



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:44 AM GMT

PDB ID : 3C0V
Title : Crystal structure of cytokinin-specific binding protein in complex with cytokinin and Ta6Br12
Authors : Pasternak, O.; Bujacz, A.; Biesiadka, J.; Bujacz, G.; Sikorski, M.; Jaskolski, M.
Deposited on : 2008-01-21
Resolution : 1.80 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

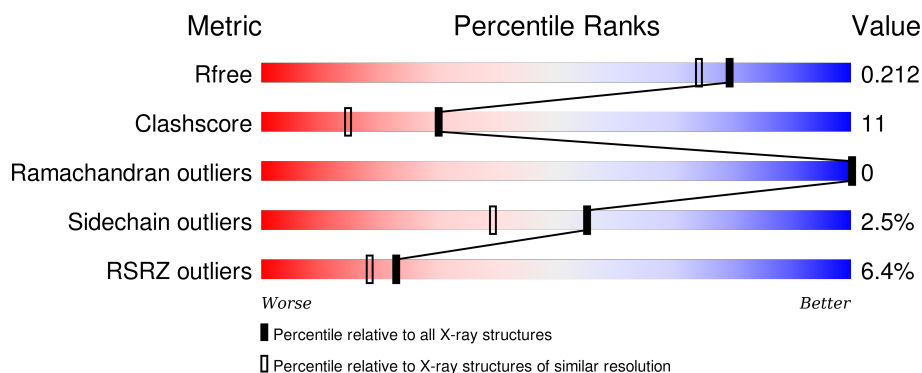
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	155	<div> <div>8%</div> <div>81%16% . .</div> </div>
1	B	155	<div> <div>5%</div> <div>88%9% . .</div> </div>
1	C	155	<div> <div>5%</div> <div>78%19% . .</div> </div>
1	D	155	<div> <div>8%</div> <div>79%19% . .</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
2	NA	B	156	-	-	-	X
3	ZEA	B	158	-	-	-	X
3	ZEA	D	157	-	-	-	X
4	TBR	A	158	-	-	X	-
4	TBR	A	159	-	-	X	-
4	TBR	C	157	-	-	X	-
4	TBR	C	158	-	-	X	-
4	TBR	D	158	-	-	X	-
5	EPE	A	160	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5729 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 Cytokinin-specific binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	3	0
			1229	789	192	245	3			
1	B	151	Total	C	N	O	S	0	3	0
			1233	791	196	243	3			
1	C	151	Total	C	N	O	S	0	9	0
			1253	807	195	248	3			
1	D	152	Total	C	N	O	S	0	2	0
			1233	789	194	247	3			

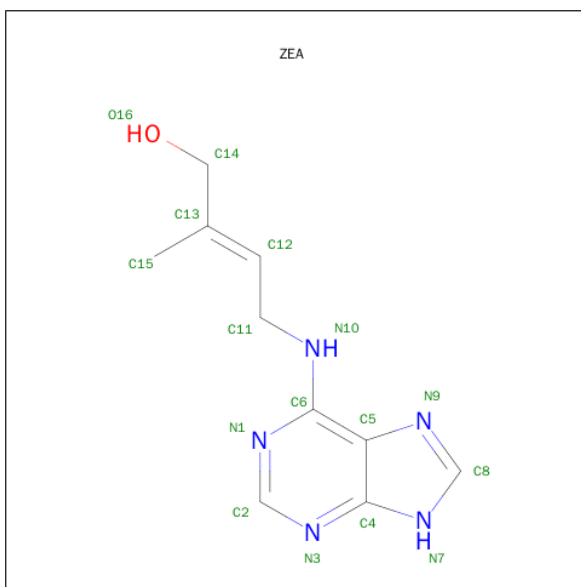
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	SER	ASN	SEE REMARK 999	UNP Q9ZWP8
B	92	SER	ASN	SEE REMARK 999	UNP Q9ZWP8
C	92	SER	ASN	SEE REMARK 999	UNP Q9ZWP8
D	92	SER	ASN	SEE REMARK 999	UNP Q9ZWP8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

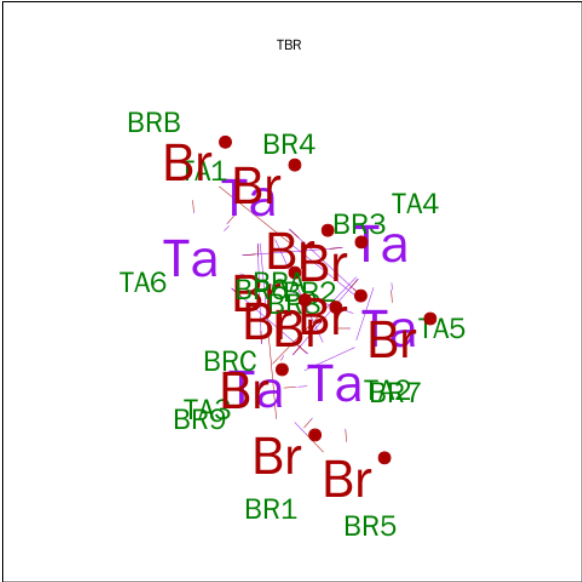
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is (2E)-2-METHYL-4-(9H-PURIN-6-YLAMINO)BUT-2-EN-1-OL (three-letter code: ZEA) (formula: C₁₀H₁₃N₅O).



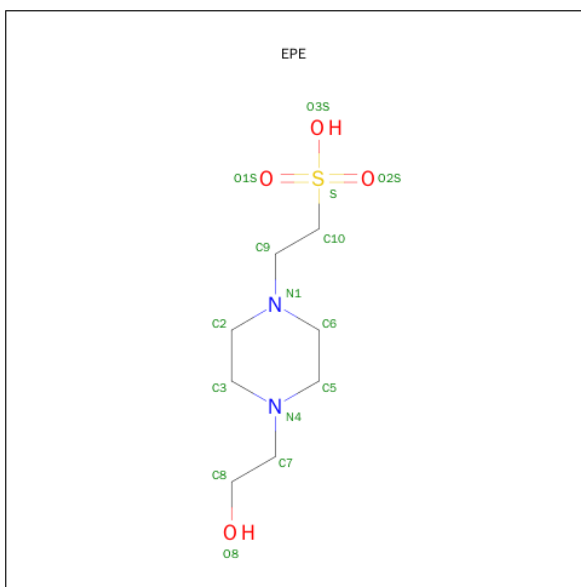
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	10	5	1		
3	A	1	Total	C	N	O	0	0
			16	10	5	1		
3	B	1	Total	C	N	O	0	0
			16	10	5	1		
3	B	1	Total	C	N	O	0	0
			16	10	5	1		
3	D	1	Total	C	N	O	0	0
			16	10	5	1		
3	D	1	Total	C	N	O	0	0
			16	10	5	1		

- Molecule 4 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $\text{Br}_{12}\text{Ta}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Br	Ta	0	0
			18	12	6		
4	C	1	Total	Br	Ta	0	0
			18	12	6		
4	A	1	Total	Br	Ta	0	0
			18	12	6		
4	D	1	Total	Br	Ta	0	0
			18	12	6		
4	C	1	Total	Br	Ta	0	0
			18	12	6		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

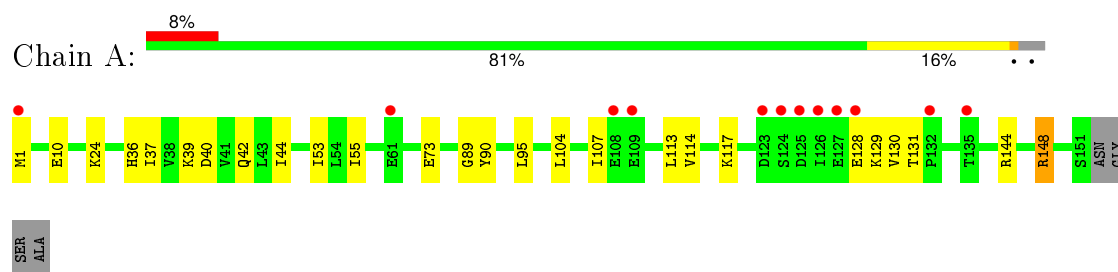
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		
6	B	159	Total	O	0	0
			159	159		
6	C	160	Total	O	0	0
			160	160		
6	D	112	Total	O	0	0
			112	112		

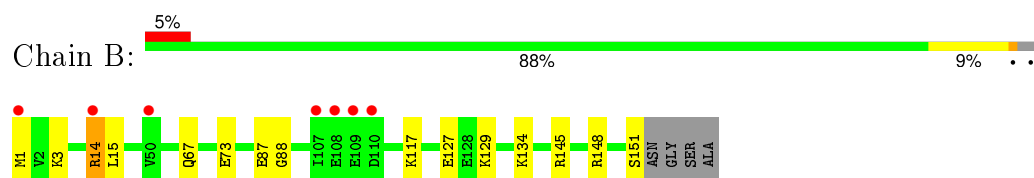
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

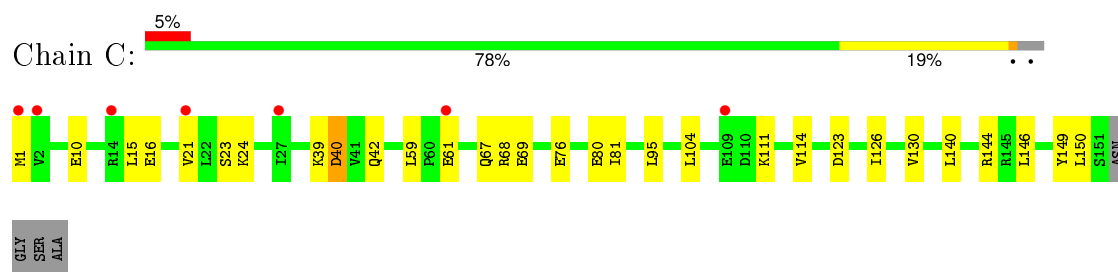
- Molecule 1: Cytokinin-specific binding protein



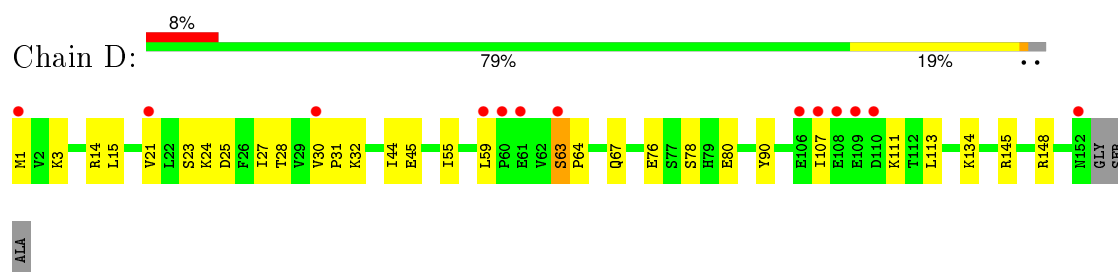
- Molecule 1: Cytokinin-specific binding protein



- Molecule 1: Cytokinin-specific binding protein



- Molecule 1: Cytokinin-specific binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	113.22Å 113.22Å 85.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.31 – 1.80 28.30 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (28.31-1.80) 98.5 (28.30-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.158 , 0.207 0.160 , 0.212	Depositor DCC
R_{free} test set	1160 reflections (2.09%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 56534 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5729	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: EPE, NA, ZEA, TBR

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	0.87	0/1264	0.86	2/1711 (0.1%)
1	B	0.90	0/1267	0.84	0/1713
1	C	0.93	1/1310 (0.1%)	0.88	1/1773 (0.1%)
1	D	0.82	0/1263	0.80	0/1710
All	All	0.88	1/5104 (0.0%)	0.84	3/6907 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	GLU	CG-CD	5.05	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	144	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	148	ARG	NE-CZ-NH2	-5.45	117.58	120.30

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	1229	0	1232	31	0
1	B	1233	0	1241	17	0
1	C	1253	0	1262	22	0
1	D	1233	0	1229	32	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	32	0	26	2	0
3	B	32	0	26	2	0
3	D	32	0	26	4	0
4	A	36	0	0	18	0
4	C	36	0	0	15	0
4	D	18	0	0	7	0
5	A	15	0	17	1	0
6	A	147	0	0	8	0
6	B	159	0	0	5	0
6	C	160	0	0	5	0
6	D	112	0	0	4	0
All	All	5729	0	5059	114	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 11.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:CD	4:A:158:TBR:BR4	2.23	1.31
1:A:40:ASP:OD2	4:A:158:TBR:BR3	2.21	1.12
1:C:42[B]:GLN:NE2	4:C:157:TBR:BR9	2.38	1.11
1:A:42:GLN:CG	4:A:158:TBR:BR4	2.54	1.11
1:C:80:GLU:OE1	4:C:158:TBR:BR1	2.24	1.10
1:A:42:GLN:NE2	4:A:158:TBR:BR4	2.41	1.09
4:A:158:TBR:BR2	6:A:278:HOH:O	2.29	1.06
1:D:80:GLU:OE2	4:D:158:TBR:BR1	2.31	1.04
1:A:95:LEU:HD11	1:A:130:VAL:HB	1.33	1.04
1:A:42:GLN:HG3	4:A:158:TBR:BR4	2.20	0.94
4:C:158:TBR:BR3	6:C:265:HOH:O	2.42	0.90
4:C:158:TBR:BR2	6:C:265:HOH:O	2.44	0.89
1:A:37:ILE:HD11	6:A:243:HOH:O	1.74	0.87
3:D:157:ZEA:H141	6:D:255:HOH:O	1.75	0.87
1:C:42[B]:GLN:NE2	4:C:157:TBR:BR5	2.62	0.86
1:D:78:SER:OG	4:D:158:TBR:BR1	2.51	0.83
1:B:1[B]:MET:HE3	6:B:314:HOH:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:158:TBR:BR4	6:C:297:HOH:O	2.53	0.82
4:C:158:TBR:BR6	6:C:257:HOH:O	2.53	0.81
1:A:95:LEU:CD1	1:A:130:VAL:HB	2.12	0.79
1:A:39:LYS:NZ	4:A:159:TBR:BR9	2.71	0.79
1:D:44:ILE:CG1	1:D:55:ILE:HD13	2.12	0.79
1:D:23:SER:OG	1:D:24:LYS:HE3	1.83	0.79
4:A:159:TBR:BRC	6:A:278:HOH:O	2.57	0.77
1:A:42:GLN:NE2	4:A:158:TBR:BR1	2.74	0.74
4:C:157:TBR:BR5	6:C:266:HOH:O	2.61	0.73
1:D:44:ILE:CG1	1:D:55:ILE:CD1	2.68	0.71
6:B:305:HOH:O	4:C:157:TBR:BRA	2.63	0.71
1:D:44:ILE:HG13	1:D:55:ILE:CD1	2.21	0.70
3:D:157:ZEA:H10	3:D:157:ZEA:H151	1.56	0.69
4:A:159:TBR:BR3	1:B:151:SER:O	2.67	0.68
1:A:39:LYS:HG3	4:A:159:TBR:BRC	2.50	0.66
1:D:44:ILE:HG12	1:D:55:ILE:HD13	1.78	0.66
1:C:21[B]:VAL:HG22	1:D:28:THR:OG1	1.98	0.64
1:C:23:SER:HA	1:C:81:ILE:HD13	1.80	0.64
1:D:44:ILE:HG12	1:D:55:ILE:CD1	2.29	0.63
1:D:3:LYS:HE3	6:D:232:HOH:O	1.99	0.63
1:D:80:GLU:OE1	4:D:158:TBR:BR4	2.72	0.62
1:A:10:GLU:HG3	1:A:107:ILE:HD12	1.82	0.61
1:A:44[B]:ILE:HD11	1:A:53:ILE:HG22	1.82	0.61
1:A:39:LYS:CG	4:A:159:TBR:BRC	3.04	0.60
1:A:24:LYS:HE3	6:A:228:HOH:O	2.02	0.60
1:D:44:ILE:HG13	1:D:55:ILE:HD13	1.81	0.60
1:A:36:HIS:CD2	1:A:36:HIS:H	2.20	0.59
4:A:158:TBR:BR5	1:B:14[B]:ARG:NE	2.91	0.59
1:B:3:LYS:HE3	6:B:317:HOH:O	2.03	0.57
1:D:67:GLN:HE21	1:D:90:TYR:H	1.51	0.57
4:A:158:TBR:BR5	1:B:14[B]:ARG:CZ	3.07	0.57
4:D:158:TBR:BR5	6:D:248:HOH:O	2.73	0.57
1:D:24:LYS:HE2	1:D:76:GLU:OE2	2.05	0.56
1:B:67:GLN:OE1	3:B:158:ZEA:H2	2.06	0.56
1:D:67:GLN:NE2	1:D:90:TYR:H	2.04	0.55
1:D:44:ILE:HG22	1:D:45:GLU:HG2	1.89	0.55
1:C:15:LEU:HD23	1:C:15:LEU:C	2.26	0.55
1:C:67[B]:GLN:NE2	1:C:69:GLU:OE2	2.41	0.54
1:D:63:SER:HA	1:D:64:PRO:O	2.08	0.54
1:A:44[B]:ILE:HD12	1:A:55:ILE:HG12	1.90	0.53
1:D:107:ILE:HD11	1:D:113:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:157:ZEA:N10	3:D:157:ZEA:H151	2.20	0.52
1:A:39:LYS:NZ	4:A:159:TBR:BRC	2.85	0.52
1:B:145:ARG:CD	1:B:148:ARG:HH21	2.23	0.52
1:C:10:GLU:HB3	1:C:111[A]:LYS:HE3	1.91	0.51
1:C:21[B]:VAL:HG11	1:C:146:LEU:HD11	1.92	0.50
1:A:73:GLU:HG3	6:A:206:HOH:O	2.11	0.50
1:C:42[B]:GLN:CD	4:C:157:TBR:BRA	3.04	0.50
1:C:95:LEU:HD21	1:C:130[B]:VAL:HG23	1.94	0.49
1:D:80:GLU:OE2	4:D:158:TBR:BR4	2.86	0.48
1:C:21[B]:VAL:HG21	1:C:150:LEU:HD21	1.94	0.48
1:C:40:ASP:OD1	4:C:157:TBR:BR9	2.86	0.48
1:C:123:ASP:HB3	1:C:126:ILE:HD12	1.95	0.48
1:D:111:LYS:HE2	1:D:111:LYS:HB3	1.65	0.48
1:B:15:LEU:HD23	1:B:15:LEU:C	2.34	0.48
1:C:42[B]:GLN:NE2	4:C:157:TBR:BRA	3.03	0.47
4:C:157:TBR:BRC	1:D:14:ARG:HD3	2.70	0.47
1:A:148:ARG:HB2	1:A:148:ARG:HE	1.41	0.47
1:A:148:ARG:HD3	6:A:296:HOH:O	2.14	0.47
5:A:160:EPE:H51	6:A:220:HOH:O	2.14	0.47
1:A:117:LYS:HE2	1:A:117:LYS:HB3	1.73	0.47
1:B:127:GLU:HB2	4:C:157:TBR:BR7	2.71	0.46
1:D:145:ARG:HD2	1:D:148:ARG:NH2	2.31	0.46
1:A:128:GLU:HA	1:A:131:THR:HG23	1.97	0.46
1:A:39:LYS:HG2	4:A:159:TBR:BRC	2.71	0.46
1:C:149:TYR:CZ	1:D:32:LYS:HD2	2.51	0.46
1:A:90:TYR:HB3	1:A:95:LEU:HD13	1.98	0.45
1:D:44:ILE:HG13	1:D:55:ILE:HD11	1.94	0.45
1:C:140:LEU:O	1:C:144:ARG:HG2	2.17	0.45
1:D:63:SER:HA	1:D:64:PRO:C	2.37	0.44
1:A:40:ASP:CG	4:A:158:TBR:BR3	3.07	0.44
1:B:145:ARG:HD2	6:B:204:HOH:O	2.16	0.44
1:D:55:ILE:N	1:D:55:ILE:HD12	2.32	0.44
1:C:39:LYS:HB2	1:C:59:LEU:HD23	1.98	0.44
3:D:157:ZEA:C14	6:D:255:HOH:O	2.50	0.44
1:A:44[B]:ILE:CD1	1:A:55:ILE:HG12	2.48	0.44
1:A:89:GLY:HA2	3:A:157:ZEA:H153	1.99	0.43
1:D:30:VAL:HB	1:D:31:PRO:HD3	2.00	0.43
1:C:24:LYS:NZ	1:D:27:ILE:HD12	2.33	0.43
4:A:158:TBR:BR1	1:B:14[B]:ARG:NH2	3.06	0.43
1:B:87:GLU:HG2	1:B:88:GLY:N	2.34	0.43
1:D:80:GLU:CD	4:D:158:TBR:BR4	3.12	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:156:ZEA:H112	3:A:156:ZEA:H151	1.71	0.43
1:C:104:LEU:HD22	1:C:114:VAL:HG22	2.01	0.42
1:C:24:LYS:HZ2	1:D:27:ILE:HD12	1.84	0.42
1:A:73:GLU:CD	6:A:170:HOH:O	2.58	0.41
1:B:117[A]:LYS:NZ	6:B:300:HOH:O	2.53	0.41
1:B:127:GLU:OE1	4:C:157:TBR:BRB	2.94	0.41
1:A:104:LEU:HD22	1:A:114:VAL:HG22	2.02	0.41
1:C:61:GLU:H	1:C:61:GLU:CD	2.22	0.41
1:D:21:VAL:HA	1:D:25:ASP:HB2	2.02	0.41
1:D:78:SER:CB	4:D:158:TBR:BR1	3.24	0.41
3:B:157:ZEA:H151	3:B:157:ZEA:H112	1.84	0.40
1:A:107:ILE:HD11	1:A:113:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/155 (97%)	148 (98%)	3 (2%)	0	100	100
1	B	151/155 (97%)	149 (99%)	2 (1%)	0	100	100
1	C	157/155 (101%)	153 (98%)	4 (2%)	0	100	100
1	D	151/155 (97%)	150 (99%)	1 (1%)	0	100	100
All	All	610/620 (98%)	600 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	144/143 (101%)	141 (98%)	3 (2%)	61	47
1	B	144/143 (101%)	139 (96%)	5 (4%)	43	25
1	C	150/143 (105%)	146 (97%)	4 (3%)	52	36
1	D	144/143 (101%)	138 (96%)	6 (4%)	36	18
All	All	582/572 (102%)	564 (97%)	18 (3%)	55	30

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	129	LYS
1	B	14[A]	ARG
1	B	14[B]	ARG
1	B	73	GLU
1	B	129	LYS
1	B	134	LYS
1	C	1[A]	MET
1	C	1[B]	MET
1	C	40	ASP
1	C	76	GLU
1	D	1[A]	MET
1	D	1[B]	MET
1	D	15	LEU
1	D	59	LEU
1	D	63	SER
1	D	134	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	D	42	GLN
1	D	67	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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$
3	ZEA	A	156	-	12,17,17	1.13	1 (8%)	12,22,22	4.49	5 (41%)
3	ZEA	A	157	-	12,17,17	1.11	1 (8%)	12,22,22	3.56	3 (25%)
4	TBR	A	158	-	0,36,36	0.00	-	0,180,180	0.00	-
4	TBR	A	159	-	0,36,36	0.00	-	0,180,180	0.00	-
5	EPE	A	160	-	14,15,15	0.62	0	18,20,20	1.25	2 (11%)
3	ZEA	B	157	-	12,17,17	0.99	0	12,22,22	4.28	5 (41%)
3	ZEA	B	158	-	12,17,17	1.25	1 (8%)	12,22,22	4.06	5 (41%)
4	TBR	C	157	-	0,36,36	0.00	-	0,180,180	0.00	-
4	TBR	C	158	-	0,36,36	0.00	-	0,180,180	0.00	-
3	ZEA	D	156	-	12,17,17	1.19	1 (8%)	12,22,22	4.59	5 (41%)
3	ZEA	D	157	-	12,17,17	1.16	2 (16%)	12,22,22	3.84	3 (25%)
4	TBR	D	158	-	0,36,36	0.00	-	0,180,180	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZEA	A	156	-	-	0/8/8/8	0/2/2/2
3	ZEA	A	157	-	-	0/8/8/8	0/2/2/2
4	TBR	A	158	-	-	0/0/696/696	0/0/19/19
4	TBR	A	159	-	-	0/0/696/696	0/0/19/19
5	EPE	A	160	-	-	0/9/19/19	0/1/1/1
3	ZEA	B	157	-	-	0/8/8/8	0/2/2/2
3	ZEA	B	158	-	-	0/8/8/8	0/2/2/2
4	TBR	C	157	-	-	0/0/696/696	0/0/19/19
4	TBR	C	158	-	-	0/0/696/696	0/0/19/19
3	ZEA	D	156	-	-	0/8/8/8	0/2/2/2
3	ZEA	D	157	-	-	1/8/8/8	0/2/2/2
4	TBR	D	158	-	-	0/0/696/696	0/0/19/19

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	157	ZEA	C2-N3	2.01	1.35	1.32
3	A	157	ZEA	C6-N1	2.04	1.37	1.34
3	A	156	ZEA	C6-N1	2.16	1.37	1.34
3	D	157	ZEA	C6-N1	2.20	1.37	1.34
3	B	158	ZEA	C6-N1	2.45	1.37	1.34
3	D	156	ZEA	C6-N1	2.83	1.38	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	156	ZEA	N3-C2-N1	-12.12	119.61	128.89
3	A	156	ZEA	N3-C2-N1	-11.21	120.31	128.89
3	D	157	ZEA	N3-C2-N1	-10.46	120.88	128.89
3	B	157	ZEA	N3-C2-N1	-10.40	120.93	128.89
3	B	158	ZEA	N3-C2-N1	-9.95	121.28	128.89
3	A	157	ZEA	N3-C2-N1	-9.01	122.00	128.89
3	B	157	ZEA	O16-C14-C13	-5.11	101.02	111.76
3	A	156	ZEA	C11-C12-C13	-4.69	118.41	126.96
3	A	157	ZEA	C4-C5-N9	-3.95	105.84	109.48
3	A	156	ZEA	C4-C5-N9	-3.75	106.03	109.48
3	D	157	ZEA	C4-C5-N9	-3.68	106.09	109.48
3	B	157	ZEA	C4-C5-N9	-3.55	106.21	109.48
3	A	156	ZEA	O16-C14-C13	-3.29	104.85	111.76
3	B	157	ZEA	C11-C12-C13	-2.92	121.64	126.96
3	D	156	ZEA	O16-C14-C13	-2.49	106.53	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	158	ZEA	C4-C5-N9	-2.03	107.61	109.48
3	D	156	ZEA	C12-C11-N10	2.06	119.87	112.93
3	B	158	ZEA	O16-C14-C13	2.17	116.33	111.76
5	A	160	EPE	C6-C5-N4	2.54	115.18	110.63
5	A	160	EPE	C5-N4-C3	3.21	115.84	108.90
3	D	156	ZEA	N10-C6-N1	3.67	124.22	119.14
3	B	158	ZEA	N10-C6-N1	3.79	124.38	119.14
3	D	157	ZEA	C2-N1-C6	6.74	121.34	116.48
3	A	157	ZEA	C2-N1-C6	6.78	121.36	116.48
3	B	157	ZEA	C2-N1-C6	7.24	121.70	116.48
3	A	156	ZEA	C2-N1-C6	7.55	121.92	116.48
3	B	158	ZEA	C2-N1-C6	8.12	122.33	116.48
3	D	156	ZEA	C2-N1-C6	8.35	122.50	116.48

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	157	ZEA	C13-C12-C11-N10

There are no ring outliers.

11 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	156	ZEA	1	0
3	A	157	ZEA	1	0
4	A	158	TBR	11	0
4	A	159	TBR	7	0
5	A	160	EPE	1	0
3	B	157	ZEA	1	0
3	B	158	ZEA	1	0
4	C	157	TBR	10	0
4	C	158	TBR	5	0
3	D	157	ZEA	4	0
4	D	158	TBR	7	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 ⓘ

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	151/155 (97%)	0.49	12 (7%) 15 12	21, 27, 39, 46	4 (2%)
1	B	151/155 (97%)	0.26	7 (4%) 36 30	21, 27, 35, 40	0
1	C	151/155 (97%)	0.18	7 (4%) 36 30	19, 26, 36, 44	0
1	D	152/155 (98%)	0.43	13 (8%) 13 10	20, 28, 41, 50	0
All	All	605/620 (97%)	0.34	39 (6%) 23 18	19, 27, 37, 50	4 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	ILE	7.4
1	D	1[A]	MET	6.1
1	A	1[A]	MET	5.9
1	C	1[A]	MET	5.7
1	A	128	GLU	5.7
1	A	123	ASP	4.9
1	B	109	GLU	4.5
1	B	1[A]	MET	4.4
1	D	108	GLU	4.3
1	A	127	GLU	4.2
1	A	124	SER	3.8
1	C	2	VAL	3.6
1	A	125	ASP	3.6
1	D	110[A]	ASP	3.4
1	D	61	GLU	3.3
1	D	60	PRO	3.2
1	D	63	SER	3.2
1	D	152	ASN	3.0
1	B	110	ASP	2.9
1	D	109	GLU	2.9
1	A	61	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	50	VAL	2.6
1	B	14[A]	ARG	2.5
1	C	109	GLU	2.5
1	D	21	VAL	2.4
1	D	30	VAL	2.4
1	A	109	GLU	2.4
1	A	135	THR	2.4
1	C	27	ILE	2.3
1	B	108	GLU	2.3
1	C	61	GLU	2.3
1	D	59	LEU	2.3
1	D	107	ILE	2.2
1	C	14	ARG	2.2
1	B	107	ILE	2.2
1	D	106	GLU	2.1
1	A	132	PRO	2.1
1	A	108	GLU	2.0
1	C	21[A]	VAL	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	ZEAL	B	158	16/16	0.66	0.25	4.92	39,42,44,44	0
2	NA	B	156	1/1	0.98	0.37	4.89	29,29,29,29	0
5	EPE	A	160	15/15	0.90	0.25	4.05	26,30,36,42	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZEA	D	157	16/16	0.57	0.29	3.11	49,54,56,56	16
3	ZEA	A	157	16/16	0.86	0.15	1.47	33,36,40,42	0
4	TBR	C	158	18/18	0.87	0.12	0.46	34,34,36,36	18
4	TBR	D	158	18/18	0.84	0.13	-0.24	30,32,33,34	18
4	TBR	A	159	18/18	0.70	0.16	-0.34	34,36,37,38	18
4	TBR	A	158	18/18	0.89	0.10	-0.72	28,32,36,36	18
4	TBR	C	157	18/18	0.93	0.09	-0.86	21,26,28,30	18
3	ZEA	D	156	16/16	0.95	0.10	-0.98	23,26,31,33	0
3	ZEA	A	156	16/16	0.94	0.11	-1.07	22,25,30,32	0
3	ZEA	B	157	16/16	0.96	0.07	-2.37	19,20,22,23	0
2	NA	C	156	1/1	0.96	0.21	-	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.