

Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 08:08 PM JST

PDB ID	:	7XRF
Title	:	Crystal structaure of DgpB/C complex
Authors	:	Ma, M.; He, P.
Deposited on	:	2022-05-10
Resolution	:	2.14 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
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.14 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	Δ	204	9%		
	A	324	83%	15%	•
	a	224	7%		
	C	324	84%	15%	•
			10%		
1	E	324	91%	1	9%
	~		10%		
1	G	324	81%	13%	6%
	_		4%		_
2	В	142	88%	10%	6•
			2%		
2	D	142	90%	89	% •



Mol	Chain	Length	Quality of chain		
2	F	142	89%	8%	•••
2	Н	142	90%	8%	•



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14639 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	202	Total	С	Ν	0	S	0	0	0
	A	323	2546	1615	421	483	27	0	0	0
1	C	202	Total	С	Ν	0	S	0	0	0
1	U	∂ ∠ ∂	2550	1617	421	485	27	0	0	0
1	Б	292	Total	С	Ν	0	S	0	0	0
	E	323	2539	1611	420	481	27	0	0	0
1	C	205	Total	С	Ν	0	S	0	0	0
	I G	505	2318	1465	387	443	23	0 0	U	

• Molecule 1 is a protein called AP_endonuc_2 domain-containing protein.

• Molecule 2 is a protein called DgpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	р	120	Total	С	Ν	0	S	0	0	0
	D	139	1111	714	179	214	4	0	0	0
0	П	120	Total	С	Ν	0	S	0	0	0
	D	159	1111	714	179	214	4	0	0	0
0	Б	120	Total	С	Ν	0	S	0	0	0
	Г	159	1111	714	179	214	4	0	0	U
0	ц	120	Total	С	Ν	0	S	0	0	0
	п	109	1111	714	179	214	4	0		U

• Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mn 1 1	0	0
3	С	1	Total Mn 1 1	0	0
3	Ε	1	Total Mn 1 1	0	0
3	G	1	Total Mn 1 1	0	0





• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	24	Total O 24 24	0	0
4	В	27	$\begin{array}{cc} \text{Total} & \text{O} \\ 27 & 27 \end{array}$	0	0
4	С	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0
4	D	27	TotalO2727	0	0
4	Е	33	Total O 33 33	0	0
4	F	32	$\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
4	G	30	$\begin{array}{cc} \text{Total} & \text{O} \\ 30 & 30 \end{array}$	0	0
4	Н	23	TotalO2323	0	0



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: AP_endonuc_2 domain-containing protein



• Molecule 1: AP_endonuc_2 domain-containing protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	78.08Å 159.70Å 176.17Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{Basolution}\left(\mathbf{\mathring{A}}\right)$	19.84 - 2.14	Depositor
Resolution (A)	19.84 - 2.14	EDS
% Data completeness	96.0 (19.84-2.14)	Depositor
(in resolution range)	97.8(19.84-2.14)	EDS
R_{merge}	0.20	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	14.91 (at 2.13Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
B B.	0.206 , 0.251	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.207 , 0.248	DCC
R_{free} test set	2000 reflections $(1.67%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	48.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , 49.9	EDS
L-test for $twinning^2$	$ < L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14639	wwPDB-VP
Average B, all atoms $(Å^2)$	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: MN

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).

Mal	Chain	Bond	lengths	Bo	ond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.38	0/2602	0.52	0/3512
1	С	0.48	0/2606	0.54	0/3517
1	Е	0.42	0/2595	0.52	0/3504
1	G	0.44	0/2368	0.59	1/3202~(0.0%)
2	В	0.38	0/1137	0.53	0/1543
2	D	0.39	0/1137	0.54	0/1543
2	F	0.39	0/1137	0.56	1/1543~(0.1%)
2	Н	0.37	0/1137	0.54	0/1543
All	All	0.42	0/14719	0.54	2/19907~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	6	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	G	227	VAL	C-N-CA	5.08	134.39	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	С	144	ASN	Peptide

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	А	2546	0	2467	40	0
1	С	2550	0	2471	31	0
1	Е	2539	0	2454	18	0
1	G	2318	0	2153	25	0
2	В	1111	0	1072	7	0
2	D	1111	0	1072	8	0
2	F	1111	0	1072	7	0
2	Н	1111	0	1072	7	0
3	А	1	0	0	0	0
3	С	1	0	0	0	0
3	Е	1	0	0	0	0
3	G	1	0	0	0	0
4	А	24	0	0	0	0
4	В	27	0	0	0	0
4	С	42	0	0	1	0
4	D	27	0	0	0	0
4	Е	33	0	0	1	0
4	F	32	0	0	0	0
4	G	30	0	0	5	0
4	Н	23	0	0	0	0
All	All	14639	0	13833	137	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 5.

All (137) 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:285:LYS:HD2	1:A:289:GLU:OE1	1.70	0.90
1:A:194:ALA:HA	1:A:227:VAL:HG21	1.64	0.79
1:A:285:LYS:O	1:A:289:GLU:HB2	1.83	0.77



	lo de pagen	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:172:PRO:HG2	1:C:262:MET:HG2	1.72	0.71
1:G:62:LYS:NZ	4:G:503:HOH:O	2.24	0.70
1:C:212:TYR:O	1:C:216:VAL:HG22	1.92	0.68
1:A:307:HIS:HB2	1:A:311:MET:CE	2.24	0.67
1:E:288:SER:OG	4:E:501:HOH:O	2.15	0.65
1:C:94:MET:HE1	1:C:119:MET:HA	1.79	0.64
1:A:307:HIS:HB2	1:A:311:MET:HE2	1.78	0.64
1:G:2:SER:N	4:G:504:HOH:O	2.31	0.63
1:C:10:LEU:HD22	1:C:27:CYS:HB3	1.82	0.61
1:C:56:LYS:O	1:C:60:GLU:HG3	2.00	0.60
1:C:51:PRO:HG2	1:C:52:TYR:CE2	2.36	0.60
2:F:6:ARG:NH1	2:F:133:CYS:O	2.29	0.58
1:A:269:MET:HE1	1:A:275:GLU:HG2	1.85	0.58
1:G:42:VAL:HG13	1:G:45:GLN:HB3	1.85	0.57
1:G:251:GLY:O	1:G:255:MET:HG3	2.04	0.57
1:E:50:TYR:CG	1:E:51:PRO:HA	2.39	0.57
1:A:194:ALA:CA	1:A:227:VAL:HG21	2.34	0.57
1:C:262:MET:HB2	1:C:296:ILE:HG12	1.87	0.57
1:C:256:ILE:HG21	1:C:290:SER:HB2	1.88	0.56
1:A:51:PRO:HG2	1:A:52:TYR:CE2	2.42	0.55
1:A:229:LEU:H	1:A:229:LEU:HD12	1.72	0.55
1:A:190:LEU:HD21	1:A:199:LEU:HD12	1.89	0.54
1:E:79:CYS:SG	1:E:94:MET:HE2	2.47	0.54
1:A:194:ALA:HA	1:A:227:VAL:CG2	2.37	0.54
1:A:225:LYS:O	1:A:229:LEU:HD12	2.08	0.53
1:C:94:MET:CE	1:C:119:MET:HA	2.39	0.53
1:E:225:LYS:O	1:E:229:LEU:HD12	2.08	0.53
1:A:50:TYR:CG	1:A:51:PRO:HA	2.43	0.53
1:G:310:GLU:OE2	1:G:313:ARG:NH1	2.41	0.52
1:A:207:TYR:CD1	1:A:243:LYS:HB2	2.44	0.52
1:C:202:ALA:HA	1:C:232:MET:HE2	1.92	0.52
1:A:252:LEU:O	1:A:256:ILE:HG12	2.10	0.52
2:F:18:LEU:HD11	2:F:102:LEU:HD12	1.91	0.52
1:C:50:TYR:CG	1:C:51:PRO:HA	2.45	0.52
1:A:124:PHE:CD1	1:A:140:ILE:HD11	2.45	0.51
1:C:172:PRO:HD2	1:C:261:HIS:O	2.11	0.51
1:G:2:SER:HB2	1:G:290:SER:O	2.10	0.51
2:B:53:LYS:HE2	2:B:56:GLY:HA2	1.91	0.51
2:D:12:VAL:O	2:D:34:VAL:HA	2.11	0.51
1:E:81:ARG:HB2	1:E:94:MET:HE1	1.93	0.51
1:E:172:PRO:HB3	1:E:255:MET:HE1	1.93	0.51



	lo de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:190:LEU:HD23	1:A:194:ALA:HB3	1.93	0.50
1:A:234:ASP:HB3	1:A:239:LEU:HD12	1.92	0.50
1:C:216:VAL:O	1:C:220:THR:HG23	2.11	0.50
1:G:99:VAL:HG12	1:G:103:LYS:HE3	1.94	0.50
1:C:219:LEU:HD13	1:C:232:MET:HE1	1.93	0.50
1:C:237:THR:O	1:C:237:THR:OG1	2.21	0.49
2:F:6:ARG:HD2	2:F:131:ASP:O	2.12	0.49
1:A:153:THR:O	1:A:157:ILE:HG13	2.11	0.49
1:G:196:LYS:O	1:G:218:ARG:CB	2.60	0.49
2:D:83:ASN:OD1	2:H:83:ASN:ND2	2.46	0.49
1:A:128:ALA:HB2	1:A:168:LEU:HD11	1.94	0.49
1:G:50:TYR:CG	1:G:51:PRO:HA	2.48	0.48
1:C:114:ARG:HG2	1:C:171:ILE:HD12	1.95	0.48
1:E:172:PRO:HG2	1:E:262:MET:HG2	1.96	0.47
1:G:51:PRO:HG2	1:G:52:TYR:CE2	2.50	0.47
1:C:125:ALA:HB1	1:C:163:THR:HG21	1.96	0.47
1:C:128:ALA:HB2	1:C:168:LEU:HD11	1.96	0.47
1:A:225:LYS:HD2	1:A:226:LYS:NZ	2.30	0.47
1:A:113:VAL:HG23	1:A:136:VAL:HG11	1.97	0.47
1:C:245:VAL:O	1:C:245:VAL:HG23	2.15	0.47
1:A:108:MET:HB3	1:A:108:MET:HE2	1.69	0.46
1:C:107:LYS:HB3	1:C:107:LYS:HE3	1.58	0.46
1:C:172:PRO:HB3	1:C:255:MET:HE3	1.97	0.46
2:H:46:THR:HA	2:H:116:ARG:NH1	2.30	0.46
1:E:214:GLU:OE2	1:E:218:ARG:NH1	2.47	0.46
1:G:114:ARG:HG2	1:G:171:ILE:HD12	1.97	0.46
1:C:210:VAL:HG23	1:C:215:ALA:HB2	1.97	0.46
1:C:137:LYS:HG2	1:C:167:TYR:HA	1.99	0.45
1:A:6:LEU:HD12	1:A:320:HIS:CE1	2.52	0.45
2:B:46:THR:HA	2:B:116:ARG:NH1	2.32	0.45
1:G:78:ASN:OD1	4:G:501:HOH:O	2.21	0.45
1:A:99:VAL:HG12	1:A:103:LYS:HE3	1.98	0.45
1:G:50:TYR:CD1	1:G:51:PRO:HA	2.52	0.45
1:C:83:LEU:HD11	2:D:43:PHE:CD1	2.52	0.44
2:F:53:LYS:HB3	2:F:110:ASP:HB2	2.00	0.44
2:H:68:LEU:HD12	2:H:68:LEU:HA	1.81	0.44
1:A:184:MET:O	1:A:188:ASN:ND2	2.39	0.44
1:A:300:TYR:CZ	1:A:302:GLU:HB2	2.53	0.44
1:C:75:TYR:HB3	1:C:113:VAL:HG22	1.99	0.44
1:A:58:LEU:HD22	1:A:107:LYS:HG2	1.98	0.44
1:A:225:LYS:O	1:A:229:LEU:CD1	2.66	0.44



	le de pagen	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:307:HIS:CB	1:A:311:MET:CE	2.96	0.44
2:B:3:LEU:HD12	2:B:4:ALA:H	1.82	0.44
1:E:8:VAL:O	1:E:39:PHE:HA	2.18	0.43
2:F:28:ILE:HA	2:F:99:PRO:HA	2.00	0.43
2:B:12:VAL:O	2:B:34:VAL:HA	2.18	0.43
1:E:183:LYS:NZ	1:E:187:ASP:OD2	2.50	0.43
2:B:123:SER:OG	2:B:126:GLU:HG2	2.19	0.43
2:H:53:LYS:HE3	2:H:56:GLY:HA2	1.99	0.43
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.88	0.43
1:A:124:PHE:CG	1:A:140:ILE:HD11	2.53	0.43
1:C:62:LYS:HA	1:C:62:LYS:HD2	1.68	0.43
1:E:205:MET:SD	1:E:218:ARG:HD2	2.58	0.43
2:H:110:ASP:OD1	2:H:135:SER:HB3	2.19	0.43
2:D:71:LYS:HD3	1:G:52:TYR:CD2	2.54	0.43
1:E:9:THR:HB	1:E:40:GLU:HB3	2.00	0.42
1:G:172:PRO:HG2	1:G:262:MET:HG2	2.00	0.42
1:G:316:LEU:HD23	1:G:316:LEU:HA	1.89	0.42
1:A:265:LYS:HE3	1:A:265:LYS:HB2	1.90	0.42
2:F:67:CYS:HB2	2:F:93:THR:HB	2.01	0.42
1:G:270:TYR:O	1:G:314:ARG:HD3	2.20	0.42
1:G:93:GLU:O	1:G:97:MET:HG3	2.18	0.42
1:A:144:ASN:OD1	1:A:176:CYS:HA	2.19	0.42
1:A:166:LYS:N	1:A:166:LYS:HD2	2.35	0.42
1:G:155:ASP:OD1	4:G:502:HOH:O	2.21	0.42
1:E:172:PRO:HD2	1:E:261:HIS:O	2.20	0.42
1:A:285:LYS:HD2	1:A:289:GLU:CD	2.37	0.42
1:C:185:ASN:ND2	4:C:501:HOH:O	2.13	0.42
1:E:81:ARG:HD3	1:E:94:MET:HE1	2.01	0.42
1:A:269:MET:HE1	1:A:275:GLU:CG	2.49	0.42
1:E:252:LEU:O	1:E:256:ILE:HG12	2.19	0.41
2:H:28:ILE:HA	2:H:99:PRO:HA	2.02	0.41
2:B:83:ASN:HB3	2:F:83:ASN:HD21	1.83	0.41
1:C:214:GLU:C	1:C:216:VAL:N	2.74	0.41
1:E:230:THR:HA	1:E:233:ARG:HB2	2.02	0.41
1:G:44:THR:HG23	4:G:501:HOH:O	2.21	0.41
1:C:45:GLN:HG2	1:C:46:MET:HG3	2.03	0.41
1:C:166:LYS:HD3	1:C:166:LYS:HA	1.79	0.41
1:E:251:GLY:O	1:E:255:MET:HB2	2.20	0.41
1:E:79:CYS:SG	1:E:94:MET:CE	3.08	0.41
1:G:95:VAL:O	1:G:99:VAL:HG23	2.20	0.41
1:A:219:LEU:HG	1:A:224:ALA:HB2	2.03	0.41



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
1:A:225:LYS:N	1:A:228:GLU:OE1	2.53	0.41
2:B:39:TYR:HH	2:B:119:TYR:HH	1.57	0.41
1:G:81:ARG:NH1	1:G:118:LEU:HD22	2.36	0.41
1:G:172:PRO:HD2	1:G:261:HIS:O	2.21	0.41
2:D:71:LYS:HD3	1:G:52:TYR:CE2	2.55	0.41
1:C:135:GLY:HA3	2:H:24:ASN:ND2	2.36	0.40
2:D:67:CYS:HA	2:D:71:LYS:O	2.21	0.40
1:G:195:ASP:C	1:G:197:LYS:N	2.75	0.40
2:D:17:SER:HB2	2:D:33:ASP:H	1.85	0.40
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.92	0.40
2:D:46:THR:HA	2:D:116:ARG:NH1	2.36	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	Perce	entiles
1	А	321/324~(99%)	305~(95%)	16 (5%)	0	100	100
1	С	321/324~(99%)	304 (95%)	16 (5%)	1 (0%)	41	36
1	Е	321/324~(99%)	310 (97%)	11 (3%)	0	100	100
1	G	301/324~(93%)	275 (91%)	23 (8%)	3 (1%)	15	8
2	В	137/142~(96%)	134 (98%)	3 (2%)	0	100	100
2	D	137/142~(96%)	135 (98%)	2 (2%)	0	100	100
2	F	137/142~(96%)	135 (98%)	2 (2%)	0	100	100
2	Н	137/142~(96%)	132 (96%)	5 (4%)	0	100	100
All	All	1812/1864 (97%)	1730 (96%)	78 (4%)	4 (0%)	47	45

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	С	238	PHE
1	G	228	GLU
1	G	187	ASP
1	G	191	ALA

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	270/277~(98%)	263~(97%)	7 (3%)	46 45
1	С	271/277~(98%)	266~(98%)	5(2%)	59 60
1	Ε	268/277~(97%)	265~(99%)	3~(1%)	73 76
1	G	231/277~(83%)	226~(98%)	5(2%)	52 53
2	В	123/125~(98%)	122~(99%)	1 (1%)	81 85
2	D	123/125~(98%)	122~(99%)	1 (1%)	81 85
2	F	123/125~(98%)	122~(99%)	1 (1%)	81 85
2	Η	123/125~(98%)	123 (100%)	0	100 100
All	All	1532/1608~(95%)	1509 (98%)	23 (2%)	65 68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	117	TRP
1	А	119	MET
1	А	166	LYS
1	А	192	ASP
1	А	226	LYS
1	А	227	VAL
1	А	311	MET
2	В	80	ASP
1	С	107	LYS
1	С	143	HIS
1	С	216	VAL
1	С	291	ASP



Mol	Chain	Res	Type
1	С	324	ASP
2	D	129	SER
1	Е	83	LEU
1	Е	117	TRP
1	Е	184	MET
2	F	24	ASN
1	G	117	TRP
1	G	152	SER
1	G	255	MET
1	G	280	TYR
1	G	285	LYS

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

Mol	Chain	Res	Type
1	С	3	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (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, 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	А	323/324~(99%)	0.64	29 (8%) 9 12	44, 60, 90, 104	0
1	С	323/324~(99%)	0.55	23 (7%) 16 20	46, 60, 90, 103	0
1	E	323/324~(99%)	0.69	31 (9%) 8 10	48, 62, 88, 101	0
1	G	305/324~(94%)	0.73	33 (10%) 5 7	44, 61, 100, 113	0
2	В	139/142~(97%)	0.35	6 (4%) 35 43	43, 52, 65, 82	0
2	D	139/142~(97%)	0.36	3 (2%) 62 68	42, 50, 63, 75	0
2	F	139/142~(97%)	0.48	7 (5%) 28 35	43, 55, 70, 81	0
2	Н	139/142~(97%)	0.44	7 (5%) 28 35	44, 54, 68, 83	0
All	All	1830/1864 (98%)	0.58	139 (7%) 13 17	42, 58, 89, 113	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res Type		RSRZ
1	Е	2	SER	8.0
1	G	230	THR	7.5
1	G	229	LEU	6.3
1	G	190	LEU	5.8
1	А	238	PHE	5.6
1	G	186	TRP	5.4
1	А	191	ALA	5.2
1	Е	213	ASP	4.8
1	G	237	THR	4.8
1	Е	307	HIS	4.8
1	Е	238	PHE	4.5
1	А	221	ALA	4.5
1	Е	171	ILE	4.4
1	С	2	SER	4.4
1	G	221	ALA	4.4
2	Н	3	LEU	4.3



Mol	Chain	Res	Type	RSRZ
1	С	324	ASP	4.3
1	С	212	TYR	4.2
1	G	219	LEU	4.2
1	Е	322	PHE	4.2
1	Е	191	ALA	4.1
2	F	3	LEU	4.0
2	D	3	LEU	3.9
1	G	145	PRO	3.9
1	А	324	ASP	3.8
1	С	213	ASP	3.8
1	С	238	PHE	3.7
2	В	3	LEU	3.6
1	А	276	ALA	3.6
1	G	220	THR	3.6
1	G	223	GLY	3.6
1	А	192	ASP	3.5
1	С	191	ALA	3.4
1	С	298	SER	3.4
1	G	306	GLY	3.3
1	С	202	ALA	3.3
2	Н	36	LEU	3.2
1	Е	170	LEU	3.2
1	Е	244	ASP	3.1
2	F	36	LEU	3.1
2	В	109	VAL	3.1
1	G	228	GLU	3.0
1	G	218	ARG	3.0
1	С	307	HIS	3.0
2	В	104	GLU	3.0
1	G	323	VAL	3.0
1	А	207	TYR	3.0
1	Ε	254	ASP	3.0
1	G	189	ALA	2.9
1	А	291	ASP	2.9
1	А	8	VAL	2.8
1	G	321	ASN	2.8
1	Е	270	TYR	2.8
1	A	211	PRO	2.8
1	G	224	ALA	2.8
1	G	270	TYR	2.8
1	Е	262	MET	2.8
1	G	194	ALA	2.7



Mol	Chain	Res	Type	RSRZ
1	Е	226	LYS	2.7
1	Е	207	TYR	2.7
1	G	232	MET	2.7
1	G	238	PHE	2.7
1	Е	212	TYR	2.6
1	С	237	THR	2.6
1	Е	194	ALA	2.6
2	D	41	GLY	2.6
1	С	312	LEU	2.6
1	А	209	ASN	2.6
2	F	7	LEU	2.6
1	С	170	LEU	2.6
1	G	198	LEU	2.6
1	G	226	LYS	2.5
1	G	199	LEU	2.5
1	G	312	LEU	2.5
1	А	307	HIS	2.5
2	Н	32	PHE	2.5
1	А	190	LEU	2.4
1	А	223	GLY	2.4
2	В	32	PHE	2.4
1	G	196	LYS	2.4
2	Н	122	LEU	2.4
1	А	296	ILE	2.4
1	G	231	THR	2.4
1	А	122	GLU	2.4
2	Н	4	ALA	2.4
1	G	254	ASP	2.4
1	С	233	ARG	2.3
1	С	235	MET	2.3
1	Е	291	ASP	2.3
2	Н	70	GLY	2.3
2	F	94	ILE	2.3
1	Е	172	PRO	2.3
1	Е	174	PHE	2.3
1	А	139	GLY	2.3
1	С	219	LEU	2.3
1	G	241	PHE	2.3
1	С	296	ILE	2.3
1	А	193	GLY	2.3
1	Е	149	ILE	2.3
2	F	88	ILE	2.3



Mol	Chain	Res	Type	RSRZ
1	Е	232	MET	2.2
1	А	233	ARG	2.2
2	F	132	SER	2.2
2	Н	88	ILE	2.2
1	А	224	ALA	2.2
1	С	232	MET	2.2
2	В	36	LEU	2.2
1	С	323	VAL	2.2
1	С	254	ASP	2.2
1	Е	208	ASP	2.2
1	Е	127	LEU	2.2
1	Е	3	ASN	2.2
1	А	169	GLY	2.2
1	G	271	GLU	2.2
1	Е	143	HIS	2.1
1	С	244	ASP	2.1
1	А	236	TYR	2.1
2	В	38	TYR	2.1
1	А	235	MET	2.1
1	С	252	LEU	2.1
1	Е	151	GLN	2.1
1	С	193	GLY	2.1
1	А	311	MET	2.1
1	А	202	ALA	2.1
2	D	130	ILE	2.1
1	А	145	PRO	2.1
1	G	269	MET	2.1
1	А	174	PHE	2.1
1	Е	292	TYR	2.1
1	G	188	ASN	2.0
1	A	10	LEU	2.0
2	F	69	ASP	2.0
1	A	226	LYS	2.0
1	Е	202	ALA	2.0
1	Е	287	VAL	2.0
1	G	280	TYR	2.0
1	Е	230	THR	2.0
1	E	252	LEU	2.0
1	С	216	VAL	2.0

Continued from previous page...



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 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	MN	G	401	1/1	0.97	0.09	$57,\!57,\!57,\!57$	0
3	MN	Е	401	1/1	0.98	0.10	62,62,62,62	0
3	MN	А	401	1/1	0.99	0.10	$53,\!53,\!53,\!53$	0
3	MN	С	401	1/1	0.99	0.07	54,54,54,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

















6.5 Other polymers (i)

There are no such residues in this entry.

