



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2019 – 01:30 PM EDT

PDB ID : 6GX9
Title : Crystal structure of the TNPO3 - CPSF6 RSLD complex
Authors : Cherepanov, P.; Cook, N.
Deposited on : 2018-06-26
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

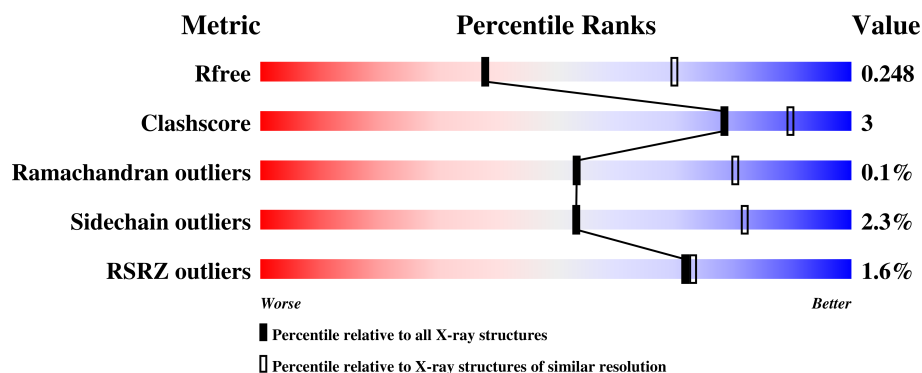
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	923	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 88%; width: 12%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 99%; width: 1%; height: 10px; background-color: orange;"></div> </div> <div> 88% 11% .. </div> </div>
1	B	923	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 89%; width: 11%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 99%; width: 1%; height: 10px; background-color: orange;"></div> </div> <div> 89% 10% .. </div> </div>
2	C	70	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 11%; width: 8%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 87%; width: 13%; height: 10px; background-color: grey;"></div> </div> <div> 11% 87% </div> </div>
2	D	70	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 13%; width: 74%; height: 10px; background-color: grey;"></div> </div> <div> 13% 87% </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
4	BCN	B	1003	-	-	-	X
5	BEN	B	1004	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14667 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 Transportin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	912	Total	C	N	O	S	0	0	0
			7222	4597	1231	1340	54			
1	B	911	Total	C	N	O	S	0	0	0
			7205	4588	1227	1336	54			

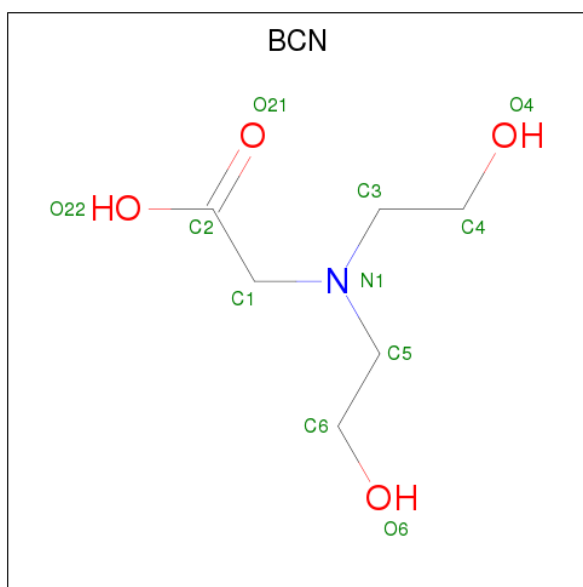
- Molecule 2 is a protein called Cleavage and polyadenylation specificity factor subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			83	46	18	18	1			
2	D	9	Total	C	N	O	P	0	0	0
			83	46	18	18	1			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

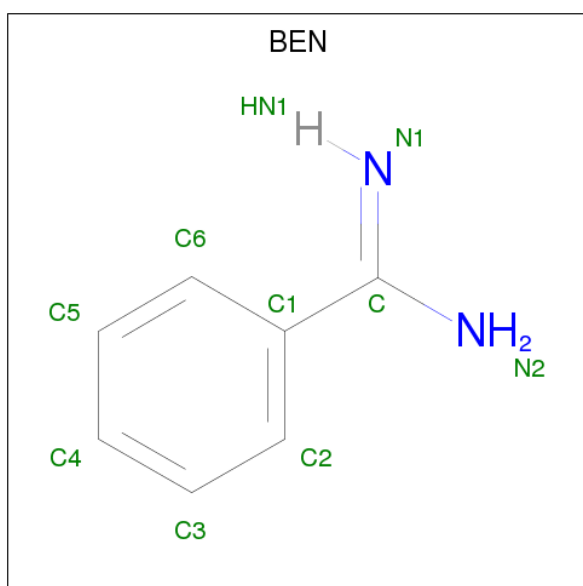
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is BICINE (three-letter code: BCN) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	6	1	4		
4	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 5 is BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			9	7	2		
5	B	1	Total	C	N	0	0
			9	7	2		

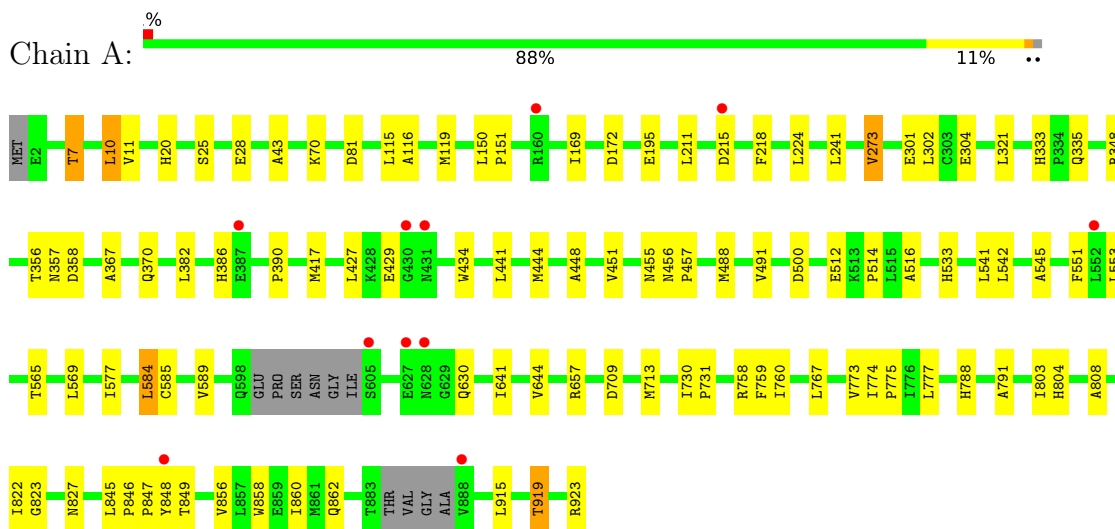
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total 20	O 20	0	0
6	B	10	Total 10	O 10	0	0

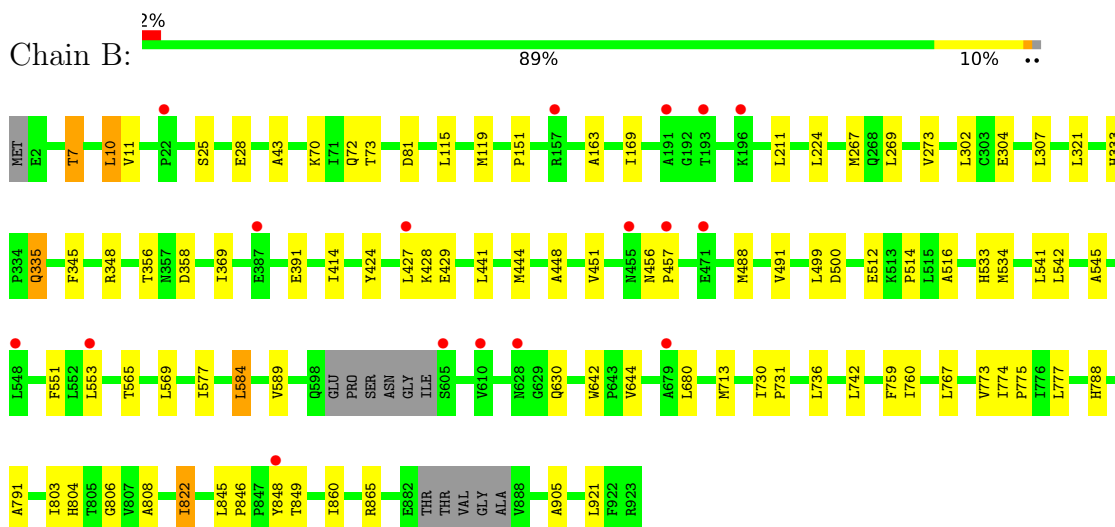
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Transportin-3

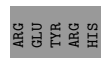


• Molecule 1: Transportin-3

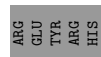
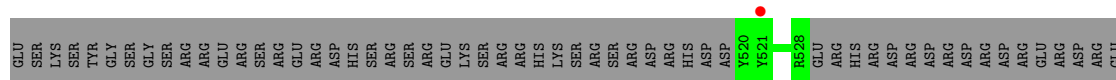


• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6





- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	200.34Å 200.34Å 234.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.65 – 2.70 50.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.65-2.70) 93.7 (50.65-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.214 , 0.248 0.214 , 0.248	Depositor DCC
R_{free} test set	3194 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14667	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCN, BEN, MG, SEP

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	0.24	0/7365	0.38	0/10002
1	B	0.23	0/7348	0.37	0/9980
2	C	0.18	0/72	0.34	0/92
2	D	0.19	0/72	0.35	0/92
All	All	0.23	0/14857	0.37	0/20166

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 [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	7222	0	7242	49	0
1	B	7205	0	7220	41	0
2	C	83	0	67	1	0
2	D	83	0	67	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	11	0	12	4	0
4	B	11	0	12	2	0
5	A	9	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	9	0	7	0	0
6	A	20	0	0	0	0
6	B	10	0	0	0	0
All	All	14667	0	14633	91	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 3.

All (91) 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:169:ILE:HD13	4:B:1003:BCN:H11	1.71	0.72
1:B:43:ALA:HB3	1:B:70:LYS:HD2	1.77	0.67
1:A:169:ILE:HD13	4:A:1003:BCN:H11	1.79	0.64
1:A:43:ALA:HB3	1:A:70:LYS:HD2	1.79	0.63
1:B:589:VAL:HG13	1:B:644:VAL:HG11	1.80	0.63
1:B:541:LEU:HB3	1:B:565:THR:HG22	1.81	0.62
1:A:512:GLU:HG2	1:A:514:PRO:HD2	1.82	0.61
1:A:823:GLY:O	1:A:827:ASN:ND2	2.35	0.60
1:B:512:GLU:HG2	1:B:514:PRO:HD2	1.84	0.58
1:A:589:VAL:HG13	1:A:644:VAL:HG11	1.84	0.58
1:A:541:LEU:HB3	1:A:565:THR:HG22	1.85	0.56
1:B:304:GLU:OE1	1:B:348:ARG:NH1	2.38	0.52
1:B:441:LEU:HD23	1:B:444:MET:HE3	1.90	0.52
1:A:569:LEU:HD11	1:A:577:ILE:HA	1.91	0.52
1:B:7:THR:HG22	1:B:10:LEU:HB2	1.92	0.52
1:B:151:PRO:HB3	1:B:211:LEU:HD22	1.91	0.51
1:B:730:ILE:HB	1:B:731:PRO:HD3	1.92	0.51
1:A:456:ASN:N	1:A:457:PRO:HD2	2.25	0.51
1:B:273:VAL:HG11	1:B:302:LEU:HD13	1.92	0.51
1:A:356:THR:O	1:A:358:ASP:N	2.45	0.50
1:A:304:GLU:OE1	1:A:348:ARG:NH1	2.39	0.49
1:A:382:LEU:HD11	1:A:390:PRO:HG3	1.95	0.49
1:A:386:HIS:HB3	1:A:434:TRP:HH2	1.78	0.49
1:A:803:ILE:HD13	1:A:860:ILE:HG12	1.93	0.49
1:A:367:ALA:HA	1:A:370:GLN:HE21	1.76	0.49
1:A:20:HIS:CD2	1:B:267:MET:HG3	2.48	0.49
1:B:788:HIS:HB3	1:B:791:ALA:HB3	1.94	0.49
1:A:151:PRO:HB3	1:A:211:LEU:HD22	1.94	0.49
1:A:516:ALA:HB1	1:A:553:LEU:HD23	1.95	0.48
1:B:774:ILE:HB	1:B:775:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HG	1:A:119:MET:HE2	1.96	0.48
1:A:760:ILE:HD13	1:A:767:LEU:HD23	1.95	0.48
1:B:865:ARG:NH2	1:B:905:ALA:O	2.47	0.48
1:A:441:LEU:HD23	1:A:444:MET:HE3	1.95	0.48
1:A:774:ILE:HB	1:A:775:PRO:HD3	1.96	0.48
1:A:215:ASP:HB3	1:A:218:PHE:HB3	1.96	0.48
1:B:25:SER:HA	1:B:28:GLU:HG2	1.96	0.48
1:A:730:ILE:HB	1:A:731:PRO:HD3	1.96	0.47
1:A:7:THR:HG22	1:A:10:LEU:HB2	1.95	0.47
1:B:448:ALA:O	1:B:451:VAL:HG12	2.14	0.47
1:A:448:ALA:O	1:A:451:VAL:HG12	2.14	0.47
1:A:847:PRO:HG3	1:A:923:ARG:NH2	2.30	0.47
1:B:456:ASN:N	1:B:457:PRO:HD2	2.30	0.47
1:A:545:ALA:HB1	1:A:584:LEU:HD21	1.96	0.46
1:A:488:MET:O	1:A:491:VAL:HG12	2.14	0.46
1:B:488:MET:O	1:B:491:VAL:HG12	2.15	0.46
1:A:116:ALA:HB1	4:A:1003:BCN:H42	1.97	0.46
1:A:417:MET:SD	1:A:455:ASN:ND2	2.88	0.46
1:B:545:ALA:HB1	1:B:584:LEU:HD21	1.98	0.46
1:B:803:ILE:HD13	1:B:860:ILE:HG12	1.98	0.46
1:B:804:HIS:CD2	1:B:808:ALA:HB2	2.51	0.46
4:A:1003:BCN:O22	4:A:1003:BCN:O4	2.23	0.45
1:B:499:LEU:HD21	1:B:534:MET:HG2	1.99	0.45
1:B:845:LEU:HD13	1:B:849:THR:HG21	1.99	0.45
1:A:845:LEU:HD13	1:A:849:THR:HG21	2.00	0.44
1:B:163:ALA:HB3	1:B:921:LEU:HA	2.00	0.44
1:A:788:HIS:HB3	1:A:791:ALA:HB3	1.99	0.44
1:A:804:HIS:CD2	1:A:808:ALA:HB2	2.53	0.44
1:B:269:LEU:O	1:B:273:VAL:HG12	2.18	0.44
1:A:25:SER:HA	1:A:28:GLU:HG2	2.00	0.44
1:B:333:HIS:CE1	1:B:335:GLN:HB2	2.53	0.43
1:B:569:LEU:HD11	1:B:577:ILE:HA	2.00	0.43
1:A:333:HIS:CE1	1:A:335:GLN:HB2	2.54	0.43
1:A:386:HIS:HB3	1:A:434:TRP:CH2	2.54	0.43
4:B:1003:BCN:O21	4:B:1003:BCN:O4	2.32	0.43
1:B:356:THR:O	1:B:358:ASP:N	2.51	0.43
1:B:424:TYR:CE2	1:B:428:LYS:HE3	2.54	0.43
1:A:172:ASP:HB3	4:A:1003:BCN:H12	2.00	0.42
1:B:736:LEU:HD22	1:B:742:LEU:HD23	2.00	0.42
1:B:516:ALA:HB1	1:B:553:LEU:HD23	2.00	0.42
1:B:760:ILE:HD13	1:B:767:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:VAL:HG22	1:B:777:LEU:HD23	2.02	0.42
1:A:301:GLU:OE1	5:A:1004:BEN:N1	2.52	0.42
1:A:195:GLU:HG3	1:A:241:LEU:HD22	2.02	0.42
1:A:858:TRP:O	1:A:862:GLN:HG2	2.19	0.42
1:A:915:LEU:O	1:A:919:THR:HB	2.20	0.42
1:B:72:GLN:HG3	1:B:73:THR:HG23	2.02	0.42
1:B:846:PRO:HB2	1:B:848:TYR:CD2	2.55	0.41
1:A:709:ASP:HB2	1:A:758:ARG:HD2	2.02	0.41
1:A:150:LEU:HB3	1:A:151:PRO:HD3	2.03	0.41
1:B:115:LEU:HG	1:B:119:MET:HE2	2.02	0.41
1:B:307:LEU:HD23	1:B:345:PHE:CE1	2.56	0.41
1:B:642:TRP:HB2	1:B:680:LEU:HD21	2.03	0.41
1:A:273:VAL:HG11	1:A:302:LEU:HD13	2.01	0.41
1:A:773:VAL:HG22	1:A:777:LEU:HD23	2.02	0.41
1:B:369:ILE:HG22	1:B:414:ILE:HD11	2.02	0.41
1:A:657:ARG:HG3	2:C:521:TYR:CG	2.56	0.41
1:A:585:CYS:HB3	1:A:641:ILE:HD11	2.03	0.41
1:A:846:PRO:HB2	1:A:848:TYR:CD2	2.55	0.41
1:A:856:VAL:O	1:A:860:ILE:HG13	2.21	0.40
1:B:806:GLY:HA3	1:B:822:ILE:HG21	2.04	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	906/923 (98%)	883 (98%)	22 (2%)	1 (0%)	53	80
1	B	905/923 (98%)	882 (98%)	23 (2%)	0	100	100
2	C	6/70 (9%)	6 (100%)	0	0	100	100
2	D	6/70 (9%)	6 (100%)	0	0	100	100
All	All	1823/1986 (92%)	1777 (98%)	45 (2%)	1 (0%)	53	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	ASN

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	810/821 (99%)	791 (98%)	19 (2%)	53	82
1	B	807/821 (98%)	788 (98%)	19 (2%)	52	81
2	C	6/67 (9%)	6 (100%)	0	100	100
2	D	6/67 (9%)	6 (100%)	0	100	100
All	All	1629/1776 (92%)	1591 (98%)	38 (2%)	53	82

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	10	LEU
1	A	11	VAL
1	A	81	ASP
1	A	224	LEU
1	A	273	VAL
1	A	321	LEU
1	A	427	LEU
1	A	429	GLU
1	A	500	ASP
1	A	533	HIS
1	A	542	LEU
1	A	551	PHE
1	A	584	LEU
1	A	630	GLN
1	A	713	MET
1	A	759	PHE
1	A	822	ILE
1	A	919	THR

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Mol	Chain	Res	Type
1	B	7	THR
1	B	10	LEU
1	B	11	VAL
1	B	81	ASP
1	B	224	LEU
1	B	321	LEU
1	B	335	GLN
1	B	391	GLU
1	B	427	LEU
1	B	429	GLU
1	B	500	ASP
1	B	533	HIS
1	B	542	LEU
1	B	551	PHE
1	B	584	LEU
1	B	630	GLN
1	B	713	MET
1	B	759	PHE
1	B	822	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	824	GLN

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
2	SEP	C	525	2	9,9,10	1.60	2 (22%)	9,12,14	1.76	2 (22%)
2	SEP	D	525	2	9,9,10	1.59	2 (22%)	9,12,14	1.62	2 (22%)

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	SEP	C	525	2	-	0/5/8/10	0/0/0/0
2	SEP	D	525	2	-	0/5/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	525	SEP	CA-C	2.09	1.53	1.50
2	C	525	SEP	CA-C	2.27	1.53	1.50
2	C	525	SEP	P-O1P	3.27	1.61	1.50
2	D	525	SEP	P-O1P	3.29	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	525	SEP	P-OG-CB	-2.95	110.18	118.30
2	D	525	SEP	P-OG-CB	-2.84	110.48	118.30
2	D	525	SEP	OG-CB-CA	3.06	111.12	108.14
2	C	525	SEP	OG-CB-CA	3.58	111.63	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	BCN	A	1003	-	7,10,10	0.29	0	8,11,11	0.85	0
5	BEN	A	1004	1	9,9,9	1.34	1 (11%)	9,11,11	1.39	1 (11%)
4	BCN	B	1003	-	7,10,10	0.28	0	8,11,11	0.88	0
5	BEN	B	1004	1	9,9,9	1.39	1 (11%)	9,11,11	0.74	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
4	BCN	A	1003	-	-	0/8/10/10	0/0/0/0
5	BEN	A	1004	1	-	0/4/4/4	0/1/1/1
4	BCN	B	1003	-	-	0/8/10/10	0/0/0/0
5	BEN	B	1004	1	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	BEN	C1-C	-3.80	1.40	1.47
5	A	1004	BEN	C1-C	-3.69	1.40	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1004	BEN	C1-C-N2	3.47	123.30	118.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	BCN	4	0
5	A	1004	BEN	1	0
4	B	1003	BCN	2	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 [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	912/923 (98%)	0.08	11 (1%) 79 80	28, 67, 104, 142	0
1	B	911/923 (98%)	0.15	17 (1%) 66 68	39, 73, 106, 134	0
2	C	8/70 (11%)	0.31	1 (12%) 4 3	64, 82, 100, 109	0
2	D	8/70 (11%)	0.14	1 (12%) 4 3	68, 85, 99, 103	0
All	All	1839/1986 (92%)	0.12	30 (1%) 72 73	28, 70, 104, 142	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	ALA	3.7
1	A	431	ASN	3.1
1	B	427	LEU	2.8
1	A	888	VAL	2.8
1	A	430	GLY	2.8
1	B	387	GLU	2.7
1	A	552	LEU	2.6
1	B	193	THR	2.6
1	A	848	TYR	2.6
1	B	457	PRO	2.6
1	A	627	GLU	2.5
1	A	160	ARG	2.5
1	B	157	ARG	2.5
1	A	387	GLU	2.4
1	A	605	SER	2.4
1	B	605	SER	2.3
1	B	471	GLU	2.3
1	B	196	LYS	2.2
1	B	548	LEU	2.2
1	A	215	ASP	2.2
1	A	628	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	679	ALA	2.2
1	B	628	ASN	2.1
1	B	455	ASN	2.1
2	D	521	TYR	2.1
2	C	521	TYR	2.1
1	B	610	VAL	2.0
1	B	22	PRO	2.0
1	B	848	TYR	2.0
1	B	553	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
2	SEP	D	525	10/11	0.97	0.13	53,65,73,73	0
2	SEP	C	525	10/11	0.98	0.14	53,64,68,77	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
5	BEN	A	1004	9/9	0.64	0.35	68,78,82,87	0
4	BCN	B	1003	11/11	0.70	0.43	83,94,112,116	0
5	BEN	B	1004	9/9	0.72	0.45	68,83,92,94	0
4	BCN	A	1003	11/11	0.80	0.37	69,83,91,93	0
3	MG	A	1001	1/1	0.93	0.21	93,93,93,93	0
3	MG	B	1001	1/1	0.94	0.19	88,88,88,88	0
3	MG	B	1002	1/1	0.98	0.26	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	1002	1/1	0.98	0.33	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.