

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

#### May 15, 2020 – 03:30 pm BST

PDB ID	:	4DSA
$\operatorname{Title}$	:	Crystal Structure of DPP-IV with Compound C1
Authors	:	Xiong, B.; Zhu, L.R.; Chen, D.Q.; Zhao, Y.L.; Jiang, F.; Shen, J.K.
Deposited on	:	2012-02-18
Resolution	:	3.25  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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 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 <sub>free</sub>	130704	$1191 \ (3.30-3.22)$		
Clashscore	141614	1251 (3.30-3.22)		
Ramachandran outliers	138981	1229 (3.30-3.22)		
Sidechain outliers	138945	1228 (3.30-3.22)		
RSRZ outliers	127900	1154 (3.30-3.22)		

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 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	728	3% 73%	23%	••		
1	В	728	72%	25%	••		



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11891 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	724	Total 5931	$ m C \ 3807$	N 975	O 1123	S 26	0	0	0
1	В	724	Total 5931	$ m C \\ 3807$	N 975	O 1123	S 26	0	0	0

• Molecule 2 is  $4-[(\{[(2R)-2-amino-3-(2,4,5-trifluorophenyl)propyl]sulfamoyl\}amino)methyl]$ be nzenesulfonamide (three-letter code: D1C) (formula:  $C_{16}H_{19}F_3N_4O_4S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	А	1	Total 29	C 16	F 3	N 4	0 4	${ m S} { m 2}$	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: Dipeptidyl peptidase 4

#### 7364 1365 1366 P478 L479 0339 1.340 W402 E403 390 390 E361 T600 F601 /480 1626 W627 G628 P676 E677 D678 N679 L680 <mark>V724</mark> D725 V726 G727 I751 <u>Y752</u> E602 F695 R69: L70 W735 LEU PRO



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants	78.68Å 78.68Å 289.85Å	Deneiten
$\mathrm{a,b,c,\alpha,\beta,\gamma}$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}\left(\hat{\boldsymbol{\lambda}}\right)$	29.37 - 3.25	Depositor
Resolution (A)	29.37 - 3.25	EDS
% Data completeness	97.2 (29.37-3.25)	Depositor
(in resolution range)	$97.3\ (29.37‐3.25)$	EDS
$R_{merge}$	0.07	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.09 (at 3.24 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
B B .	0.198 , $0.266$	Depositor
$n, n_{free}$	0.193 , $0.265$	DCC
$R_{free}$ test set	1544 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	122.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , $93.4$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.34$	Xtriage
	0.000 for -h,-k,l	
Estimated twinning fraction	0.056  for  h,-h-k,-l	Xtriage
	0.024 for -k,-h,-l	
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11891	wwPDB-VP
Average B, all atoms $(Å^2)$	144.0	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:  $\rm D1C$ 

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	Bo	ond lengths	Bond angles		
10101		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.61	13/6102~(0.2%)	0.67	0/8299	
1	В	0.62	10/6102~(0.2%)	0.67	0/8299	
All	All	0.61	23/12204~(0.2%)	0.67	0/16598	

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	337	TRP	CD2-CE2	6.13	1.48	1.41
1	А	157	TRP	CD2-CE2	5.96	1.48	1.41
1	В	337	TRP	CD2-CE2	5.92	1.48	1.41
1	В	563	TRP	CD2-CE2	5.69	1.48	1.41
1	А	187	TRP	CD2-CE2	5.65	1.48	1.41
1	А	154	TRP	CD2-CE2	5.53	1.48	1.41
1	В	157	TRP	CD2-CE2	5.52	1.48	1.41
1	В	525	TRP	CD2-CE2	5.51	1.48	1.41
1	А	315	TRP	CD2-CE2	5.50	1.48	1.41
1	А	627	TRP	CD2-CE2	5.47	1.48	1.41
1	А	62	TRP	CD2-CE2	5.44	1.47	1.41
1	В	154	TRP	CD2-CE2	5.42	1.47	1.41
1	В	187	TRP	CD2-CE2	5.38	1.47	1.41
1	В	734	TRP	CD2-CE2	5.30	1.47	1.41
1	В	305	TRP	CD2-CE2	5.27	1.47	1.41
1	В	315	TRP	CD2-CE2	5.25	1.47	1.41
1	А	734	TRP	CD2-CE2	5.21	1.47	1.41
1	В	353	TRP	CD2-CE2	5.12	1.47	1.41
1	А	353	TRP	CD2-CE2	5.10	1.47	1.41
1	A	305	TRP	CD2-CE2	5.10	1.47	1.41
1	A	525	TRP	CD2-CE2	5.06	1.47	1.41
1	A	168	TRP	CD2-CE2	5.03	1.47	1.41
1	A	216	TRP	CD2-CE2	5.00	1.47	1.41



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	5931	0	5649	118	0
1	В	5931	0	5649	121	0
2	А	29	0	19	0	0
All	All	11891	0	11317	231	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 10.

All (231) 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	${ m distance}~({ m \AA})$	overlap (Å)
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.52	0.90
1:B:175:LYS:HG3	1:B:182:SER:HB3	1.56	0.86
1:B:383:HIS:HD2	1:B:399:LYS:HA	1.41	0.85
1:A:383:HIS:HD2	1:A:399:LYS:HA	1.41	0.84
1:A:383:HIS:CD2	1:A:399:LYS:HA	2.15	0.81
1:B:383:HIS:CD2	1:B:399:LYS:HA	2.14	0.80
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.61	0.80
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.63	0.79
1:A:253:ARG:HH12	1:B:253:ARG:HH12	1.35	0.74
1:A:43:TYR:CD2	1:A:565:THR:HG22	2.21	0.74
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.70	0.72
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.26	0.71
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.73	0.70
1:A:369:ASN:HA	1:A:389:ILE:HD12	1.72	0.70
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.26	0.70
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.75	0.69
1:B:369:ASN:HA	1:B:389:ILE:HD12	1.73	0.69
1:B:516:PHE:HD1	1:B:523:LYS:HB2	1.57	0.68
1:A:149:PRO:HG2	1:A:168:TRP:CD1	2.27	0.68



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlan (Å)	
1·A·340·LEU·HB2	1·A·343·ABG·HD2	1 76	0.68	
1:B:522:THB:HG21	1:B:590:ILE:HD11	1.77	0.67	
1.B.596.ABG.NH2	$1 \cdot B \cdot 678 \cdot ASP \cdot OD1$	2.28	0.66	
1:B:115:LEU:HD21	1:B:155:VAL:HG11	1 76	0.66	
1:B:43:TYB:CD2	1:B:565:THB:HG22	2 29	0.66	
1.A.516.PHE.HD1	$1 \cdot A \cdot 523 \cdot LYS \cdot HB2$	1.61	0.66	
1.B.149.PRO.HG2	$1 \cdot B \cdot 168 \cdot TBP \cdot CD1$	2 29	0.66	
1.A.382.ABG.H	1.A.403.GLU.HG2	1 61	0.65	
1·B·232·GLU·HB2	1.B.262.VAL.HG11	1.01	0.65	
1.B.382.ABG.H	1.B.202.011L.HG11	1.0	0.65	
$1 \cdot B \cdot 195 \cdot TYB \cdot HB2$	1.B.228.PHE.HB2	1.00	0.64	
$1 \cdot \underline{A} \cdot \underline{290} \cdot \underline{PR0} \cdot \underline{HD3}$	1:A:326:ASP:OD2	1.15	0.01	
1.R.250.1 RO.HD0	1.R.480.LVS.HE2	1.50	0.00	
$1.\Delta.403.\text{GLU}.\text{OE1}$	$\frac{1.0.405.0105.012}{1.0.585.000}$	1.00	0.00	
1.R.340.1 FU.HB2	1.R.3/3·ABC·HD2	1.95	0.00	
1.D.340.DE0.IID2	1. A • 969 · VAI • HC11	1.81	0.03	
1.A.232.GLU.IID2	1.A.202.VAL.IIG11	1.82	0.02	
1.A.720.VAL.IIG23	1.A. 720. VAL.IIG23	1.02	0.02	
1.D.231.1 II.II. 1.A.115.1 FU.HD91	1.1.232.GLU.IIG3	1.02	0.01	
$1:A:110:LEU:\Pi D21$	1.A.155.VAL.HGI1	1.00	0.01	
1:A:040:LEU:HD11	1:A:000:GLY:HA3	1.85	0.60	
1:A:100:A5N:U	1:A:101:A5N:HB2	2.01	0.60	
1:A:55:LEU:HD22	1:A:478:PRO:HG2	1.84	0.60	
1:A:487:ASN:HD21	1:A:489:LY S:HE2	1.67	0.60	
1:A:195:1YR:HB2	1:A:228:PHE:HB2	1.85	0.59	
1:A:364:PHE:CD1	1:A:371:PHE:HB3	2.37	0.59	
1:B:146:GLU:O	I:B:175:LYS:NZ	2.34	0.59	
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.85	0.59	
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.38	0.59	
1:B:115:LEU:HD21	1:B:155:VAL:CG1	2.33	0.59	
1:A:231:THR:HG22	1:A:232:GLU:HG3	1.84	0.59	
1:B:598:LEU:HD22	1:B:631:TYR:OH	2.03	0.59	
1:B:170:ASN:O	1:B:196:ASN:HB2	2.04	0.58	
1:B:163:LYS:NZ	1:B:220:GLY:O	2.34	0.58	
1:A:482:LEU:HD23	1:A:483:HIS:H	1.69	0.58	
1:A:107:ILE:HG13	1:A:114:ILE:HG13	1.86	0.58	
1:B:383:HIS:HE1	1:B:402:TRP:O	1.86	0.58	
1:A:383:HIS:HE1	1:A:402:TRP:O	1.87	0.57	
1:B:107:ILE:HG13	1:B:114:ILE:HG13	1.86	0.57	
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.39	0.57	
1:A:163:LYS:NZ	1:A:220:GLY:O	2.33	0.57	
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.05	0.57	



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:600:THR:OG1	1:A:601:PHE:N	2.38	0.56
1:B:482:LEU:HD23	1:B:483:HIS:H	1.70	0.56
1:B:385:CYS:HB3	1:B:387:PHE:HE1	1.70	0.56
1:A:115:LEU:HD21	1:A:155:VAL:CG1	2.35	0.56
1:B:290:PRO:HD3	1:B:326:ASP:OD2	2.05	0.56
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.38	0.56
1:B:364:PHE:CD1	1:B:371:PHE:HB3	2.41	0.56
1:A:258:LYS:HD2	1:B:248:TYR:CE1	2.41	0.55
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.06	0.55
1:A:88:VAL:HG21	1:A:91:GLU:HG2	1.88	0.55
1:B:516:PHE:HD2	1:B:516:PHE:H	1.54	0.55
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.88	0.55
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.42	0.54
1:B:88:VAL:HG21	1:B:91:GLU:HG2	1.90	0.54
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.43	0.54
1:A:636:THR:HG21	1:A:651:ILE:O	2.08	0.53
1:B:74:ASN:HB3	1:B:92:ASN:HB2	1.90	0.53
1:A:528:MET:HE1	1:A:530:LEU:HD21	1.90	0.53
1:B:55:LEU:HD22	1:B:478:PRO:HG2	1.91	0.53
1:A:216:TRP:HZ3	1:A:273:THR:HG21	1.73	0.53
1:B:540:TYR:N	1:B:618:PHE:O	2.33	0.53
1:B:216:TRP:HZ3	1:B:273:THR:HG21	1.74	0.53
1:B:516:PHE:CD1	1:B:523:LYS:HB2	2.42	0.53
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.90	0.52
1:A:516:PHE:H	1:A:516:PHE:HD2	1.56	0.52
1:B:580:GLY:O	1:B:583:SER:OG	2.26	0.52
1:A:74:ASN:HB3	1:A:92:ASN:HB2	1.92	0.52
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.09	0.52
1:B:113:PHE:CZ	1:B:178:PRO:HG2	2.45	0.52
1:B:594:ILE:HD11	1:B:602:GLU:OE1	2.09	0.51
1:B:600:THR:OG1	1:B:601:PHE:N	2.43	0.51
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.11	0.51
1:A:385:CYS:HB3	1:A:387:PHE:HE1	1.71	0.51
1:A:750:HIS:CD2	1:B:724:VAL:HG22	2.46	0.51
1:B:538:LYS:O	1:B:618:PHE:HA	2.11	0.51
1:B:334:SER:OG	1:B:336:ARG:HG2	2.11	0.51
1:B:594:ILE:HD11	1:B:602:GLU:H	1.76	0.51
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.46	0.50
1:A:146:GLU:O	1:A:175:LYS:NZ	2.42	0.50
1:B:191:GLU:O	1:B:193:ILE:HG13	2.11	0.50
1:A:224:ALA:HB1	1:A:268:PHE:HZ	1.74	0.50



	t a c	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.42	0.50
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.47	0.50
1:B:224:ALA:HB1	1:B:268:PHE:HZ	1.75	0.50
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.12	0.50
1:A:402:TRP:NE1	1:A:421:GLU:HG3	2.27	0.50
1:A:461:PHE:CD1	1:A:468:TYR:HB3	2.47	0.50
1:A:594:ILE:HD11	1:A:602:GLU:H	1.77	0.50
1:B:330:TYR:CE1	1:B:335:GLY:HA2	2.47	0.50
1:A:594:ILE:HD11	1:A:602:GLU:OE1	2.12	0.49
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.43	0.49
1:A:538:LYS:O	1:A:618:PHE:HA	2.13	0.49
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.12	0.49
1:A:258:LYS:HD2	1:B:248:TYR:CZ	2.48	0.49
1:B:402:TRP:NE1	1:B:421:GLU:HG3	2.28	0.49
1:B:68:TYR:HE2	1:B:482:LEU:HD11	1.77	0.49
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.48	0.49
1:B:640:LEU:HB3	1:B:698:VAL:HG21	1.95	0.49
1:A:195:TYR:HB3	1:A:198:ILE:O	2.13	0.48
1:B:169:ASN:O	1:B:170:ASN:HB2	2.13	0.48
1:A:65:ASP:O	1:A:466:LYS:HB2	2.13	0.48
1:A:68:TYR:HE2	1:A:482:LEU:HD11	1.78	0.48
1:A:701:LEU:HA	1:A:731:GLN:HB2	1.95	0.48
1:B:125:ARG:HD2	1:B:126:HIS:NE2	2.28	0.48
1:B:235:LEU:HD13	1:B:253:ARG:HB3	1.95	0.48
1:B:516:PHE:HD1	1:B:523:LYS:CB	2.25	0.48
1:A:235:LEU:HD13	1:A:253:ARG:HB3	1.94	0.48
1:A:334:SER:OG	1:A:336:ARG:HG2	2.13	0.48
1:A:237:GLU:HG2	1:A:253:ARG:CG	2.44	0.48
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.43	0.48
1:A:594:ILE:HA	1:A:594:ILE:HD12	1.78	0.48
1:A:714:GLN:HA	1:B:241:TYR:CE1	2.48	0.48
1:B:184:ARG:HH21	1:B:187:TRP:HA	1.79	0.48
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.95	0.48
1:B:150:ASN:O	1:B:151:ASN:HB2	2.14	0.47
1:A:248:TYR:CE1	1:B:258:LYS:HD2	2.49	0.47
1:B:735:TYR:OH	1:B:751:ILE:HA	2.13	0.47
1:A:598:LEU:HD22	1:A:631:TYR:OH	2.15	0.47
1:B:365:THR:O	1:B:368:GLY:N	2.46	0.47
1:A:522:THR:HG21	1:A:590:ILE:HD11	1.96	0.47
1:A:516:PHE:CD1	1:A:523:LYS:HB2	2.46	0.47
1:B:594:ILE:HD12	1:B:594:ILE:HA	1.82	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:524:PHE:HE1	1:A:590:ILE:HG12	1.80	0.47
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.29	0.47
1:B:528:MET:HE2	1:B:528:MET:HB3	1 74	0.46
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.96	0.46
1:B:524:PHE:HE1	1:B:590:ILE:HG12	1.81	0.46
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.50	0.46
1:A:528:MET:HE2	1:A:528:MET:HB3	1.68	0.46
1:A:402:TRP:CD1	1:A:421:GLU:HG3	2.50	0.46
1:A:644:SER:O	1:A:646:VAL:N	2.49	0.46
1:A:305:TRP:CZ2	1:A:311:ILE:HD12	2.51	0.45
1:A:170:ASN:O	1:A:196:ASN:HB2	2.16	0.45
1:A:159:PRO:HD3	1:A:216:TRP:CG	2.51	0.45
1:A:184:ARG:HH21	1:A:187:TRP:HA	1.82	0.45
1:A:461:PHE:CE1	1:A:468:TYR:HB3	2.52	0.45
1:A:509:MET:O	1:A:532:PRO:HB3	2.17	0.45
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.46	0.45
1:B:383:HIS:CE1	1:B:402:TRP:O	2.69	0.45
1:A:528:MET:CE	1:A:530:LEU:HD21	2.46	0.45
1:A:735:TYR:OH	1:A:751:ILE:HA	2.17	0.45
1:B:153:GLN:OE1	1:B:198:ILE:HD13	2.17	0.45
1:B:471:ARG:HD3	1:B:480:TYR:CE2	2.52	0.44
1:A:72:GLN:O	1:A:74:ASN:N	2.50	0.44
1:B:117:GLU:OE1	1:B:128:TYR:HE1	2.00	0.44
1:A:725:ASP:HA	1:B:746:THR:HG21	1.99	0.44
1:A:383:HIS:CE1	1:A:402:TRP:O	2.69	0.44
1:A:241:TYR:CE1	1:B:714:GLN:HA	2.52	0.44
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.17	0.44
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.99	0.44
1:B:48:TYR:CE1	1:B:562:ASN:HA	2.53	0.44
1:A:330:TYR:CE1	1:A:335:GLY:HA2	2.53	0.44
1:A:531:PRO:HB3	1:A:572:ASN:HA	2.00	0.44
1:A:43:TYR:CD2	1:A:565:THR:CG2	2.97	0.44
1:B:676:PRO:HD2	1:B:677:GLU:OE1	2.18	0.44
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.84	0.43
1:B:482:LEU:HD12	1:B:494:LEU:HD21	2.00	0.43
1:A:369:ASN:HA	1:A:389:ILE:CD1	2.44	0.43
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.48	0.43
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.53	0.43
1:A:516:PHE:HD1	1:A:523:LYS:CB	2.30	0.43
1:B:95:PHE:HB3	1:B:98:PHE:HB2	2.00	0.43
1:B:162:HIS:NE2	1:B:177:GLU:OE1	2.51	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:84:GLY:HA3	1:A:492:ARG:HH22	1.83	0.43	
1:A:658:ARG:HB2	1:A:689:MET:CE	2.49	0.43	
1:B:237:GLU:HG2	1:B:253:ARG:CG	2.41	0.43	
1:B:734:TRP:C	1:B:734:TRP:CD1	2.90	0.43	
1:A:169:ASN:O	1:A:170:ASN:HB2	2.19	0.42	
1:A:48:TYR:CE1	1:A:562:ASN:HA	2.54	0.42	
1:B:701:LEU:HA	1:B:731:GLN:HB2	2.00	0.42	
1:B:65:ASP:O	1:B:466:LYS:HB2	2.19	0.42	
1:A:446:SER:HA	1:A:449:LEU:HG	2.01	0.42	
1:B:468:TYR:CE2	1:B:483:HIS:HB2	2.54	0.42	
1:B:72:GLN:O	1:B:74:ASN:N	2.51	0.42	
1:A:301:CYS:SG	1:A:359:PRO:HD2	2.59	0.42	
1:A:45:LEU:HG	1:A:49:LEU:HD22	2.01	0.42	
1:B:528:MET:CE	1:B:574:ILE:HG21	2.50	0.42	
1:A:677:GLU:N	1:A:677:GLU:OE1	2.51	0.42	
1:B:256:TYR:CZ	1:B:663:ASP:HB3	2.54	0.42	
1:A:471:ARG:HD3	1:A:480:TYR:CE2	2.55	0.42	
1:B:195:TYR:HB3	1:B:198:ILE:O	2.19	0.42	
1:B:109:PRO:HG2	1:B:158:SER:O	2.18	0.42	
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.55	0.42	
1:B:735:TYR:CE2	1:B:751:ILE:HG13	2.55	0.41	
1:A:612:GLN:O	1:A:616:MET:HG3	2.20	0.41	
1:A:540:TYR:N	1:A:618:PHE:O	2.36	0.41	
1:A:256:TYR:CZ	1:A:663:ASP:HB3	2.55	0.41	
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.50	0.41	
1:A:365:THR:O	1:A:368:GLY:N	2.53	0.41	
1:A:95:PHE:HB3	1:A:98:PHE:HB2	2.02	0.41	
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.19	0.41	
1:A:676:PRO:HD2	1:A:677:GLU:OE1	2.21	0.41	
1:A:562:ASN:O	1:A:565:THR:HB	2.20	0.41	
1:B:157:TRP:HA	1:B:163:LYS:O	2.21	0.41	
1:B:369:ASN:HA	1:B:389:ILE:CD1	2.46	0.41	
1:B:191:GLU:C	1:B:193:ILE:H	2.24	0.41	
1:B:641:GLY:O	1:B:691:ARG:HB3	2.21	0.41	
1:A:383:HIS:CD2	1:A:399:LYS:CA	2.98	0.41	
1:B:612:GLN:O	1:B:616:MET:HG3	2.21	0.41	
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.99	0.41	
1:A:302:ASP:HB3	1:A:314:GLN:HB2	2.03	0.40	
1:A:509:MET:HB3	1:A:509:MET:HE2	1.98	0.40	
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.40	
1:A:117:GLU:OE1	1:A:128:TYR:HE1	2.05	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.40
1:B:461:PHE:CE1	1:B:468:TYR:HB3	2.57	0.40
1:B:695:PHE:HB3	1:B:728:VAL:HG11	2.04	0.40
1:B:752:TYR:HA	1:B:755:MET:HE2	2.02	0.40
1:B:113:PHE:CE2	1:B:178:PRO:HG2	2.56	0.40
1:B:631:TYR:O	1:B:634:TYR:HB3	2.20	0.40
1:B:356:ARG:HD3	1:B:551:CYS:SG	2.61	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	Pe	erce	entiles
1	А	722/728~(99%)	643~(89%)	69~(10%)	10 (1%)		11	40
1	В	722/728~(99%)	640 (89%)	75 (10%)	7 (1%)		15	47
All	All	1444/1456~(99%)	1283 (89%)	144 (10%)	17 (1%)		13	43

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	178	PRO
1	А	644	SER
1	А	645	GLY
1	В	169	ASN
1	В	178	PRO
1	В	644	SER
1	А	73	GLU
1	А	169	ASN
1	А	341	VAL
1	А	551	CYS
1	А	760	LYS



Continued from previous page...

Mol	Chain	$\mathbf{Res}$	Type
1	В	73	GLU
1	А	565	THR
1	В	551	CYS
1	А	279	VAL
1	В	279	VAL
1	В	450	ASN

#### 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	Perce	ntiles
1	А	649/653~(99%)	615~(95%)	34~(5%)	23	53
1	В	649/653~(99%)	613 (94%)	36 (6%)	21	52
All	All	1298/1306~(99%)	1228~(95%)	70~(5%)	22	53

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	49	LEU
1	А	51	ASN
1	А	87	SER
1	А	156	THR
1	А	180	LEU
1	А	182	SER
1	А	231	THR
1	А	242	SER
1	А	244	GLU
1	А	288	THR
1	А	301	CYS
1	А	312	SER
1	А	329	ASP
1	А	361	GLU
1	А	366	LEU
1	А	382	ARG
1	А	385	CYS



Mol	Chain	Res	Type
1	А	390	ASP
1	А	410	LEU
1	А	412	SER
1	А	425	MET
1	А	443	THR
1	А	450	ASN
1	А	471	ARG
1	А	479	LEU
1	А	482	LEU
1	А	486	VAL
1	А	506	ASN
1	А	516	PHE
1	А	522	THR
1	A	618	PHE
1	А	627	TRP
1	A	704	HIS
1	A	751	ILE
1	В	49	LEU
1	В	51	ASN
1	В	87	SER
1	В	156	THR
1	В	169	ASN
1	В	180	LEU
1	В	182	SER
1	В	211	TYR
1	В	231	THR
1	В	242	SER
1	В	244	GLU
1	В	284	SER
1	В	288	THR
1	B	299	TYR
1	B	329	ASP
1	B	361	GLU
1	B	366	LEU
1	B	385	CYS
1	В	390	ASP
1	В	410	LEU
1	В	425	MET
1	B	443	THR
1	В	449	LEU
1	В	450	ASN
1	В	471	ARG



Mol	Chain	Res	Type
1	В	472	CYS
1	В	479	LEU
1	В	482	LEU
1	В	486	VAL
1	В	506	ASN
1	В	516	PHE
1	В	618	PHE
1	В	627	TRP
1	В	704	HIS
1	В	751	ILE
1	В	757	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	138	ASN
1	А	247	GLN
1	А	430	ASN
1	А	748	HIS
1	В	66	HIS
1	В	138	ASN
1	В	247	GLN

#### 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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

1 ligand is 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).

Mal	Mol Type Chain	Chain Bes Lin		Tink	Bond lengths			Bond angles		
Mol Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
2	D1C	А	800	-	29,30,30	<mark>5.39</mark>	11 (37%)	36,44,44	2.33	8 (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	D1C	А	800	-	-	7/21/22/22	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	А	800	D1C	SBA-NAZ	-17.48	1.40	1.61
2	А	800	D1C	SBA-NAL	14.08	1.78	1.61
2	А	800	D1C	CAV-CAP	-10.41	1.37	1.51
2	А	800	D1C	OBC-SBA	7.49	1.54	1.43
2	А	800	D1C	OBB-SBA	7.07	1.53	1.43
2	А	800	D1C	OAJ-SAH	5.54	1.54	1.43
2	А	800	D1C	OAK-SAH	5.42	1.53	1.43
2	А	800	D1C	CAA-CAB	-4.71	1.41	1.51
2	А	800	D1C	CAE-SAH	-4.49	1.70	1.77
2	А	800	D1C	FAU-CAN	-2.73	1.28	1.35
2	A	800	D1C	FAS-CAQ	2.20	1.41	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	800	D1C	OBC-SBA-OBB	-8.95	107.01	120.40
2	А	800	D1C	OAK-SAH-OAJ	-4.66	111.09	118.76
2	А	800	D1C	CAO-CAP-CAQ	4.58	121.91	116.58
2	А	800	D1C	OBB-SBA-NAL	4.06	113.89	106.73
2	А	800	D1C	CAR-CAQ-CAP	-3.43	119.48	123.98
2	А	800	D1C	OBC-SBA-NAL	2.58	111.27	106.73



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	800	D1C	FAT-CAM-CAR	2.48	123.55	118.61
2	А	800	D1C	FAU-CAN-CAO	2.24	123.07	118.61

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	800	D1C	CAX-NAZ-SBA-OBC
2	А	800	D1C	CAX-NAZ-SBA-NAL
2	А	800	D1C	CAA-NAL-SBA-OBC
2	А	800	D1C	CAV-CAW-CAX-NAZ
2	А	800	D1C	CAA-NAL-SBA-NAZ
2	А	800	D1C	CAA-NAL-SBA-OBB
2	А	800	D1C	CAX-NAZ-SBA-OBB

There are no ring outliers.

No monomer is involved in short contacts.

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.





### 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	724/728~(99%)	0.04	22 (3%) 50 48	87, 141, 186, 246	0
1	В	724/728~(99%)	0.06	23 (3%) 47 45	86, 144, 192, 229	0
All	All	1448/1456~(99%)	0.05	45 (3%) 49 47	86, 143, 189, 246	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	524	PHE	5.5
1	А	82	GLU	4.9
1	В	309	GLU	4.7
1	А	83	TYR	4.5
1	В	138	ASN	3.7
1	А	455	GLN	3.7
1	А	628	GLY	3.4
1	А	632	GLY	3.2
1	В	467	TYR	3.2
1	А	545	ASP	3.1
1	В	100	HIS	3.0
1	А	42	THR	3.0
1	В	618	PHE	3.0
1	А	633	GLY	2.8
1	В	628	GLY	2.8
1	В	103	ASN	2.7
1	В	97	GLU	2.7
1	В	101	SER	2.7
1	В	429	ARG	2.7
1	В	179	ASN	2.6
1	В	334	SER	2.6
1	A	630	SER	2.5
1	В	96	ASP	2.5
1	A	471	ARG	2.5



Mol	Chain	Res	Type	RSRZ
1	А	636	THR	2.4
1	А	138	ASN	2.4
1	В	42	THR	2.4
1	В	545	ASP	2.3
1	А	674	PRO	2.3
1	А	657	SER	2.3
1	В	617	GLY	2.2
1	А	122	LYS	2.2
1	А	309	GLU	2.2
1	А	91	GLU	2.2
1	В	122	LYS	2.1
1	А	222	PHE	2.1
1	В	125	ARG	2.1
1	В	338	ASN	2.1
1	В	41	LYS	2.1
1	А	41	LYS	2.1
1	А	726	VAL	2.1
1	В	422	TYR	2.0
1	В	89	PHE	2.0
1	В	508	GLN	2.0
1	А	539	LYS	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. 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	$\mathbf{Res}$	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	$\mathbf{Q}{<}0.9$
2	D1C	А	800	29/29	0.90	0.27	$98,\!148,\!204,\!207$	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.

