

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

#### Jun 4, 2024 – 08:13 PM EDT

PDB ID	:	8VZP
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in
		complex with k-403
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		R.; Kim, S.H.; Ziegler, Y.; Rangarajan, E.S.; Izard, T.; Katzenellenbogen,
		B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on	:	2024-02-12
Resolution	:	1.72 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2



# 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 1.72 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	5722(1.74-1.70)
Clashscore	141614	6152(1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	242	84%	11% ••
1	В	242	82%	11% 6%
1	С	242	13%	18% • •
1	D	242	73%	15% • 10%



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## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14774 atoms, of which 7237 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		Atoms						AltConf	Trace
1	Δ	234	Total	С	Η	Ν	0	$\mathbf{S}$	0	1	0
	Л	204	3611	1158	1805	311	320	17	0		0
1	В	227	Total	С	Η	Ν	0	S	0	0	0
		221	3541	1130	1777	302	316	16			
1	С	0.25	Total	С	Η	Ν	0	S	0	1	0
	200	3668	1175	1832	313	331	17	0	1	0	
1 D	217	Total	С	Н	Ν	0	S	0	0	0	
	217	3419	1089	1722	291	301	16		0	U	

• Molecule 1 is a protein called Estrogen receptor.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	372	SER	LEU	engineered mutation	UNP P03372
А	536	SER	LEU	engineered mutation	UNP P03372
В	372	SER	LEU	engineered mutation	UNP P03372
В	536	SER	LEU	engineered mutation	UNP P03372
С	372	SER	LEU	engineered mutation	UNP P03372
С	536	SER	LEU	engineered mutation	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

• Molecule 2 is (1S,2R,4S)-N-(2-hydroxyethyl)-5,6-bis(4-hydroxyphenyl)-N-(4-methoxyph enyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (three-letter code: A1AHW) (formula: C<sub>27</sub>H<sub>27</sub>NO<sub>7</sub>S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
0	Λ	٨	1	Total	С	Η	Ν	0	S	0	0
	A	1	61	27	26	1	6	1	0	0	
9	В	1	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	
	D	1	58	26	24	1	6	1		0	
9	С	1	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	
	U		58	26	24	1	6	1	0	0	
0	Л	D 1	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	
	D	1	63	27	27	1	7	1	0	0	

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	76	Total         O           76         76	0	0
3	В	64	Total         O           64         64	0	0
3	С	85	Total O 85 85	0	0
3	D	70	Total O 70 70	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: Estrogen receptor







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	53.56Å $58.91$ Å $93.24$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$86.76^{\circ}$ $74.95^{\circ}$ $63.05^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	37.20 - 1.72	Depositor
Resolution (A)	38.36 - 1.72	EDS
% Data completeness	59.3 (37.20-1.72)	Depositor
(in resolution range)	59.3(38.36-1.72)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 1.72 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D	0.181 , 0.222	Depositor
$\Pi, \Pi_{free}$	0.181 , $0.221$	DCC
$R_{free}$ test set	3104 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	28.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.43 , $50.5$	EDS
L-test for $twinning^2$	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.117 for h,h-k,h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14774	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.57% 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: A1AHW

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bo	nd lengths	Bond angles		
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.47	1/1850~(0.1%)	0.78	8/2507~(0.3%)	
1	В	0.40	0/1793	0.63	1/2425~(0.0%)	
1	С	0.65	5/1881~(0.3%)	1.35	26/2548~(1.0%)	
1	D	0.52	3/1724~(0.2%)	1.81	10/2330~(0.4%)	
All	All	0.52	9/7248~(0.1%)	1.22	45/9810~(0.5%)	

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	2
1	D	0	5
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	А	401	LYS	CD-CE	9.42	1.74	1.51
1	D	425	PHE	CE1-CZ	-8.63	1.21	1.37
1	С	498	GLN	CD-OE1	-8.29	1.05	1.24
1	С	477	ARG	CZ-NH1	-7.87	1.22	1.33
1	С	498	GLN	CD-NE2	6.85	1.50	1.32
1	D	425	PHE	CE2-CZ	-6.80	1.24	1.37
1	С	416	LYS	CE-NZ	5.50	1.62	1.49
1	D	425	PHE	CB-CG	-5.39	1.42	1.51
1	С	414	GLN	CD-OE1	-5.26	1.12	1.24

All (45) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	425	PHE	CB-CG-CD2	-59.18	79.37	120.80
1	D	425	PHE	CB-CG-CD1	48.85	154.99	120.80
1	С	498	GLN	CG-CD-OE1	29.14	179.88	121.60
1	D	425	PHE	CD1-CG-CD2	-17.88	95.06	118.30
1	С	414	GLN	CG-CD-OE1	15.37	152.34	121.60
1	С	498	GLN	N-CA-CB	15.21	137.97	110.60
1	С	498	GLN	CG-CD-NE2	-14.61	81.64	116.70
1	С	477	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	С	477	ARG	CD-NE-CZ	14.40	143.76	123.60
1	С	498	GLN	CB-CA-C	-13.78	82.85	110.40
1	С	412	ARG	NE-CZ-NH2	-13.59	113.50	120.30
1	А	425	PHE	CB-CG-CD1	-13.47	111.37	120.80
1	С	414	GLN	CG-CD-NE2	-13.41	84.52	116.70
1	А	425	PHE	CB-CG-CD2	11.90	129.13	120.80
1	С	498	GLN	OE1-CD-NE2	-10.23	98.36	121.90
1	D	542	GLU	CA-CB-CG	-9.26	93.03	113.40
1	С	412	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	С	335	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	С	416	LYS	CG-CD-CE	8.37	137.01	111.90
1	D	425	PHE	CG-CD1-CE1	8.18	129.80	120.80
1	С	498	GLN	N-CA-C	-7.81	89.92	111.00
1	С	335	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	D	425	PHE	CG-CD2-CE2	7.37	128.91	120.80
1	А	326	ILE	CG1-CB-CG2	7.20	127.24	111.40
1	D	526	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	С	498	GLN	CA-C-O	7.04	134.89	120.10
1	А	401	LYS	CB-CG-CD	-6.83	93.84	111.60
1	В	423	GLU	CB-CA-C	-6.51	97.39	110.40
1	С	477	ARG	CG-CD-NE	-6.41	98.34	111.80
1	С	412	ARG	CD-NE-CZ	6.21	132.29	123.60
1	D	542	GLU	CG-CD-OE2	-6.19	105.92	118.30
1	С	434	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	497	LEU	CB-CG-CD2	-5.99	100.81	111.00
1	D	526	TYR	N-CA-CB	5.94	121.29	110.60
1	С	414	GLN	OE1-CD-NE2	-5.68	108.84	121.90
1	А	401	LYS	CD-CE-NZ	-5.67	98.65	111.70
1	C	335	ARG	CG-CD-NE	5.61	123.57	111.80
1	A	401	LYS	N-CA-CB	-5.59	$100.5\overline{3}$	110.60
1	A	323	GLU	CA-CB-CG	5.51	125.53	113.40
1	А	326	ILE	CA-CB-CG1	-5.45	100.64	111.00
1	С	416	LYS	CD-CE-NZ	-5.38	99.32	111.70
1	$\mathbf{C}$	434	ARG	CA-CB-CG	-5.34	101.65	113.40
1	С	335	ARG	CB-CG-CD	-5.21	98.06	111.60



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	414	GLN	CB-CA-C	5.09	120.58	110.40
1	С	412	ARG	CB-CA-C	-5.08	100.24	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	414	GLN	Sidechain
1	С	497	LEU	Peptide
1	D	413	ASN	Peptide
1	D	414	GLN	Sidechain
1	D	425	PHE	Sidechain
1	D	526	TYR	Sidechain
1	D	542	GLU	Sidechain

### 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	1806	1805	1796	29	2
1	В	1764	1777	1777	19	2
1	С	1836	1832	1823	41	0
1	D	1697	1722	1722	27	0
2	А	35	26	0	4	0
2	В	34	24	0	0	0
2	С	34	24	0	2	0
2	D	36	27	0	3	0
3	А	76	0	0	4	0
3	В	64	0	0	4	0
3	С	85	0	0	3	2
3	D	70	0	0	5	2
All	All	7537	7237	7118	113	4

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 8.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
	1. A. 401. IVS. CF	$\frac{\text{distance (A)}}{1.74}$	1.57
1.A.401.L15.CD	1.A.401.L15.UE	1.74	1.07
1.D.475.A51.0D1 1.D.369.IVS.N7	3.D.701.HOH.O	2.03	1.10
1.D.302.LIS.NZ	1.D.414.CI N.OE1	2.03	0.92
1.D.411.A5F.N	$\frac{1.D.414.GLN.OE1}{2.D.702.UOU.O}$	2.04	0.90
1:D:352:A5N:N	3:D:702:HOH:O	2.05	0.89
1:0:381:015:5G	3:D:700:HUH:U	2.32	0.80
1:D:370:LEU:HD11	1:D:4/5:ILE:HD11	1.58	0.80
1:D:520:LY 5:NZ	1:D:523:GLU:OE2	2.11	0.83
1:B:412:ARG:NH1	1:B:420:ASP:0D1	2.16	0.79
1:A:401:LYS:CE	1:A:401:LYS:CG	2.61	0.78
1:A:401:LYS:CD	1:A:401:LYS:NZ	2.47	0.78
1:C:485:THR:O	1:C:489:LEU:HD13	1.85	0.76
1:C:473:ASP:OD1	I:C:477:ARG:NHI	2.18	0.76
1:C:316:VAL:HG21	1:C:489:LEU:HD11	1.68	0.75
1:C:525:LEU:HD12	2:C:601:A1AHW:C24	2.17	0.75
1:C:401:LYS:HE2	1:C:411:ASP:OD1	1.91	0.71
1:C:501:HIS:CD2	1:D:501:HIS:CE1	2.80	0.70
1:B:441:GLN:OE1	3:B:701:HOH:O	2.08	0.69
1:A:354:LEU:O	1:A:358:ILE:HD12	1.93	0.69
1:D:353:GLU:OE1	3:D:703:HOH:O	2.10	0.67
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.78	0.66
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.79	0.64
1:C:532:ASN:N	3:C:703:HOH:O	2.30	0.64
1:A:461:PHE:O	3:A:701:HOH:O	2.14	0.63
1:C:501:HIS:NE2	1:D:501:HIS:CE1	2.67	0.63
1:D:485:THR:O	1:D:489:LEU:HD13	1.99	0.62
1:B:485:THR:O	1:B:489:LEU:HD23	1.99	0.62
1:B:363:ARG:NH1	3:B:703:HOH:O	2.26	0.62
1:A:525:LEU:HD22	2:A:601:A1AHW:C24	2.30	0.61
1:A:369:ASP:OD2	3:A:702:HOH:O	2.16	0.61
1:B:385:GLU:HG3	3:B:731:HOH:O	1.98	0.60
1:C:413:ASN:N	1:C:413:ASN:OD1	2.32	0.60
1:C:326:ILE:HD12	1:C:394:ARG:HD3	1.83	0.60
1:C:412:ARG:HA	1:C:425:PHE:CE1	2.36	0.60
1:A:525:LEU:HD22	2:A:601:A1AHW:O6	2.02	0.60
1:A:326:ILE:HD13	3:A:737:HOH:O	2.01	0.59
1:C:376:VAL:HG22	1:C:544:LEU:HD12	1.85	0.59
1:C:342:MET:CE	1:C:417:CYS:HB2	2.33	0.59
1:C:411:ASP:HB3	1:C:413:ASN:OD1	2.03	0.58
1:A:376:VAL:HG22	1:A:544:LEU:HD12	1.86	0.58
1:C:415:GLY:O	1:C:421:MET:HB2	2.04	0.57
1:A:421:MET:O	1:A:425:PHE:HB2	2.05	0.56



A + 1	<b>A t</b> and <b>D</b>	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:368:VAL:HG22	3:B:710:HOH:O	2.05	0.56	
1:B:486:LEU:O	1:B:490:MET:HG3	2.05	0.56	
1:D:476:HIS:HB3	1:D:477:ARG:HH21	1.70	0.56	
1:C:374:ASP:OD1	1:C:471:GLU:OE1	2.23	0.55	
1:A:520:LYS:NZ	3:A:703:HOH:O	2.38	0.55	
1:A:413:ASN:HA	1:A:416:LYS:NZ	2.22	0.54	
1:C:501:HIS:CD2	1:D:501:HIS:ND1	2.76	0.54	
1:D:316:VAL:HG21	1:D:489:LEU:HD11	1.91	0.53	
1:C:316:VAL:CG2	1:C:489:LEU:HD11	2.39	0.51	
1:A:358:ILE:HG23	1:A:544:LEU:HD23	1.91	0.51	
1:B:466:LEU:C	1:B:466:LEU:HD23	2.31	0.51	
1:D:410:LEU:HA	1:D:414:GLN:OE1	2.11	0.51	
1:D:490:MET:HB3	1:D:495:LEU:HD22	1.92	0.51	
1:C:342:MET:HE1	1:C:417:CYS:HB2	1.93	0.50	
1:D:423:GLU:O	1:D:427:MET:HG3	2.12	0.50	
1:B:403:LEU:O	1:B:403:LEU:HD23	2.13	0.49	
1:C:501:HIS:CE1	1:D:487:ILE:HG21	2.47	0.49	
1:C:326:ILE:HD13	3:C:750:HOH:O	2.13	0.49	
1:D:373:HIS:ND1	1:D:537:TYR:OH	2.45	0.49	
1:A:326:ILE:HD12	1:A:394:ARG:HD3	1.96	0.48	
1:C:342:MET:HE3	1:C:417:CYS:HB2	1.95	0.48	
1:B:538:ASP:O	1:B:542:GLU:HG3	2.14	0.47	
1:B:490:MET:HB3	1:B:495:LEU:HD22	1.97	0.47	
1:A:333:PRO:HB3	1:A:345:LEU:HD21	1.97	0.46	
1:A:516:HIS:O	1:A:520:LYS:HG2	2.14	0.46	
1:A:421:MET:SD	2:A:601:A1AHW:C19	3.04	0.46	
1:A:403:LEU:CD1	1:A:409:LEU:HD13	2.46	0.45	
1:C:465:THR:HG23	1:C:468:SER:H	1.81	0.45	
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.97	0.45	
1:C:384:LEU:O	1:C:388:MET:HG3	2.17	0.45	
1:C:402:LEU:HD12	1:C:425:PHE:CE2	2.51	0.45	
2:D:601:A1AHW:O5	2:D:601:A1AHW:O7	2.35	0.45	
1:C:403:LEU:HD12	1:C:405:ALA:O	2.16	0.45	
1:D:343:MET:HE1	1:D:346:LEU:HD12	1.99	0.45	
1:D:421:MET:HG2	2:D:601:A1AHW:C20	2.46	0.45	
1:A:421:MET:SD	2:A:601:A1AHW:O1	2.75	0.45	
1:A:402:LEU:HD12	1:A:425:PHE:CE2	2.52	0.45	
1:C:473:ASP:CG	1:C:477:ARG:NH1	2.69	0.44	
1:C:403:LEU:HD13	1:C:409:LEU:HD13	2.00	0.44	
2:D:601:A1AHW:O7	2:D:601:A1AHW:C20	2.66	0.44	
1:B:463:SER:HB3	1:B:468:SER:OG	2.18	0.43	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:423:GLU:OE2	1:B:520:LYS:HE3	2.18	0.43	
1:B:533:VAL:O	1:B:533:VAL:HG12	2.17	0.43	
1:C:456:SER:HA	1:C:515:ARG:NH2	2.33	0.43	
1:B:412:ARG:NH1	1:B:426:ASP:CG	2.70	0.43	
1:C:358:ILE:HG23	1:C:544:LEU:HD23	2.01	0.43	
1:C:435:PHE:HE1	1:C:510:ILE:HG21	1.83	0.43	
1:C:353:GLU:OE1	2:C:601:A1AHW:O2	2.37	0.43	
1:C:434:ARG:O	1:C:434:ARG:HG3	2.18	0.43	
1:A:326:ILE:HD13	1:A:326:ILE:HA	1.75	0.42	
1:A:400:GLY:C	1:A:401:LYS:HG3	2.38	0.42	
1:C:434:ARG:NH1	3:C:701:HOH:O	2.18	0.42	
1:A:471:GLU:O	1:A:475:ILE:HG13	2.19	0.42	
1:C:335:ARG:HA	1:C:336:PRO:C	2.40	0.42	
1:C:411:ASP:CB	1:C:413:ASN:OD1	2.66	0.42	
1:A:413:ASN:HA	1:A:416:LYS:HZ2	1.84	0.42	
1:B:376:VAL:CG2	1:B:544:LEU:HD12	2.50	0.42	
1:D:368:VAL:HG22	3:D:722:HOH:O	2.19	0.42	
1:C:396:MET:O	1:C:436:ARG:HD3	2.20	0.42	
1:D:486:LEU:O	1:D:490:MET:HG3	2.19	0.42	
1:D:343:MET:CE	1:D:346:LEU:HD12	2.50	0.41	
1:C:376:VAL:HG22	1:C:544:LEU:CD1	2.49	0.41	
1:D:315:MET:SD	1:D:365:PRO:HG2	2.60	0.41	
1:B:539:LEU:O	1:B:543:MET:HG3	2.20	0.41	
1:C:333:PRO:HG3	1:C:345:LEU:HD11	2.02	0.41	
1:C:501:HIS:HD2	1:D:501:HIS:ND1	2.16	0.40	
1:A:434:ARG:O	1:A:438:MET:HG3	2.21	0.40	
1:D:390:GLY:O	1:D:394:ARG:HG3	2.21	0.40	
1:D:473:ASP:O	1:D:477:ARG:HG2	2.21	0.40	
1:A:316:VAL:HG21	1:A:489:LEU:HD21	2.03	0.40	
1:A:401:LYS:CG	1:A:401:LYS:NZ	2.84	0.40	

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TYR:OH	1:B:359:ASN:ND2[1_645]	1.81	0.39
1:A:328:TYR:OH	$1:B:359:ASN:HD21[1_645]$	1.54	0.06
3:C:774:HOH:O	3:D:760:HOH:O[1_655]	2.14	0.06
3:C:774:HOH:O	3:D:719:HOH:O[1_655]	2.17	0.03

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## 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	ntiles
1	А	229/242~(95%)	227~(99%)	2(1%)	0	100	100
1	В	219/242~(90%)	217~(99%)	2(1%)	0	100	100
1	С	230/242~(95%)	225~(98%)	5(2%)	0	100	100
1	D	207/242~(86%)	205~(99%)	1 (0%)	1 (0%)	29	13
All	All	885/968~(91%)	874 (99%)	10 (1%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	414	GLN

#### 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	194/218~(89%)	194 (100%)	0	100	100
1	В	192/218~(88%)	192 (100%)	0	100	100
1	С	200/218~(92%)	200 (100%)	0	100	100
1	D	186/218~(85%)	186 (100%)	0	100	100
All	All	772/872 (88%)	772 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	Res	Type
1	В	439	ASN
1	С	501	HIS
1	D	501	HIS
1	D	519	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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol True	Turne	Chain	Dec	T : 1-	Bo	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	A1AHW	D	601	-	38,40,40	1.57	4 (10%)	46,59,59	1.32	6 (13%)	
2	A1AHW	А	601	-	37,39,40	1.59	5 (13%)	44,58,59	1.38	5 (11%)	
2	A1AHW	В	601	-	35,38,40	1.70	4 (11%)	44,57,59	1.27	5 (11%)	
2	A1AHW	С	601	-	35,38,40	1.76	4 (11%)	44,57,59	1.52	5 (11%)	

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	A1AHW	D	601	-	-	8/27/53/53	0/6/5/5
2	A1AHW	А	601	-	-	7/26/52/53	0/6/5/5
2	A1AHW	В	601	-	-	10/24/50/53	0/6/5/5
2	A1AHW	С	601	-	-	7/24/50/53	0/6/5/5

All (17) bond length outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	D	601	A1AHW	S1-N1	6.21	1.79	1.67
2	С	601	A1AHW	C19-N1	-5.79	1.36	1.47
2	В	601	A1AHW	C19-N1	-5.57	1.36	1.47
2	А	601	A1AHW	S1-N1	5.41	1.78	1.67
2	С	601	A1AHW	01-S1	5.27	1.48	1.43
2	В	601	A1AHW	07-S1	5.04	1.47	1.43
2	А	601	A1AHW	01-S1	4.92	1.47	1.43
2	D	601	A1AHW	07-S1	4.83	1.47	1.43
2	В	601	A1AHW	S1-N1	4.47	1.76	1.67
2	С	601	A1AHW	S1-N1	4.17	1.75	1.67
2	А	601	A1AHW	07-S1	4.04	1.47	1.43
2	С	601	A1AHW	07-S1	4.03	1.47	1.43
2	В	601	A1AHW	01-S1	3.64	1.46	1.43
2	D	601	A1AHW	01-S1	3.28	1.46	1.43
2	A	601	A1AHW	C21-N1	-3.09	1.40	1.44
2	D	601	A1AHW	C21-N1	-2.49	1.41	1.44
2	A	601	A1AHW	O4-C18	-2.23	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	601	A1AHW	07-S1-O1	6.38	123.32	119.22
2	А	601	A1AHW	07-S1-O1	5.40	122.69	119.22
2	D	601	A1AHW	O4-C3-C2	-4.44	95.92	104.64
2	В	601	A1AHW	O4-C3-C2	-4.03	96.70	104.64
2	А	601	A1AHW	O4-C3-C2	-3.63	97.49	104.64
2	С	601	A1AHW	O4-C3-C2	-3.57	97.61	104.64
2	D	601	A1AHW	C10-C5-C4	-3.43	116.47	120.91
2	D	601	A1AHW	C20-C19-N1	3.39	118.33	112.46
2	А	601	A1AHW	C20-C19-N1	3.23	120.21	111.73
2	С	601	A1AHW	C19-N1-S1	-3.19	112.70	117.86
2	В	601	A1AHW	07-S1-O1	3.18	121.26	119.22
2	В	601	A1AHW	C10-C5-C4	-2.96	117.08	120.91
2	С	601	A1AHW	C10-C5-C4	-2.93	117.11	120.91



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	601	A1AHW	07-S1-N1	2.86	111.06	107.56
2	В	601	A1AHW	01-S1-N1	2.33	109.88	107.08
2	D	601	A1AHW	C6-C5-C4	2.22	123.78	120.91
2	С	601	A1AHW	C3-C2-C1	-2.18	98.69	100.61
2	В	601	A1AHW	C19-N1-S1	-2.12	114.42	117.86
2	А	601	A1AHW	C3-C2-C1	-2.11	98.75	100.61
2	D	601	A1AHW	C3-C2-C1	-2.07	98.78	100.61
2	А	601	A1AHW	C17-C12-C11	-2.02	118.29	120.91

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There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	601	A1AHW	C20-C19-N1-C21
2	А	601	A1AHW	C19-N1-S1-O7
2	А	601	A1AHW	C21-N1-S1-O7
2	В	601	A1AHW	C19-N1-S1-C1
2	В	601	A1AHW	C19-N1-S1-O1
2	С	601	A1AHW	C19-N1-S1-C1
2	С	601	A1AHW	C19-N1-S1-O7
2	С	601	A1AHW	C21-N1-S1-C1
2	D	601	A1AHW	C20-C19-N1-C21
2	D	601	A1AHW	C20-C19-N1-S1
2	D	601	A1AHW	C19-N1-S1-O1
2	D	601	A1AHW	C19-N1-S1-O7
2	D	601	A1AHW	C21-N1-S1-O1
2	А	601	A1AHW	C22-C21-N1-S1
2	D	601	A1AHW	C22-C21-N1-S1
2	D	601	A1AHW	C27-C21-N1-S1
2	В	601	A1AHW	C26-C24-O6-C25
2	В	601	A1AHW	C23-C24-O6-C25
2	А	601	A1AHW	C19-N1-S1-C1
2	D	601	A1AHW	C19-N1-S1-C1
2	В	601	A1AHW	C27-C21-N1-S1
2	С	601	A1AHW	C22-C21-N1-S1
2	В	601	A1AHW	C19-N1-S1-O7
2	С	601	A1AHW	C27-C21-N1-C19
2	А	601	A1AHW	C21-N1-S1-C1
2	С	601	A1AHW	C21-N1-S1-O7
2	В	601	A1AHW	C22-C21-N1-S1
2	А	601	A1AHW	C27-C21-N1-S1
2	В	601	A1AHW	C22-C21-N1-C19



Contr	Contentaca from prettoas page									
Mol	Chain	$\mathbf{Res}$	Type	Atoms						
2	В	601	A1AHW	C18-C11-C12-C13						
2	В	601	A1AHW	C18-C11-C12-C17						
2	С	601	A1AHW	C22-C21-N1-C19						

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There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	A1AHW	3	0
2	А	601	A1AHW	4	0
2	С	601	A1AHW	2	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.





















## 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	< <b>RSRZ</b> >	#RSRZ>2		$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	234/242~(96%)	0.85	28 (11%) 4	5	20,40,71,83	0
1	В	227/242~(93%)	0.84	32 (14%) 2 3	3	20,  35,  69,  95	0
1	С	235/242~(97%)	0.83	31 (13%) 3	3	20,  36,  71,  90	0
1	D	217/242~(89%)	0.94	34~(15%) 2 2	2	23,  37,  70,  96	0
All	All	913/968~(94%)	0.86	125~(13%) 3	3	20,  37,  71,  96	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res Type		RSRZ
1	В	526	TYR	8.9
1	С	526	TYR	7.5
1	В	417	CYS	6.6
1	А	466	LEU	6.3
1	D	468	SER	6.2
1	А	526	TYR	6.2
1	В	340	ALA	6.1
1	С	524	HIS	6.1
1	D	469	LEU	5.7
1	В	533	VAL	5.6
1	D	526	TYR	5.5
1	С	527	SER	5.4
1	С	417	CYS	5.2
1	D	511	LEU	5.0
1	D	510	ILE	4.9
1	С	465	THR	4.9
1	А	527	527 SER 4	
1	D	509 LEU		4.6
1	А	417 CYS		4.5
1	С	466	LEU	4.4
1	В	463	SER	4.2



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Mol	Chain	Res	Type	RSRZ
1	В	331	TYR	4.2
1	С	464	SER	4.1
1	В	524	HIS	4.1
1	С	413	ASN	4.1
1	С	525	LEU	4.1
1	С	469	LEU	4.0
1	D	306	LEU	4.0
1	А	545	ASP	3.9
1	D	532	ASN	3.9
1	В	511	LEU	3.8
1	А	494	GLY	3.8
1	А	465	THR	3.8
1	В	510	ILE	3.8
1	В	416	LYS	3.8
1	А	420	GLY	3.8
1	А	425	PHE	3.7
1	С	425	PHE	3.7
1	А	421	MET	3.7
1	С	418	VAL	3.7
1	А	511	LEU	3.6
1	D	413	ASN	3.6
1	С	420	GLY	3.5
1	D	524	HIS	3.5
1	D	342	MET	3.4
1	D	411	ASP	3.4
1	А	509	LEU	3.4
1	С	546	ALA	3.3
1	А	525	LEU	3.3
1	В	509	LEU	3.3
1	D	507	LEU	3.3
1	D	414	GLN	3.3
1	D	341	SER	3.3
1	В	505	ALA	3.3
1	D	420	GLY	3.3
1	A	458	VAL	3.2
1	В	341	SER	3.2
1	D	533	VAL	3.2
1	А	508	LEU	3.1
1	D	514	ILE	3.1
1	С	509	LEU	3.1
1	С	511	LEU	3.1
1	D	425	PHE	3.0



Mol	Chain	Res	Type	RSRZ
1	D	305	SER	3.0
1	А	307	ALA	3.0
1	D	422	VAL	3.0
1	В	425	PHE	3.0
1	С	508	LEU	3.0
1	D	421	MET	2.9
1	С	397	GLU	2.9
1	D	308	LEU	2.9
1	В	514	ILE	2.9
1	А	544	LEU	2.9
1	В	532	ASN	2.8
1	А	524	HIS	2.7
1	С	419	GLU	2.6
1	В	507	LEU	2.6
1	В	415	GLY	2.6
1	С	416	LYS	2.6
1	D	508	LEU	2.6
1	В	512	SER	2.6
1	D	512	SER	2.6
1	D	461	PHE	2.5
1	А	451	ILE	2.5
1	С	451	ILE	2.5
1	D	525	LEU	2.5
1	D	513	HIS	2.5
1	А	368	VAL	2.5
1	С	452	ILE	2.5
1	D	452	ILE	2.5
1	D	409	LEU	2.5
1	В	409	LEU	2.5
1	В	525	LEU	2.5
1	D	505	ALA	2.4
1	В	452	ILE	2.4
1	В	382	ALA	2.4
1	D	412	ARG	2.4
1	С	523	GLU	2.4
1	В	368	VAL	2.4
1	В	448	LEU	2.4
1	С	386	ILE	2.4
1	D	435	PHE	2.4
1	А	467	LYS	2.4
1	В	342	MET	2.4
1	С	510	ILE	2.4



Mol	Chain	Res	Type	RSRZ
1	С	421	MET	2.4
1	А	512	SER	2.4
1	А	413	ASN	2.4
1	С	545	ASP	2.3
1	А	452	ILE	2.3
1	D	343	MET	2.3
1	С	437	MET	2.3
1	В	462	LEU	2.3
1	В	523	GLU	2.2
1	С	411	ASP	2.2
1	В	414	GLN	2.2
1	А	308	LEU	2.2
1	А	386	ILE	2.2
1	С	544	LEU	2.1
1	В	305	SER	2.1
1	А	493	ALA	2.1
1	В	308	LEU	2.1
1	В	381	CYS	2.0
1	С	514	ILE	2.0
1	А	418	VAL	2.0

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

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

#### 6.3 Carbohydrates (i)

There are no 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	A1AHW	А	601	35/36	0.91	0.15	24,37,64,66	61
2	A1AHW	В	601	34/36	0.92	0.12	28,42,62,68	0
2	A1AHW	D	601	36/36	0.93	0.12	$25,\!47,\!64,\!77$	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
2	A1AHW	С	601	34/36	0.94	0.12	$25,\!40,\!61,\!64$	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.

