.02	0.42
2:C:100:LEU:HD22	2:C:141:HIS:CD2	2.55	0.42
2:D:105:ASP:HA	2:D:181:GLN:HG2	2.00	0.42
2:C:219:GLY:CA	2:C:246:ARG:HH12	2.32	0.42
2:D:125:ILE:HB	2:D:169:LEU:HB2	2.02	0.42
2:D:172:ASN:ND2	2:D:236:SER:HB2	2.34	0.42
1:B:161:ILE:HG12	1:B:185:ASN:HB2	2.01	0.41
2:C:94:PHE:CG	2:C:95:LEU:N	2.87	0.41
2:C:153:TYR:O	2:C:157:MET:HG2	2.20	0.41
2:D:184:PHE:O	2:D:187:GLN:HG2	2.20	0.41
1:A:254:ILE:HD11	2:C:248:ILE:HD11	2.02	0.41
1:A:22:VAL:HA	1:A:127:GLY:O	2.21	0.41
1:A:228:GLY:O	1:B:151:TYR:OH	2.36	0.41
1:B:68:VAL:HG13	1:B:68:VAL:O	2.19	0.41
1:B:105:ASN:ND2	5:B:301:HOH:O	2.26	0.41
2:C:194:SER:HB2	2:C:197:GLU:HG3	2.02	0.41
1:A:74:TYR:O	1:A:79:LYS:HE3	2.20	0.40
1:A:42:LEU:HB2	1:A:222:GLU:HB3	2.03	0.40
1:B:234:GLN:NE2	1:B:239:GLU:OE1	2.52	0.40
2:C:97:PHE:CE1	2:C:137:LEU:CD2	3.05	0.40
2:C:97:PHE:HD1	2:C:137:LEU:CD2	2.33	0.40
2:C:142:LYS:HD2	2:C:142:LYS:HA	1.84	0.40

All (4) 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:131:LYS:NZ	1:B:129:ASP:OD1[4_545]	1.81	0.39
1:A:131:LYS:NZ	1:B:129:ASP:OD2[4_545]	1.90	0.30
1:A:131:LYS:NZ	1:B:129:ASP:CG[4_545]	2.00	0.20
1:A:132:GLU:OE1	1:B:129:ASP:OD2[4_545]	2.07	0.13

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	242/259 (93%)	234 (97%)	8 (3%)	0	100 100
1	B	242/259 (93%)	236 (98%)	5 (2%)	1 (0%)	34 48
2	C	177/190 (93%)	170 (96%)	6 (3%)	1 (1%)	25 37
2	D	175/190 (92%)	168 (96%)	7 (4%)	0	100 100
All	All	836/898 (93%)	808 (97%)	26 (3%)	2 (0%)	47 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ASP
2	C	235	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	217/224 (97%)	209 (96%)	8 (4%)	34 50
1	B	216/224 (96%)	211 (98%)	5 (2%)	50 68
2	C	162/171 (95%)	158 (98%)	4 (2%)	47 66
2	D	159/171 (93%)	155 (98%)	4 (2%)	47 66
All	All	754/790 (95%)	733 (97%)	21 (3%)	43 61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	42	LEU
1	A	70	CYS
1	A	80	ARG
1	A	166	LYS
1	A	173	ASP
1	A	178	LEU
1	A	252	LYS
1	B	30	SER
1	B	70	CYS
1	B	133	ASP
1	B	168	ARG
1	B	237	ARG
2	C	176	ARG
2	C	193	SER
2	C	204	LYS
2	C	236	SER
2	D	98	PHE
2	D	143	LYS
2	D	151	GLU
2	D	242	LEU

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	164	ASN
1	B	198	ASN
1	B	212	ASN
2	C	112	GLN
2	D	172	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)

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	23,23,24	2.68	8 (34%)	30,32,34	2.88	8 (26%)
1	CRO	B	66	1	23,23,24	2.66	8 (34%)	30,32,34	2.70	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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	C1-N2	7.11	1.42	1.32
1	B	66	CRO	C1-N2	7.03	1.42	1.32
1	B	66	CRO	CA2-C2	5.95	1.54	1.48
1	A	66	CRO	CA2-C2	5.74	1.54	1.48
1	B	66	CRO	C1-N3	5.02	1.45	1.37
1	A	66	CRO	C1-N3	4.98	1.45	1.37
1	A	66	CRO	C2-N3	3.67	1.48	1.39
1	B	66	CRO	C2-N3	3.64	1.48	1.39
1	A	66	CRO	CB2-CA2	-3.64	1.32	1.35
1	A	66	CRO	CG2-CB2	3.48	1.53	1.46
1	B	66	CRO	CG2-CB2	3.47	1.53	1.46
1	B	66	CRO	CB2-CA2	-2.99	1.32	1.35
1	B	66	CRO	CA2-N2	2.45	1.43	1.38
1	A	66	CRO	O2-C2	-2.25	1.18	1.23
1	B	66	CRO	O2-C2	-2.15	1.18	1.23
1	A	66	CRO	CA2-N2	2.12	1.43	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	CRO	O2-C2-CA2	-9.13	125.83	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	CRO	CA2-C2-N3	7.97	107.14	103.37
1	B	66	CRO	CA2-C2-N3	7.74	107.03	103.37
1	B	66	CRO	O2-C2-CA2	-7.57	126.71	130.96
1	A	66	CRO	C2-N3-C1	-5.43	105.22	107.97
1	B	66	CRO	C2-N3-C1	-4.93	105.47	107.97
1	A	66	CRO	CA2-N2-C1	4.06	108.77	105.77
1	B	66	CRO	CA2-N2-C1	3.95	108.68	105.77
1	A	66	CRO	CG2-CB2-CA2	-3.89	125.18	129.94
1	B	66	CRO	CA1-C1-N3	-3.40	120.67	124.75
1	B	66	CRO	C2-CA2-N2	-3.28	106.64	108.93
1	A	66	CRO	C2-CA2-N2	-3.20	106.69	108.93
1	A	66	CRO	CA1-C1-N3	-2.39	121.88	124.75
1	B	66	CRO	CG2-CB2-CA2	-2.34	127.08	129.94
1	B	66	CRO	CA1-C1-N2	2.32	127.13	123.89
1	B	66	CRO	OG1-CB1-CA1	2.21	113.77	109.04
1	B	66	CRO	O3-C3-CA3	-2.20	119.75	126.39
1	A	66	CRO	CA3-N3-C2	2.13	128.69	123.80
1	B	66	CRO	CG1-CB1-CA1	-2.10	107.21	112.16

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	C3-CA3-N3-C1
1	A	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	N1-CA1-CB1-CG1
1	B	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	N2-CA2-CB2-CG2
1	B	66	CRO	C1-CA1-CB1-CG1
1	A	66	CRO	N2-CA2-CB2-CG2
1	B	66	CRO	N1-CA1-CB1-OG1

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	3	0
1	B	66	CRO	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	CAC	C	305	-	0,4,4	-	-	0,6,6	-	-

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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	305	CAC	4	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^{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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	248/259 (95%)	-0.01	4 (1%) 72 69	47, 67, 100, 123	0
1	B	248/259 (95%)	-0.09	5 (2%) 65 60	49, 72, 99, 122	1 (0%)
2	C	181/190 (95%)	-0.07	2 (1%) 80 79	54, 72, 108, 131	0
2	D	177/190 (93%)	-0.26	0 100 100	47, 64, 92, 106	6 (3%)
All	All	854/898 (95%)	-0.10	11 (1%) 77 75	47, 69, 101, 131	7 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	PRO	3.0
1	A	132	GLU	2.9
2	C	98	PHE	2.9
1	B	132	GLU	2.7
1	B	230	MET	2.3
1	A	76	ASP	2.2
1	A	160	GLY	2.1
1	A	192	PRO	2.1
1	B	233	LEU	2.1
2	C	244	LYS	2.0
1	B	129	ASP	2.0

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

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^{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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CRO	B	66	22/23	0.93	0.23	56,62,69,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CRO	A	66	22/23	0.94	0.19	56,66,71,78	0

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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	C	302	1/1	0.86	0.15	71,71,71,71	0
3	CA	C	304	1/1	0.91	0.07	75,75,75,75	0
3	CA	C	303	1/1	0.92	0.12	96,96,96,96	0
3	CA	D	303	1/1	0.93	0.08	84,84,84,84	0
4	CAC	C	305	5/5	0.96	0.14	77,85,86,95	0
3	CA	D	302	1/1	0.98	0.12	72,72,72,72	0
3	CA	C	301	1/1	0.98	0.16	64,64,64,64	0
3	CA	D	304	1/1	0.98	0.09	51,51,51,51	0
3	CA	D	301	1/1	0.98	0.15	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.