

# Full wwPDB X-ray Structure Validation Report (i)

#### Jun 17, 2024 – 10:12 pm BST

PDB ID	:	8PC4
Title	:	MEMBRANE TARGET COMPLEX 1
Authors	:	Garau, G.
Deposited on	:	2023-06-09
Resolution	:	2.85  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	:	2.37.1
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)	:	2.37.1

# 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 2.85 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	А	393	37%	38%	9% •	16%				
1	В	393	6%	36%	5% •	15%				

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
5	HCZ	В	608	-	-	-	Х



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5928 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 N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	А	332	Total 2752	C 1785	N 467	0 486	S 14	0	3	0
1	В	334	Total 2749	C 1776	N 465	0 494	S 14	0	3	0

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0
2	В	2	Total Zn 2 2	0	0

• Molecule 3 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	ο Λ	1	Total	С	Ν	0	Р	0	0	
D A	1	44	34	1	8	1	0	0		
2	Р	1	Total	С	Ν	Ο	Р	0	0	
0	3 B	L	44	34	1	8	1	0	0	

• Molecule 4 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula:  $C_{24}H_{40}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
4	А	1	Total C O	0	0	
		1	28 24 4	0	0	
4	Δ	1	Total C O	0	0	
		1	28 24 4	0	0	
1	Δ	1	Total C O	0	0	
T	11	1	28  24  4	0	0	
4	Λ Λ	Δ	1	Total C O	0	0
	Л	T	28  24  4	0	0	
4	4 A	Δ 1	Total C O	0	0	
4	Л	T	28  24  4	0	0	
4	Δ	1	Total C O	0	0	
4	Л	T	28  24  4	0		
4	В	1	Total C O	0	0	
4	D	T	28  24  4	0	0	
4	В	1	Total C O	0	0	
4	D		28  24  4	0	U	
4	В	B 1	Total C O	0	0	
4	D		28  24  4	0	U	



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Mol	Chain	Residues	At	$\mathbf{oms}$		ZeroOcc	AltConf
4	В	1	Total 28	C 24	0 4	0	0

• Molecule 5 is 6-chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide (three-letter code: HCZ) (formula:  $C_7H_8ClN_3O_4S_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	В	1	Total 17	$\begin{array}{c} \mathrm{C} \\ 7 \end{array}$	Cl 1	N 3	0 4	${ m S} { m 2}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	16	Total O 16 16	0	0
6	В	22	Total O 22 22	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: N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	94.39Å 94.39Å 442.32Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Bosolution (Å)	54.75 - 2.85	Depositor
Resolution (A)	54.75 - 2.85	EDS
% Data completeness	99.5 (54.75-2.85)	Depositor
(in resolution range)	99.5(54.75-2.85)	EDS
$R_{merge}$	0.14	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.18 (at 2.86 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D	0.265 , $0.301$	Depositor
II, II, <i>free</i>	0.263 , $0.299$	DCC
$R_{free}$ test set	1468 reflections $(5.17\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	87.8	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.32 , 79.1	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5928	wwPDB-VP
Average B, all atoms $(Å^2)$	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: DXC, 3PE, ZN, HCZ

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		Bond	angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.46	0/2858	0.66	0/3892
1	В	0.42	0/2851	0.67	0/3881
All	All	0.44	0/5709	0.66	0/7773

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	А	2752	0	2651	198	0
1	В	2749	0	2641	152	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	44	0	62	6	0
3	В	44	0	62	5	0
4	А	168	0	234	21	0
4	В	112	0	156	9	0
5	В	17	0	8	1	0
6	А	16	0	0	0	0
6	В	22	0	0	0	0
All	All	5928	0	5814	366	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 31.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:312:GLU:HG3	1:B:313:PRO:CD	1.80	1.11
1:B:312:GLU:HG3	1:B:313:PRO:HD2	1.31	1.09
1:B:73:LYS:HG2	1:B:288:CYS:HB2	1.45	0.95
1:A:326:GLU:HA	1:A:329:ARG:HG3	1.49	0.94
1:B:323:ASP:OD1	1:B:326:GLU:HG3	1.73	0.89
1:B:312:GLU:CG	1:B:313:PRO:HD2	2.01	0.89
1:A:142:LEU:CD2	1:A:144:PHE:HD2	1.89	0.86
1:A:82:ARG:HG2	4:A:409:DXC:H51	1.59	0.85
1:A:236:ASN:OD1	1:A:237:CYS:N	2.10	0.84
1:A:371:ASN:OD1	1:A:373:GLU:HG3	1.81	0.81
1:A:59:LYS:HE3	1:A:293:GLU:HB3	1.63	0.80
4:A:405:DXC:H211	4:B:602:DXC:H81	1.63	0.79
1:B:365:LEU:HD11	1:B:375:PHE:HB3	1.62	0.78
1:A:69:TRP:HD1	1:A:266:LEU:HD13	1.48	0.78
1:A:142:LEU:HD22	1:A:144:PHE:HD2	1.48	0.77
1:A:258:THR:HA	3:A:403:3PE:H282	1.67	0.77
1:A:67:ASN:OD1	1:A:68:PRO:HD3	1.85	0.76
1:B:312:GLU:HG2	1:B:351:ASN:HB3	1.67	0.76
1:A:101:ASP:HA	1:A:166:ARG:HH22	1.51	0.76
1:B:65:PHE:HB2	1:B:70:PRO:HG3	1.65	0.76
1:A:314:ARG:HB3	1:A:318:LYS:HE3	1.68	0.75
1:A:83:TRP:HE1	1:A:88:LYS:HA	1.53	0.74
1:A:141:GLU:O	1:A:241:HIS:CD2	2.39	0.74
1:A:314:ARG:O	1:A:318:LYS:HG2	1.89	0.72
1:A:371:ASN:ND2	1:A:374:ASP:OD1	2.23	0.72
1:B:127:VAL:HG21	1:B:340:MET:HE1	1.71	0.72
1:A:254:TRP:HA	1:A:267:TRP:CZ3	2.25	0.72
1:B:60:GLY:HA3	1:B:72:TRP:CZ3	2.25	0.71
1:A:126:ARG:HD2	1:A:138:GLU:OE2	1.90	0.71
1:A:97:LYS:HD3	1:A:101:ASP:OD1	1.91	0.70
1:A:75:PRO:HB2	1:A:252:GLN:HE22	1.56	0.70
1:A:62:ASP:HA	1:A:232:TRP:HE1	1.55	0.70
1:B:322:VAL:HB	1:B:326:GLU:HB2	1.71	0.70
1:B:312:GLU:HG3	1:B:313:PRO:HD3	1.73	0.69
1:A:326:GLU:HA	1:A:329:ARG:CG	2.21	0.69
1:A:314:ARG:HE	1:A:314:ARG:HA	1.56	0.69
1:B:67:ASN:H	1:B:68:PRO:HD2	1.57	0.69



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:287:TYR:HD1	1:B:288:CYS:N	1.90	0.69
1:A:120:VAL:HG21	1:A:139:MET:HA	1.75	0.68
1:A:141:GLU:O	1:A:241:HIS:HD2	1.76	0.67
1:A:241:HIS:ND1	1:A:241:HIS:N	2.43	0.67
1:B:172:ILE:O	1:B:175:LEU:HG	1.94	0.66
1:A:69:TRP:CD1	1:A:266:LEU:HD13	2.28	0.66
1:A:89:ASP:OD1	1:A:90:HIS:N	2.29	0.65
1:B:312:GLU:CB	1:B:313:PRO:HD2	2.27	0.64
1:B:232:TRP:CH2	1:B:250:PRO:HA	2.32	0.64
1:B:73:LYS:HG3	1:B:289:PRO:HD2	1.79	0.64
1:B:125:LEU:CD2	1:B:139:MET:HB3	2.27	0.63
1:B:251:SER:HB3	1:B:268:GLY:HA2	1.80	0.63
4:A:405:DXC:H211	4:B:602:DXC:H151	1.80	0.63
1:B:59:LYS:HA	1:B:293:GLU:OE1	1.97	0.63
1:B:149:ILE:HD12	1:B:192:ASP:HB2	1.79	0.63
1:A:254:TRP:HA	1:A:267:TRP:CE3	2.34	0.63
1:B:364:ALA:HA	1:B:367:ARG:HD3	1.81	0.63
1:B:235:GLU:HB3	1:B:247:VAL:HG22	1.81	0.63
1:A:347:PHE:HB2	1:A:349:LEU:HD11	1.80	0.62
1:A:243:LYS:H	1:A:243:LYS:HD2	1.62	0.62
1:B:80:VAL:O	1:B:82:ARG:NH2	2.32	0.62
1:A:64:ARG:HA	1:A:70:PRO:HD3	1.82	0.62
1:B:73:LYS:HB3	1:B:75:PRO:HD2	1.82	0.62
1:A:134:THR:HA	1:A:146:THR:O	1.99	0.62
1:A:238:VAL:HG13	1:A:239:PRO:HD2	1.82	0.62
1:B:312:GLU:CG	1:B:313:PRO:CD	2.66	0.61
1:B:312:GLU:O	1:B:313:PRO:C	2.38	0.61
1:A:111:PHE:CD2	1:A:176:PRO:HD3	2.34	0.61
1:A:81:LEU:HG	4:A:409:DXC:H62	1.83	0.60
1:A:232:TRP:CE3	1:A:250:PRO:HA	2.35	0.60
1:B:134:THR:HG23	1:B:148:PRO:HA	1.83	0.60
1:B:123:ALA:N	1:B:276:TRP:HE1	2.00	0.60
1:A:59:LYS:HG3	1:A:233:TRP:CZ2	2.36	0.59
1:B:355:LEU:O	1:B:358:PRO:HD2	2.02	0.59
1:A:77:ILE:HD12	1:A:319:TYR:CE1	2.38	0.59
1:A:181:VAL:HG21	1:A:209:TRP:CE3	2.37	0.59
1:B:227:VAL:O	1:B:228:ILE:HD13	2.02	0.58
1:B:200:ASN:ND2	1:B:223:GLY:O	2.37	0.58
1:B:273:LEU:HD12	1:B:278:ARG:HG2	1.86	0.57
1:A:175:LEU:HD13	1:A:178:ILE:HD11	1.85	0.57
4:A:406:DXC:H183	4:A:407:DXC:H203	1.84	0.57



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:97:LYS:O	1:A:101:ASP:OD1	2.22	0.57
1:A:126:ARG:HB3	1:A:138:GLU:HG3	1.86	0.57
1:B:65:PHE:O	1:B:66:VAL:C	2.42	0.57
1:B:305:ALA:HB1	1:B:342:ILE:HG21	1.86	0.57
1:A:341:ALA:HB2	1:A:375:PHE:HE1	1.68	0.57
4:B:601:DXC:H203	4:B:602:DXC:H182	1.86	0.57
1:A:90:HIS:CD2	1:A:93:VAL:HA	2.40	0.57
1:B:134:THR:HA	1:B:146:THR:O	2.04	0.57
1:B:65:PHE:H	1:B:70:PRO:HD3	1.68	0.56
1:A:192:ASP:O	1:A:196:VAL:HG23	2.05	0.56
1:A:185:HIS:CE1	1:A:190:HIS:CD2	2.93	0.56
1:B:312:GLU:HG2	1:B:351:ASN:CB	2.35	0.56
1:A:303:LEU:HD13	1:A:304:ALA:N	2.21	0.56
1:B:247:VAL:HG11	1:B:298:PHE:CZ	2.41	0.56
1:A:62:ASP:HA	1:A:232:TRP:NE1	2.20	0.55
1:A:82:ARG:CG	4:A:409:DXC:H51	2.32	0.55
1:A:310:ALA:N	1:A:352:GLU:OE2	2.37	0.55
1:B:123:ALA:H	1:B:276:TRP:HE1	1.53	0.55
1:B:228:ILE:HG21	1:B:236:ASN:HD22	1.71	0.55
1:B:100:LEU:HD21	1:B:165:PHE:HD2	1.71	0.55
1:B:310:ALA:N	1:B:352:GLU:OE2	2.36	0.55
1:A:238:VAL:HB	1:A:241:HIS:O	2.06	0.55
1:A:90:HIS:C	1:A:92:SER:H	2.10	0.55
1:B:216:LEU:HB2	1:B:229:GLU:HG3	1.88	0.55
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.07	0.55
1:A:207:LEU:O	1:A:226:ASN:HB3	2.07	0.55
1:A:120:VAL:HG13	1:A:121:ARG:H	1.72	0.54
1:A:185:HIS:CD2	1:A:187:HIS:ND1	2.75	0.54
1:A:290:ALA:O	1:A:294:ILE:HG13	2.07	0.54
1:B:287:TYR:HE2	1:B:329:ARG:HB3	1.73	0.54
1:A:151:SER:HA	5:B:608:HCZ:H13	1.90	0.54
1:B:73:LYS:CG	1:B:289:PRO:HD2	2.37	0.54
4:A:405:DXC:C21	4:B:602:DXC:H151	2.38	0.54
1:B:185:HIS:CD2	1:B:187:HIS:ND1	2.74	0.54
1:A:142:LEU:CD2	1:A:144:PHE:CD2	2.80	0.54
1:B:259:LEU:HD21	4:B:607:DXC:H72	1.89	0.53
1:A:120:VAL:HG21	1:A:139:MET:CA	2.38	0.53
1:A:290:ALA:HA	1:A:293:GLU:CG	2.38	0.53
1:A:194:ASN:HA	1:A:197:ILE:HG12	1.90	0.53
1:A:101:ASP:HA	1:A:166:ARG:NH2	2.21	0.53
1:A:285:THR:HG21	1:A:291:PHE:CZ	2.44	0.53



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:B:88:LYS:HD3	1:B:348:ALA:O	2.07	0.53
1:A:62:ASP:CA	1:A:232:TRP:HE1	2.21	0.53
1:B:287:TYR:CD1	1:B:288:CYS:N	2.73	0.53
1:A:233:TRP:CE3	1:A:233:TRP:HA	2.43	0.53
1:B:232:TRP:CE3	1:B:232:TRP:HA	2.44	0.53
1:A:142:LEU:HD22	1:A:144:PHE:CD2	2.38	0.53
1:A:175:LEU:HB3	1:A:178:ILE:HD11	1.91	0.53
1:A:360:LYS:HA	1:A:363:GLU:CD	2.30	0.53
1:B:183:ILE:HD12	1:B:191:LEU:HD13	1.90	0.53
1:B:280:PHE:O	1:B:304:ALA:HA	2.09	0.52
1:B:130:LEU:HA	1:B:169:PRO:HG2	1.90	0.52
1:B:308:ILE:HG12	1:B:341:ALA:HB1	1.90	0.52
1:A:347:PHE:HB2	1:A:349:LEU:CD1	2.39	0.52
1:A:314:ARG:HD3	1:A:318:LYS:HE2	1.91	0.52
1:B:343:HIS:O	1:B:344:TRP:CD1	2.63	0.52
1:A:77:ILE:CG1	1:A:78:PRO:CD	2.88	0.52
1:A:140:ASP:OD2	1:A:276:TRP:N	2.30	0.52
1:A:175:LEU:O	1:A:202:ARG:NH2	2.43	0.52
1:A:206:GLU:OE1	1:A:206:GLU:N	2.32	0.52
1:B:313:PRO:HD2	1:B:351:ASN:HB2	1.92	0.52
1:B:67:ASN:H	1:B:68:PRO:CD	2.20	0.52
1:A:280:PHE:HB2	1:A:301:PHE:CD2	2.45	0.51
1:A:77:ILE:HG12	1:A:78:PRO:HD2	1.93	0.51
3:A:403:3PE:H2A1	3:A:403:3PE:H3D2	1.91	0.51
1:B:185:HIS:CE1	1:B:284:ASP:HB2	2.46	0.51
1:A:77:ILE:CG1	1:A:78:PRO:HD2	2.40	0.51
1:A:134:THR:HB	1:A:148:PRO:HA	1.92	0.51
1:A:353:HIS:HE1	1:A:355:LEU:HD12	1.76	0.51
1:B:175:LEU:O	1:B:202:ARG:NH1	2.43	0.51
1:B:216:LEU:HB2	1:B:229:GLU:CD	2.31	0.51
1:A:216:LEU:HB2	1:A:229:GLU:CD	2.31	0.51
1:A:80:VAL:O	1:A:81:LEU:C	2.49	0.51
4:A:406:DXC:C23	4:A:406:DXC:H161	2.41	0.51
1:B:214:GLY:N	1:B:229:GLU:OE2	2.36	0.51
1:B:123:ALA:HA	1:B:276:TRP:HE1	1.75	0.51
1:B:232:TRP:CZ2	1:B:250:PRO:HA	2.46	0.51
1:B:71:THR:HG22	1:B:267:TRP:CZ2	2.46	0.50
1:B:97:LYS:HG3	1:B:167:ARG:HH22	1.75	0.50
1:A:92:SER:HB3	1:A:353:HIS:HA	1.93	0.50
1:A:83:TRP:CH2	1:A:162:PRO:HB3	2.46	0.50
1:B:308:ILE:HD12	1:B:357:PRO:CB	2.41	0.50



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:B:312:GLU:CG	1:B:351:ASN:HB3	2.40	0.50
1:B:312:GLU:HB3	1:B:351:ASN:H	1.77	0.50
1:A:196:VAL:HG13	1:A:209:TRP:CZ3	2.46	0.50
3:A:403:3PE:H3A1	4:B:601:DXC:H21	1.93	0.50
1:B:187:HIS:CG	3:B:605:3PE:H12	2.47	0.50
1:B:216:LEU:O	1:B:220:GLN:HG3	2.11	0.50
1:A:231:ASP:O	1:A:234:GLU:HB2	2.12	0.50
1:A:314:ARG:CZ	1:A:318:LYS:HA	2.42	0.50
1:B:123:ALA:CA	1:B:276:TRP:HE1	2.25	0.50
1:B:125:LEU:HD23	1:B:139:MET:HB3	1.93	0.50
1:B:308:ILE:HD12	1:B:357:PRO:HB2	1.93	0.50
1:A:83:TRP:NE1	1:A:88:LYS:HA	2.24	0.49
1:A:204:GLY:N	1:A:206:GLU:OE1	2.46	0.49
1:A:313:PRO:HD3	1:A:351:ASN:HB2	1.95	0.49
1:B:84:LEU:O	1:B:85:ILE:HG13	2.11	0.49
1:A:130:LEU:HA	1:A:169:PRO:HG2	1.94	0.49
1:A:254:TRP:NE1	1:A:320:GLN:OE1	2.44	0.49
1:A:285:THR:HG21	1:A:291:PHE:HZ	1.77	0.49
1:A:325:GLU:O	1:A:329:ARG:HG2	2.13	0.49
1:B:312:GLU:O	1:B:317:MET:HG3	2.12	0.49
1:A:104:LEU:O	1:A:166:ARG:NE	2.43	0.49
1:A:156:PRO:HD3	1:A:188:TYR:CE2	2.47	0.49
1:A:308:ILE:HD13	1:A:341:ALA:HB1	1.93	0.49
1:A:82:ARG:HD3	1:A:256:LYS:HE2	1.94	0.49
1:A:188:TYR:HD2	3:A:403:3PE:H342	1.76	0.49
1:A:314:ARG:HA	1:A:314:ARG:NE	2.26	0.49
4:A:404:DXC:H243	1:B:160:MET:HE1	1.95	0.49
1:A:82:ARG:HG3	4:A:409:DXC:H181	1.94	0.49
1:B:62:ASP:N	1:B:62:ASP:OD1	2.41	0.49
1:B:191:LEU:O	1:B:257:ARG:NH2	2.45	0.49
1:B:341:ALA:CB	1:B:377:VAL:HG12	2.43	0.49
1:A:232:TRP:O	1:A:233:TRP:HB2	2.13	0.48
1:B:97:LYS:HG3	1:B:167:ARG:NH2	2.29	0.48
1:A:92:SER:CB	1:A:353:HIS:HA	2.43	0.48
1:A:120:VAL:HG13	1:A:121:ARG:N	2.27	0.48
1:B:171:THR:OG1	1:B:174:GLU:HG3	2.13	0.48
1:B:258:THR:HB	4:B:602:DXC:H1	1.95	0.48
1:B:353:HIS:HB3	1:B:356:GLU:HB2	1.95	0.48
1:A:103:GLU:HB3	1:A:355:LEU:HD21	1.96	0.48
1:A:137:VAL:HB	1:A:144:PHE:CE1	2.48	0.48
1:A:349:LEU:HD12	1:A:349:LEU:N	2.28	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:138:GLU:HG2	1:B:143:ILE:HG23	1.95	0.48
1:B:312:GLU:O	1:B:314:ARG:N	2.46	0.48
1:A:253:HIS:CG	1:A:254:TRP:H	2.32	0.48
1:A:280:PHE:CE1	1:A:294:ILE:HD13	2.48	0.48
3:B:605:3PE:H271	3:B:605:3PE:H2A2	1.49	0.48
1:A:172:ILE:HD12	1:A:199:LEU:HD22	1.96	0.47
1:B:256:LYS:NZ	1:B:258:THR:O	2.40	0.47
1:A:77:ILE:HG13	1:A:78:PRO:CD	2.45	0.47
1:A:312:GLU:O	1:A:350:ALA:HB1	2.15	0.47
1:B:127:VAL:HG21	1:B:340:MET:CE	2.42	0.47
1:B:216:LEU:HB2	1:B:229:GLU:CG	2.44	0.47
1:A:138:GLU:HB3	1:A:143:ILE:HD13	1.95	0.47
1:B:232:TRP:HA	1:B:232:TRP:HE3	1.80	0.47
1:B:116[B]:GLU:OE1	1:B:117:GLU:N	2.45	0.47
1:B:254:TRP:CD1	1:B:254:TRP:N	2.82	0.47
1:A:363:GLU:O	1:A:366:GLU:HG3	2.13	0.47
1:B:312:GLU:HB3	1:B:313:PRO:HD2	1.97	0.47
1:A:243:LYS:HD2	1:A:243:LYS:N	2.29	0.47
1:A:187:HIS:CG	3:A:403:3PE:H12	2.50	0.47
1:A:313:PRO:HB3	1:A:315[B]:TRP:CZ3	2.50	0.47
1:B:210:PHE:HB3	1:B:270:TRP:CH2	2.50	0.47
1:A:246:PHE:CD2	1:A:272:VAL:HG22	2.50	0.46
1:B:153:ARG:HG2	1:B:155:SER:HB3	1.97	0.46
1:B:247:VAL:HG12	1:B:249:THR:HG23	1.97	0.46
1:A:123:ALA:HB1	1:A:276:TRP:CE3	2.50	0.46
1:A:178:ILE:HD12	1:A:203:PHE:HE2	1.80	0.46
1:B:172:ILE:HA	1:B:175:LEU:CD2	2.45	0.46
1:A:313:PRO:O	1:A:317:MET:HG2	2.15	0.46
1:B:105:PRO:HG2	1:B:379:LYS:HD2	1.97	0.46
1:B:259:LEU:CD2	4:B:607:DXC:H72	2.44	0.46
1:A:238:VAL:CG1	1:A:239:PRO:HD2	2.45	0.46
1:B:100:LEU:HD11	1:B:165:PHE:HB2	1.96	0.46
1:B:188:TYR:HE1	1:B:257:ARG:NH1	2.12	0.46
1:B:287:TYR:CE2	1:B:329:ARG:HB3	2.51	0.46
1:A:155:SER:HB2	1:A:161:GLY:HA3	1.97	0.46
1:A:311:TYR:O	1:A:317:MET:HB2	2.16	0.46
1:A:343:HIS:O	1:A:344:TRP:CD1	2.68	0.46
1:A:387:ASN:OD1	1:A:387:ASN:N	2.44	0.46
1:A:114:ASN:O	1:A:117:GLU:HG3	2.16	0.46
1:B:92:SER:HB3	1:B:354:TYR:H	1.80	0.46
1:A:77:ILE:CD1	1:A:319:TYR:CE1	2.99	0.46



Atom-1	Atom-2	Interatomic	Clash
	1100HI 2	distance (Å)	overlap (Å)
1:A:140:ASP:OD1	1:A:276:TRP:HB2	2.15	0.46
1:B:368:TYR:CD1	1:B:368:TYR:N	2.84	0.46
1:A:142:LEU:CD1	1:A:238:VAL:HG21	2.45	0.46
1:A:215:LEU:O	1:A:219:MET:HG2	2.16	0.46
1:B:311:TYR:HB3	1:B:322:VAL:O	2.16	0.46
1:B:312:GLU:CG	1:B:351:ASN:CB	2.94	0.45
3:B:605:3PE:H111	3:B:605:3PE:H31	1.99	0.45
1:A:106:VAL:HG21	1:A:167[B]:ARG:HH21	1.81	0.45
1:A:303:LEU:HD11	1:A:340:MET:HB2	1.98	0.45
1:B:125:LEU:HD22	1:B:139:MET:HB3	1.97	0.45
1:A:172:ILE:O	1:A:175:LEU:HB2	2.17	0.45
1:A:90:HIS:O	1:A:93:VAL:N	2.48	0.45
1:B:219:MET:HB3	1:B:227:VAL:HG11	1.98	0.45
1:A:145:LEU:O	1:A:181:VAL:HA	2.16	0.45
1:A:208:ARG:HD3	1:A:210:PHE:CZ	2.51	0.45
1:B:88:LYS:HG3	1:B:89:ASP:N	2.31	0.45
1:B:136:MET:CE	1:B:176:PRO:HG2	2.47	0.45
1:A:142:LEU:HD12	1:A:238:VAL:HG21	1.97	0.45
1:A:147:ASP:OD2	1:A:190:HIS:ND1	2.46	0.45
1:A:191:LEU:HD23	1:A:257:ARG:NH1	2.31	0.45
1:A:218:TRP:CD1	4:A:404:DXC:H3	2.52	0.45
1:A:296:LYS:N	1:A:296:LYS:HD2	2.31	0.45
1:A:361:LEU:HD21	1:A:375:PHE:CD1	2.52	0.45
1:A:228:ILE:HG21	1:A:236:ASN:ND2	2.32	0.45
1:A:136:MET:HA	1:A:145:LEU:HD23	1.98	0.45
1:A:233:TRP:HA	1:A:233:TRP:HE3	1.81	0.45
4:A:409:DXC:H221	4:A:409:DXC:H243	1.58	0.45
1:B:109:PRO:HG2	1:B:170:CYS:HB3	1.98	0.45
1:A:232:TRP:HZ3	1:A:267:TRP:CD1	2.35	0.44
1:A:314:ARG:NH2	1:A:321:HIS:O	2.44	0.44
1:A:90:HIS:C	1:A:92:SER:N	2.69	0.44
1:B:59:LYS:HE2	1:B:59:LYS:HB2	1.47	0.44
1:A:231:ASP:OD1	1:A:232:TRP:N	2.50	0.44
1:A:120:VAL:HG22	1:A:121:ARG:N	2.33	0.44
1:B:137:VAL:HB	1:B:144:PHE:CE1	2.53	0.44
1:A:77:ILE:CG2	1:A:319:TYR:HB2	2.48	0.44
1:A:98:GLU:HG2	1:A:99:GLU:H	1.83	0.44
1:A:120:VAL:HG22	1:A:121:ARG:H	1.83	0.44
1:A:172:ILE:O	1:A:202:ARG:NH1	2.50	0.44
1:A:254:TRP:CD1	1:A:254:TRP:N	2.85	0.44
1:B:123:ALA:N	1:B:276:TRP:NE1	2.65	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:185:HIS:CD2	1:A:253:HIS:CD2	3.05	0.44
1:A:185:HIS:CD2	1:A:253:HIS:HD2	2.36	0.44
1:A:340:MET:O	1:A:341:ALA:HB3	2.18	0.44
1:B:192:ASP:O	1:B:196:VAL:HG23	2.17	0.43
1:A:132:HIS:HB3	1:A:133:ALA:H	1.61	0.43
1:A:219:MET:HB3	1:A:227:VAL:HG11	2.00	0.43
1:A:173:SER:HB2	1:B:97:LYS:HD2	1.99	0.43
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.77	0.43
1:A:126:ARG:HB3	1:A:138:GLU:OE2	2.18	0.43
1:A:159:TYR:HA	1:B:193:TYR:CE2	2.54	0.43
1:A:306:ILE:HG12	1:A:330:ILE:HG21	2.00	0.43
1:A:314:ARG:O	1:A:316:PHE:N	2.52	0.43
1:B:229:GLU:O	1:B:230:LEU:HD23	2.19	0.43
1:A:90:HIS:O	1:A:90:HIS:CG	2.71	0.43
1:B:205:ASN:OD1	1:B:225:GLU:HB2	2.19	0.43
1:A:67:ASN:CG	1:A:68:PRO:HD3	2.39	0.43
1:A:296:LYS:HA	1:A:296:LYS:NZ	2.34	0.43
1:A:353:HIS:CE1	1:A:355:LEU:HD12	2.53	0.43
1:A:228:ILE:HD12	1:A:236:ASN:ND2	2.33	0.42
1:A:209:TRP:HB2	1:A:227:VAL:HG12	2.01	0.42
1:A:218:TRP:NE1	4:A:404:DXC:H3	2.34	0.42
1:A:259:LEU:HB2	4:A:406:DXC:O2	2.19	0.42
1:A:299:GLY:HA2	1:A:300:PRO:C	2.40	0.42
1:A:77:ILE:HG22	1:A:319:TYR:CB	2.48	0.42
1:A:365:LEU:HD12	1:A:365:LEU:HA	1.72	0.42
1:B:207:LEU:O	1:B:226:ASN:HB3	2.19	0.42
1:A:185:HIS:CE1	1:A:284:ASP:HB2	2.55	0.42
1:B:235:GLU:HB3	1:B:247:VAL:CG2	2.47	0.42
1:B:341:ALA:HB3	1:B:377:VAL:HG12	2.01	0.42
1:A:175:LEU:HD22	1:A:176:PRO:HD2	2.01	0.42
4:A:404:DXC:H203	1:B:159:TYR:HB3	2.01	0.42
1:A:96:SER:HB2	1:A:99:GLU:HB2	2.02	0.42
1:A:131:GLY:O	1:A:132:HIS:C	2.58	0.42
1:B:314:ARG:NH2	1:B:318:LYS:HB2	2.35	0.42
1:A:81:LEU:CD2	1:A:86:MET:HB2	2.50	0.42
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.78	0.42
1:B:64:ARG:HG3	1:B:68:PRO:O	2.20	0.42
1:B:368:TYR:N	1:B:368:TYR:HD1	2.18	0.42
1:B:177:PRO:HA	1:B:203:PHE:HE2	1.85	0.42
1:B:215:LEU:O	1:B:219:MET:HG2	2.20	0.42
4:A:404:DXC:C20	1:B:159:TYR:HB3	2.50	0.41



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
1:B:69:TRP:CH2	1:B:213:LEU:HD23	2.55	0.41
1:B:82:ARG:HG2	4:B:607:DXC:H1	2.01	0.41
1:B:136:MET:HE2	1:B:176:PRO:HG2	2.01	0.41
1:A:77:ILE:HG21	1:A:319:TYR:CG	2.55	0.41
1:A:330:ILE:HD13	1:A:330:ILE:HA	1.83	0.41
4:A:405:DXC:H161	4:A:405:DXC:H212	1.81	0.41
1:B:62:ASP:HA	1:B:63:GLY:HA3	1.67	0.41
1:A:59:LYS:HE2	1:A:297:ARG:HB2	2.01	0.41
1:A:142:LEU:HD21	1:A:144:PHE:HB3	2.02	0.41
4:A:408:DXC:H222	4:A:408:DXC:H243	1.79	0.41
1:B:230:LEU:HD13	1:B:234:GLU:O	2.19	0.41
1:A:90:HIS:O	1:A:92:SER:N	2.53	0.41
1:B:330:ILE:O	1:B:334:VAL:HG23	2.20	0.41
4:A:407:DXC:H1	3:B:605:3PE:H2D2	2.02	0.41
1:B:57:SER:C	1:B:59:LYS:H	2.23	0.41
1:B:208:ARG:NH2	1:B:228:ILE:HD11	2.36	0.41
3:A:403:3PE:H232	3:A:403:3PE:H341	2.02	0.41
1:B:285:THR:HG21	1:B:291:PHE:CZ	2.56	0.41
1:B:364:ALA:O	1:B:367:ARG:HB2	2.20	0.41
1:B:120:VAL:HG13	1:B:122:GLU:N	2.36	0.41
1:A:384:ARG:HG2	1:A:386:LEU:CD2	2.50	0.41
1:A:96:SER:HB2	1:A:99:GLU:OE1	2.21	0.41
1:A:312:GLU:HG3	1:A:313:PRO:N	2.36	0.41
4:A:405:DXC:H61	4:A:408:DXC:H243	2.02	0.41
1:B:94:PRO:HA	1:B:354:TYR:CE1	2.56	0.41
1:B:142:LEU:CD1	1:B:244:VAL:HG11	2.50	0.41
1:B:191:LEU:HB3	1:B:257:ARG:HH21	1.86	0.41
1:B:215:LEU:HD22	1:B:218:TRP:HB3	2.03	0.41
1:B:218:TRP:HE3	1:B:219:MET:HE3	1.84	0.41
1:A:156:PRO:HB3	1:A:188:TYR:OH	2.21	0.41
1:A:212:PRO:O	1:A:229:GLU:HG2	2.20	0.41
1:B:285:THR:O	1:B:322:VAL:HG13	2.21	0.41
1:B:153:ARG:CG	1:B:155:SER:HB3	2.51	0.40
1:A:77:ILE:CG2	1:A:319:TYR:CB	2.99	0.40
1:A:324:PRO:O	1:A:328:VAL:HG23	2.21	0.40
1:B:232:TRP:CZ3	1:B:250:PRO:HA	2.56	0.40
1:A:120:VAL:CG1	1:A:121:ARG:HH21	2.34	0.40
1:B:111:PHE:HZ	1:B:170:CYS:HG	1.68	0.40
1:B:241:HIS:ND1	1:B:241:HIS:N	2.69	0.40
4:A:404:DXC:H181	4:A:407:DXC:C23	2.50	0.40
1:B:92:SER:HB3	1:B:354:TYR:HD1	1.85	0.40



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Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)	
3:B:605:3PE:H281	3:B:605:3PE:H3B2	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	Perc	$\mathbf{entiles}$
1	А	333/393~(85%)	274 (82%)	47 (14%)	12~(4%)	3	11
1	В	335/393~(85%)	296 (88%)	30~(9%)	9~(3%)	5	16
All	All	668/786~(85%)	570 (85%)	77 (12%)	21 (3%)	4	14

All (21) Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	78	PRO
1	А	119	GLY
1	В	66	VAL
1	В	85	ILE
1	В	312	GLU
1	В	313	PRO
1	А	58	LYS
1	А	91	SER
1	А	120	VAL
1	А	315[A]	TRP
1	А	315[B]	TRP
1	А	79	ASN
1	В	57	SER
1	В	89	ASP
1	А	59	LYS
1	В	67	ASN
1	В	95	SER



Continued from previous page...

Mol	Chain	Res	Type
1	А	344	TRP
1	В	344	TRP
1	А	67	ASN
1	А	313	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	ers Percen	
1	А	298/352~(85%)	255~(86%)	43 (14%)	3	8
1	В	299/352~(85%)	269~(90%)	30 (10%)	7	21
All	All	597/704~(85%)	524 (88%)	73~(12%)	5	13

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	58	LYS
1	А	59	LYS
1	А	61	LYS
1	А	62	ASP
1	А	67	ASN
1	А	69	TRP
1	А	73	LYS
1	А	80	VAL
1	А	81	LEU
1	А	82	ARG
1	А	88	LYS
1	А	90	HIS
1	А	121	ARG
1	А	125	LEU
1	А	132	HIS
1	А	134	THR
1	А	140	ASP
1	А	143	ILE
1	А	155	SER



Mol	Chain	Res	Type
1	А	165	PHE
1	А	167[A]	ARG
1	А	167[B]	ARG
1	А	179	ASP
1	А	230	LEU
1	А	232	TRP
1	А	241	HIS
1	А	243	LYS
1	А	254	TRP
1	А	257	ARG
1	А	262	ASP
1	А	288	CYS
1	А	296	LYS
1	А	297	ARG
1	А	302	ASP
1	А	312	GLU
1	А	314	ARG
1	А	320	GLN
1	А	343	HIS
1	А	344	TRP
1	А	365	LEU
1	А	366	GLU
1	А	374	ASP
1	А	387	ASN
1	В	59	LYS
1	В	61	LYS
1	В	65	PHE
1	В	66	VAL
1	В	67	ASN
1	В	73	LYS
1	В	81	LEU
1	В	82	ARG
1	В	89	ASP
1	В	97	LYS
1	В	121	ARG
1	В	126	ARG
1	В	157	SER
1	В	172	ILE
1	В	199	LEU
1	В	232	TRP
1	В	241	HIS
1	В	276	TRP



Mol	Chain	$\operatorname{Res}$	Type
1	В	287	TYR
1	В	288	CYS
1	В	303	LEU
1	В	313	PRO
1	В	314	ARG
1	В	317	MET
1	В	340	MET
1	В	343	HIS
1	В	351	ASN
1	В	375	PHE
1	В	384	ARG
1	В	386	LEU

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

Mol	Chain	Res	Type
1	А	200	ASN
1	А	220	GLN
1	А	252	GLN
1	А	277	ASN
1	А	351	ASN
1	А	362	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.



8PC4

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).

Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	DXC	В	607	-	31,31,31	0.63	0	49,49,49	1.07	4 (8%)
3	3PE	А	403	2	43,43,50	0.54	0	46,48,55	0.81	1 (2%)
4	DXC	А	404	-	31,31,31	0.70	0	49,49,49	1.21	4 (8%)
4	DXC	В	606	-	31,31,31	0.67	0	49,49,49	1.24	4 (8%)
4	DXC	А	405	-	31,31,31	0.58	0	49,49,49	1.01	2 (4%)
4	DXC	А	406	-	31,31,31	0.67	0	49,49,49	1.20	2 (4%)
4	DXC	В	601	-	31,31,31	0.64	1 (3%)	49,49,49	0.85	1 (2%)
3	3PE	В	605	2	43,43,50	0.52	0	46,48,55	0.90	1 (2%)
4	DXC	А	409	-	31,31,31	0.56	0	49,49,49	1.13	5 (10%)
4	DXC	В	602	-	31,31,31	0.64	0	49,49,49	1.46	7 (14%)
5	HCZ	В	608	-	18,18,18	1.36	3 (16%)	29,29,29	1.23	3 (10%)
4	DXC	А	408	-	31,31,31	0.53	0	49,49,49	1.04	1 (2%)
4	DXC	А	407	-	31,31,31	0.62	0	49,49,49	1.20	5 (10%)

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	DXC	В	607	-	-	8/9/71/71	0/4/4/4
3	3PE	А	403	2	-	24/47/47/54	-
4	DXC	А	404	-	-	5/9/71/71	0/4/4/4
4	DXC	В	606	-	-	3/9/71/71	0/4/4/4
4	DXC	А	405	-	-	4/9/71/71	0/4/4/4
4	DXC	А	406	-	-	9/9/71/71	0/4/4/4
4	DXC	В	601	-	-	0/9/71/71	0/4/4/4
3	3PE	В	605	2	-	24/47/47/54	-
4	DXC	А	409	-	-	6/9/71/71	0/4/4/4
4	DXC	В	602	-	-	5/9/71/71	0/4/4/4



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HCZ	В	608	-	-	6/6/19/19	0/2/2/2
4	DXC	А	408	-	-	8/9/71/71	0/4/4/4
4	DXC	А	407	-	-	0/9/71/71	0/4/4/4

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All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	В	608	HCZ	S02-N01	2.67	1.65	1.60
5	В	608	HCZ	S15-N14	2.44	1.66	1.63
4	В	601	DXC	C22-C23	2.14	1.55	1.50
5	В	608	HCZ	O17-S15	2.03	1.45	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	В	602	DXC	C12-C11-C9	-4.15	110.13	114.71
4	В	602	DXC	C11-C9-C10	-4.05	103.66	109.09
4	В	602	DXC	C8-C9-C10	3.48	114.81	110.49
4	В	606	DXC	C12-C17-C19	3.45	123.61	119.50
4	В	602	DXC	C15-C11-C12	3.38	106.87	103.55
4	А	406	DXC	C14-C10-C4	3.27	117.10	113.73
4	А	406	DXC	C16-C15-C11	-3.14	98.91	105.13
3	В	605	3PE	O12-P-O14	2.90	126.59	112.24
4	В	606	DXC	C21-C19-C17	-2.89	104.31	110.28
4	А	404	DXC	O1-C13-C14	2.80	114.83	109.12
4	А	404	DXC	C11-C12-C13	2.76	109.97	107.40
5	В	608	HCZ	C05-S02-N01	-2.75	103.21	108.28
4	А	404	DXC	O1-C13-C12	-2.65	106.56	111.03
3	А	403	3PE	O12-P-O14	2.55	124.85	112.24
4	В	602	DXC	C14-C13-C12	2.51	113.82	111.24
4	А	407	DXC	C12-C17-C19	2.51	122.49	119.50
5	В	608	HCZ	O03-S02-N01	2.48	111.04	107.36
4	А	409	DXC	C10-C14-C13	-2.47	111.03	114.30
4	А	409	DXC	C4-C10-C9	2.47	115.01	112.42
4	А	407	DXC	C2-C3-C4	2.46	115.27	112.66
4	А	407	DXC	C3-C2-C1	2.45	116.35	112.76
4	А	409	DXC	C16-C17-C12	-2.45	101.15	103.55
4	В	601	DXC	C20-C12-C17	-2.43	107.41	111.21
4	В	607	DXC	C4-C10-C9	2.37	114.91	112.42
4	А	408	DXC	C18-C4-C5	-2.31	104.54	108.26
4	В	606	DXC	C18-C4-C5	-2.22	104.68	108.26
4	А	407	DXC	C10-C4-C3	2.22	111.70	108.58



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	В	606	DXC	C22-C21-C19	2.22	118.57	114.52
5	В	608	HCZ	O16-S15-N14	-2.22	105.86	107.92
4	В	607	DXC	C16-C15-C11	-2.21	100.76	105.13
4	А	405	DXC	O1-C13-C14	2.17	113.55	109.12
4	В	607	DXC	O1-C13-C12	-2.14	107.42	111.03
4	А	407	DXC	C20-C12-C11	-2.12	107.90	111.21
4	А	404	DXC	C14-C10-C4	-2.11	111.55	113.73
4	А	409	DXC	C14-C13-C12	-2.11	109.08	111.24
4	А	405	DXC	O1-C13-C12	-2.10	107.48	111.03
4	В	602	DXC	C10-C14-C13	2.08	117.05	114.30
4	В	602	DXC	C4-C10-C9	2.06	114.58	112.42
4	B	607	DXC	C18-C4-C5	-2.03	104.99	108.26
4	А	409	DXC	C17-C12-C13	2.01	119.50	117.67

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	403	3PE	C1-O11-P-O12
3	А	403	3PE	C11-O13-P-O14
3	А	403	3PE	O13-C11-C12-N
3	В	605	3PE	C1-O11-P-O12
3	В	605	3PE	C11-O13-P-O12
3	В	605	3PE	O13-C11-C12-N
4	А	409	DXC	C19-C21-C22-C23
5	В	608	HCZ	C10-C05-S02-N01
5	В	608	HCZ	C10-C05-S02-O03
5	В	608	HCZ	C10-C05-S02-O04
4	А	408	DXC	C24-C19-C21-C22
4	А	406	DXC	C19-C21-C22-C23
3	А	403	3PE	C38-C39-C3A-C3B
3	А	403	3PE	O32-C31-O31-C3
3	В	605	3PE	O32-C31-O31-C3
3	В	605	3PE	C38-C39-C3A-C3B
3	В	605	3PE	C32-C31-O31-C3
4	А	405	DXC	C17-C19-C21-C22
3	А	403	3PE	C32-C31-O31-C3
4	В	607	DXC	C24-C19-C21-C22
4	A	408	DXC	C12-C17-C19-C21
4	A	404	DXC	C24-C19-C21-C22
4	А	409	DXC	C24-C19-C21-C22
3	В	605	3PE	C29-C2A-C2B-C2C



Mol	Chain	Res	Type	Atoms
4	А	406	DXC	C17-C19-C21-C22
4	А	405	DXC	C24-C19-C21-C22
4	А	406	DXC	C24-C19-C21-C22
3	А	403	3PE	C1-O11-P-O13
3	В	605	3PE	C1-O11-P-O13
3	В	605	3PE	C11-O13-P-O11
4	А	408	DXC	C12-C17-C19-C24
3	А	403	3PE	C21-C22-C23-C24
4	А	408	DXC	C17-C19-C21-C22
3	А	403	3PE	C29-C2A-C2B-C2C
4	В	602	DXC	C19-C21-C22-C23
4	В	606	DXC	C24-C19-C21-C22
4	А	408	DXC	C16-C17-C19-C24
5	В	608	HCZ	C06-C05-S02-O03
5	В	608	HCZ	C06-C05-S02-O04
4	А	408	DXC	C16-C17-C19-C21
3	В	605	3PE	C37-C38-C39-C3A
3	В	605	3PE	C3A-C3B-C3C-C3D
3	А	403	3PE	C23-C24-C25-C26
3	А	403	3PE	C11-O13-P-O11
3	А	403	3PE	C33-C34-C35-C36
3	В	605	3PE	C32-C33-C34-C35
3	А	403	3PE	C2B-C2C-C2D-C2E
3	В	605	3PE	C2B-C2C-C2D-C2E
5	В	608	HCZ	C06-C05-S02-N01
3	А	403	3PE	C32-C33-C34-C35
3	А	403	3PE	C27-C28-C29-C2A
4	В	602	DXC	C16-C17-C19-C24
3	А	403	3PE	C3A-C3B-C3C-C3D
3	В	605	3PE	C27-C28-C29-C2A
3	А	403	3PE	O11-C1-C2-O21
3	А	403	3PE	C36-C37-C38-C39
3	А	403	3PE	O11-C1-C2-C3
3	В	605	3PE	O11-C1-C2-C3
3	В	605	3PE	O11-C1-C2-O21
4	В	$\overline{602}$	DXC	C12-C17-C19-C24
3	В	605	3PE	C36-C37-C38-C39
4	В	607	DXC	C19-C21-C22-C23
3	A	403	3PE	C1-O11-P-O14
3	A	403	3PE	C11-O13-P-O12
3	В	605	3PE	C1-O11-P-O14
3	В	605	3PE	C11-O13-P-O14

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$\mathbf{Mol}$	Chain	Res	Type	Atoms	
4	В	602	DXC	C16-C17-C19-C21	
4	А	406	DXC	C16-C17-C19-C21	
4	В	607	DXC	C16-C17-C19-C21	
4	А	406	DXC	C12-C17-C19-C24	
4	А	406	DXC	C12-C17-C19-C21	
4	А	404	DXC	C12-C17-C19-C24	
4	В	607	DXC	C12-C17-C19-C24	
4	В	607	DXC	C12-C17-C19-C21	
4	В	602	DXC	C12-C17-C19-C21	
4	В	607	DXC	C16-C17-C19-C24	
4	А	406	DXC	C16-C17-C19-C24	
4	А	406	DXC	C21-C22-C23-O4	
4	В	607	DXC	C21-C22-C23-O3	
4	А	408	DXC	C21-C22-C23-O4	
4	В	607	DXC	C21-C22-C23-O4	
4	А	406	DXC	C21-C22-C23-O3	
4	А	404	DXC	C21-C22-C23-O3	
4	А	408	DXC	C21-C22-C23-O3	
4	А	409	DXC	C12-C17-C19-C24	
4	А	404	DXC	C12-C17-C19-C21	
3	В	605	3PE	C23-C24-C25-C26	
3	А	403	3PE	C3C-C3D-C3E-C3F	
4	А	404	DXC	C21-C22-C23-O4	
3	А	403	3PE	O31-C31-C32-C33	
4	А	409	DXC	C21-C22-C23-O4	
3	В	605	3PE	O31-C31-C32-C33	
4	А	409	DXC	C21-C22-C23-O3	
4	А	405	DXC	C21-C22-C23-O4	
4	В	606	DXC	C21-C22-C23-O4	
3	В	605	3PE	C26-C27-C28-C29	
3	А	403	3PE	O32-C31-C32-C33	
3	В	605	3PE	O32-C31-C32-C33	
4	А	405	DXC	C21-C22-C23-O3	
4	В	606	DXC	C21-C22-C23-O3	
4	А	409	DXC	C12-C17-C19-C21	
3	В	605	3PE	O21-C21-C22-C23	

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There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	607	DXC	3	0
				<i>a</i> .:	7 1



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	403	3PE	6	0
4	А	404	DXC	6	0
4	А	405	DXC	5	0
4	А	406	DXC	3	0
4	В	601	DXC	2	0
3	В	605	3PE	5	0
4	А	409	DXC	5	0
4	В	602	DXC	5	0
5	В	608	HCZ	1	0
4	А	408	DXC	2	0
4	А	407	DXC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.























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### 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	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	332/393~(84%)	0.55	34 (10%) 6 4	69, 105, 151, 183	0
1	В	334/393~(84%)	0.38	23 (6%) 16 12	62, 87, 142, 174	0
All	All	666/786~(84%)	0.46	57 (8%) 10 7	62, 97, 147, 183	0

All (57) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	В	88	LYS	9.8
1	В	85	ILE	9.1
1	А	72[A]	TRP	7.3
1	А	59	LYS	6.1
1	В	89	ASP	5.9
1	А	244	VAL	5.1
1	А	83	TRP	5.0
1	В	72	TRP	4.6
1	А	82	ARG	4.4
1	А	89	ASP	4.3
1	В	92	SER	4.1
1	В	233	TRP	4.1
1	В	84	LEU	3.9
1	В	83	TRP	3.9
1	А	121	ARG	3.8
1	А	79	ASN	3.7
1	А	88	LYS	3.6
1	А	287	TYR	3.5
1	А	69	TRP	3.5
1	А	298	PHE	3.4
1	А	388	ASN	3.3
1	А	57	SER	3.2
1	В	100	LEU	3.1
1	В	69	TRP	3.1



Mol	Chain	Res	Type	RSRZ
1	В	65	PHE	3.1
1	А	142	LEU	3.0
1	А	87	GLU	3.0
1	В	87	GLU	3.0
1	А	85	ILE	2.9
1	В	230	LEU	2.9
1	А	294	ILE	2.8
1	В	86	MET	2.7
1	В	59	LYS	2.7
1	В	297	ARG	2.7
1	В	237	CYS	2.7
1	А	301	PHE	2.6
1	А	233	TRP	2.6
1	А	90	HIS	2.6
1	А	273	LEU	2.6
1	А	77	ILE	2.5
1	В	97	LYS	2.5
1	А	93	VAL	2.5
1	А	340	MET	2.5
1	А	144	PHE	2.4
1	В	91	SER	2.4
1	А	125	LEU	2.4
1	В	298	PHE	2.3
1	А	314	ARG	2.3
1	А	363	GLU	2.2
1	В	93	VAL	2.2
1	A	315[A]	TRP	2.2
1	A	65	PHE	2.1
1	В	236	ASN	2.1
1	В	367	ARG	2.1
1	A	248	PHE	2.1
1	A	139	MET	2.0
1	A	319	TYR	2.0

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#### 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
4	DXC	В	607	28/28	0.72	0.40	114,118,130,137	0
5	HCZ	В	608	17/17	0.73	0.42	109,126,141,146	0
4	DXC	А	409	28/28	0.74	0.37	129,138,157,159	0
4	DXC	А	406	28/28	0.87	0.36	92,98,102,103	28
4	DXC	В	606	28/28	0.91	0.28	86,91,105,113	0
4	DXC	А	404	28/28	0.91	0.25	81,85,99,102	0
4	DXC	А	405	28/28	0.91	0.24	87,94,100,106	0
4	DXC	В	602	28/28	0.93	0.28	83,88,92,96	28
4	DXC	В	601	28/28	0.93	0.28	77,83,86,87	0
4	DXC	А	408	28/28	0.94	0.21	74,79,92,101	0
4	DXC	А	407	28/28	0.95	0.23	77,81,84,86	0
3	3PE	В	605	44/51	0.96	0.30	80,89,95,96	0
3	3PE	А	403	44/51	0.96	0.24	82,90,95,98	0
2	ZN	А	402	1/1	0.98	0.22	88,88,88,88	0
2	ZN	В	603	1/1	0.98	0.21	82,82,82,82	0
2	ZN	A	401	1/1	0.98	0.18	85,85,85,85	0
2	ZN	B	604	1/1	0.99	0.21	89,89,89,89	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.

