

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8VZ0
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in
		complex with k-400
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		B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on	:	2024-02-09
Resolution	:	1.86 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:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.36.2
:	1.1.7(2018)
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.36.2
	: : : : : : : : : : : : : : : : : : : :



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 1.86 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	2469(1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592(1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	10%	20%	
1	В	242	71%	18%	 9%
1	С	242	75%	18%	
1	D	242	72%	18%	 8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14395 atoms, of which 7083 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					ZeroOcc	AltConf	Trace
1	Δ	237	Total	С	Η	Ν	0	\mathbf{S}	0	1	0
1	Π	201	3637	1168	1818	316	318	17	0	T	0
1	В	220	Total	С	Η	Ν	Ο) S	0	0	0
1	D	220	3320	1068	1650	289	298	15	0	0	0
1	С	233	Total	С	Η	Ν	0	S	0	3	0
1			3559	1153	1768	309	313	16			0
1	1 D	222	Total	С	Η	Ν	0	S	0	0	0
	223	3481	1110	1750	298	308	15	0	0	0	

• 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-(cyclopropylmethyl)-5,6-bis(4-hydroxyphenyl)-N-(4-methoxyp henyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (three-letter code: A1AHO) (formula: C₂₉H₂₉NO₆S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
0	Λ	1	Total	С	Η	Ν	0	S	0	0
	A	1	40	18	15	1	5	1	0	0
0	В	1	Total	С	Η	Ν	0	S	0	0
	D	1	66	29	29	1	6	1		0
9	С	1	Total	С	Η	Ν	0	\mathbf{S}	0	0
	U		66	29	29	1	6	1	0	0
0	Л	1	Total	С	Η	Ν	0	S	0	0
	D	1	58	26	24	1	6	1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	48	Total O 48 48	0	0
3	В	36	Total O 36 36	0	0
3	С	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0
3	D	37	$\begin{array}{cc} \text{Total} & \text{O} \\ 37 & 37 \end{array}$	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





• Molecule 1: Estrogen receptor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	53.26Å 58.89 Å 93.04 Å	Deperitor
a, b, c, α , β , γ	80.10° 75.02° 63.17°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	33.05 - 1.86	Depositor
Resolution (A)	38.20 - 1.86	EDS
% Data completeness	59.5 (33.05-1.86)	Depositor
(in resolution range)	59.6 (38.20-1.86)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.55 (at 1.85 Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D	0.207 , 0.249	Depositor
Λ, Λ_{free}	0.207 , 0.249	DCC
R_{free} test set	2400 reflections $(4.93%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	31.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.43, 56.9	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.124 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14395	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.98% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1AHO

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	nd lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.47	1/1864~(0.1%)	0.97	21/2527~(0.8%)	
1	В	0.48	2/1696~(0.1%)	1.29	13/2297~(0.6%)	
1	С	0.77	8/1839~(0.4%)	1.29	18/2495~(0.7%)	
1	D	0.46	2/1759~(0.1%)	1.26	9/2378~(0.4%)	
All	All	0.56	13/7158~(0.2%)	1.21	61/9697~(0.6%)	

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	А	0	4
1	В	0	1
1	С	0	6
1	D	0	3
All	All	0	14

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	С	477	ARG	CZ-NH1	19.32	1.58	1.33
1	В	520	LYS	CD-CE	9.15	1.74	1.51
1	С	421	MET	CG-SD	-8.97	1.57	1.81
1	А	421	MET	CG-SD	-8.72	1.58	1.81
1	D	472	LYS	CD-CE	6.76	1.68	1.51
1	С	363	ARG	CG-CD	-6.76	1.35	1.51
1	С	414	GLN	CB-CG	-5.87	1.36	1.52
1	С	351	ASP	CB-CG	-5.56	1.40	1.51
1	D	401	LYS	CE-NZ	-5.36	1.35	1.49
1	С	477	ARG	NE-CZ	5.15	1.39	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	477	ARG	CZ-NH2	5.12	1.39	1.33
1	В	520	LYS	CG-CD	5.11	1.69	1.52
1	С	473	ASP	CB-CG	-5.03	1.41	1.51

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	523	GLU	OE1-CD-OE2	-36.36	79.67	123.30
1	D	538	ASP	CB-CG-OD1	34.71	149.54	118.30
1	С	351	ASP	CB-CG-OD1	28.33	143.79	118.30
1	D	538	ASP	OD1-CG-OD2	-25.91	74.08	123.30
1	D	411	ASP	CB-CG-OD1	21.69	137.82	118.30
1	С	308	LEU	CB-CG-CD1	18.84	143.03	111.00
1	В	525	LEU	CB-CG-CD1	18.71	142.80	111.00
1	В	523	GLU	CG-CD-OE1	18.32	154.94	118.30
1	С	477	ARG	NH1-CZ-NH2	-17.30	100.37	119.40
1	В	523	GLU	CG-CD-OE2	-16.43	85.44	118.30
1	А	313	ASP	CB-CG-OD1	14.54	131.38	118.30
1	С	351	ASP	OD1-CG-OD2	-14.25	96.22	123.30
1	В	497	LEU	CB-CG-CD1	13.85	134.55	111.00
1	С	351	ASP	CB-CG-OD2	-13.46	106.19	118.30
1	С	473	ASP	CB-CG-OD1	12.81	129.83	118.30
1	С	525	LEU	CB-CG-CD2	12.50	132.25	111.00
1	D	466	LEU	CB-CG-CD2	12.37	132.02	111.00
1	В	477	ARG	CG-CD-NE	11.44	135.83	111.80
1	А	525	LEU	CB-CG-CD2	11.28	130.17	111.00
1	D	411	ASP	OD1-CG-OD2	-10.55	103.25	123.30
1	D	538	ASP	CB-CG-OD2	-10.51	108.84	118.30
1	D	411	ASP	CB-CG-OD2	-10.48	108.87	118.30
1	С	308	LEU	CA-CB-CG	-10.21	91.81	115.30
1	А	313	ASP	OD1-CG-OD2	-9.88	104.53	123.30
1	С	363	ARG	CD-NE-CZ	9.85	137.39	123.60
1	С	477	ARG	CG-CD-NE	9.60	131.96	111.80
1	С	473	ASP	OD1-CG-OD2	-9.43	105.38	123.30
1	С	414	GLN	CB-CG-CD	9.30	135.79	111.60
1	А	354	LEU	CB-CG-CD1	8.78	125.93	111.00
1	А	335	ARG	CG-CD-NE	8.55	129.76	111.80
1	С	473	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	A	310	LEU	CB-CG-CD1	8.33	125.16	111.00
1	А	354	LEU	CB-CG-CD2	-7.82	97.71	111.00
1	А	421	MET	CB-CG-SD	-7.81	88.96	112.40
1	A	506	GLN	CB-CA-C	7.68	125.77	110.40



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	497	LEU	CB-CG-CD2	-7.66	97.98	111.00
1	В	409	LEU	CB-CG-CD2	7.58	123.89	111.00
1	D	497	LEU	CB-CG-CD2	-7.42	98.39	111.00
1	В	492	LYS	CA-CB-CG	-7.38	97.17	113.40
1	С	525	LEU	CA-CB-CG	-6.82	99.63	115.30
1	А	421	MET	CG-SD-CE	6.76	111.01	100.20
1	А	506	GLN	N-CA-CB	-6.75	98.45	110.60
1	В	354	LEU	CB-CG-CD2	6.67	122.34	111.00
1	А	525	LEU	CA-CB-CG	-6.61	100.09	115.30
1	С	363	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	В	520	LYS	CG-CD-CE	-6.32	92.93	111.90
1	А	472	LYS	CB-CG-CD	-6.18	95.53	111.60
1	А	506	GLN	CA-CB-CG	5.95	126.49	113.40
1	А	421	MET	CA-CB-CG	-5.83	103.39	113.30
1	А	506	GLN	CB-CG-CD	-5.76	96.64	111.60
1	С	363	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	А	335	ARG	N-CA-CB	5.60	120.68	110.60
1	В	520	LYS	CB-CG-CD	5.53	125.99	111.60
1	А	421	MET	CA-C-O	-5.49	108.57	120.10
1	В	409	LEU	CB-CG-CD1	5.48	120.32	111.00
1	А	310	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	А	313	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	С	414	GLN	CG-CD-NE2	-5.23	104.15	116.70
1	С	363	ARG	$C\overline{A}-C\overline{B}-C\overline{G}$	5.10	124.62	113.40
1	D	472	LYS	CD-CE-NZ	-5.05	100.09	111.70
1	А	313	ASP	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	313	ASP	Sidechain
1	А	335	ARG	Sidechain
1	А	421	MET	Mainchain
1	А	506	GLN	Sidechain
1	В	523	GLU	Sidechain
1	С	351	ASP	Sidechain
1	С	363	ARG	Sidechain
1	С	414	GLN	Sidechain
1	С	473	ASP	Sidechain, Mainchain
1	С	477	ARG	Sidechain
1	D	411	ASP	Sidechain



Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	537	TYR	Peptide
1	D	538	ASP	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	1819	1818	1809	43	1
1	В	1670	1650	1649	31	2
1	С	1791	1768	1760	40	0
1	D	1731	1750	1749	39	0
2	А	25	15	0	5	0
2	В	37	29	0	2	0
2	С	37	29	0	2	0
2	D	34	24	0	4	0
3	А	48	0	0	7	0
3	В	36	0	0	4	0
3	С	47	0	0	7	1
3	D	37	0	0	3	1
All	All	7312	7083	6967	149	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (149) 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 (\AA)	overlap (Å)
1:D:401:LYS:NZ	1:D:411:ASP:OD2	1.94	0.98
1:D:373:HIS:HD1	1:D:537:TYR:HH	1.18	0.88
1:C:307:ALA:N	3:C:702:HOH:O	2.06	0.87
1:D:381:CYS:SG	3:D:733:HOH:O	2.32	0.86
1:B:484:ASP:OD1	3:B:701:HOH:O	1.94	0.85
1:C:490:MET:HB3	1:C:495:LEU:HD12	1.59	0.85
1:C:501:HIS:ND1	3:C:703:HOH:O	2.11	0.81
1:C:333:PRO:O	3:C:701:HOH:O	2.00	0.80
1:B:533:VAL:HG11	2:B:600:A1AHO:O3	1.82	0.78



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:368:VAL:HG22	3:C:721:HOH:O	1.84	0.77
1:A:421:MET:HE2	3:A:701:HOH:O	1.84	0.76
1:A:421:MET:CE	2:A:600:A1AHO:N1	2.50	0.74
1:D:348:ASN:OD1	3:D:701:HOH:O	2.06	0.73
1:A:458:VAL:HG21	1:A:475:ILE:HG21	1.71	0.73
1:A:525:LEU:HD11	1:A:531:LYS:N	2.06	0.71
2:A:600:A1AHO:O6	3:A:701:HOH:O	2.07	0.71
1:D:408:LEU:HD12	1:D:410:LEU:HD21	1.72	0.71
1:A:376:VAL:HG22	1:A:544:LEU:HD12	1.72	0.70
1:A:413:ASN:ND2	3:A:705:HOH:O	2.26	0.68
1:D:487:ILE:HA	1:D:490:MET:HE3	1.75	0.68
1:C:421:MET:HG3	2:C:600:A1AHO:C21	2.25	0.67
1:D:423:GLU:OE1	1:D:520:LYS:NZ	2.27	0.67
1:A:480:ASP:OD1	3:A:702:HOH:O	2.13	0.67
1:B:354:LEU:O	1:B:358:ILE:HD12	1.94	0.66
1:A:335:ARG:HB3	1:A:336:PRO:HA	1.79	0.65
1:C:515:ARG:NH1	1:D:512:SER:OG	2.30	0.65
1:C:333:PRO:HB3	1:C:345:LEU:HD11	1.79	0.65
1:B:539:LEU:CB	3:B:727:HOH:O	2.44	0.64
1:C:342:MET:CE	1:C:417:CYS:HB2	2.27	0.64
1:A:487:ILE:HD11	1:A:504:LEU:HD22	1.80	0.64
1:D:408:LEU:CD1	1:D:410:LEU:HD21	2.27	0.63
1:C:376:VAL:O	1:C:380:GLU:HG3	2.00	0.61
1:D:424:ILE:HD12	1:D:424:ILE:H	1.65	0.61
1:C:316:VAL:HG21	1:C:489:LEU:HD21	1.83	0.60
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.83	0.60
1:A:458:VAL:CG2	1:A:475:ILE:HG21	2.32	0.60
1:D:373:HIS:ND1	1:D:537:TYR:OH	2.17	0.58
1:B:460:THR:HG22	1:B:460:THR:O	2.03	0.58
1:C:501:HIS:HB2	3:C:703:HOH:O	2.04	0.58
1:A:334:THR:O	3:A:703:HOH:O	2.17	0.57
1:C:342:MET:HE1	1:C:417:CYS:HB2	1.84	0.57
1:B:368:VAL:HG22	3:B:706:HOH:O	2.03	0.56
1:C:333:PRO:CB	1:C:345:LEU:HD11	2.34	0.56
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.87	0.56
1:D:463:SER:OG	1:D:465:THR:HG23	2.05	0.56
1:B:353:GLU:OE2	2:B:600:A1AHO:O2	2.24	0.56
1:A:354:LEU:O	1:A:358:ILE:HD12	2.06	0.56
1:A:376:VAL:HG22	1:A:544:LEU:CD1	2.34	0.56
1:C:380:GLU:HG2	1:C:540:LEU:HD12	1.88	0.55
3:A:745:HOH:O	1:B:381:CYS:SG	2.58	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:312:ALA:O	1:D:316:VAL:HG23	2.07	0.55
1:A:506:GLN:NE2	1:B:480:ASP:OD1	2.40	0.55
1:B:474:HIS:O	1:B:478:VAL:HG23	2.07	0.55
1:B:434:ARG:O	1:B:438:MET:HG3	2.07	0.55
1:C:306:LEU:C	3:C:702:HOH:O	2.43	0.54
1:C:487:ILE:HD11	1:C:504:LEU:HD22	1.90	0.54
1:D:310:LEU:O	1:D:481:LYS:HE3	2.06	0.54
1:D:509:LEU:O	1:D:512:SER:HB3	2.08	0.54
1:B:350:ALA:O	1:B:354:LEU:HD22	2.08	0.54
1:C:385:GLU:HG2	1:C:514:ILE:HG22	1.90	0.54
1:D:353:GLU:OE2	2:D:600:A1AHO:O2	2.27	0.53
1:B:456:SER:HA	1:B:515:ARG:NH2	2.23	0.53
1:C:353:GLU:OE1	2:C:600:A1AHO:O2	2.27	0.53
1:A:385:GLU:HG2	1:A:514:ILE:HG22	1.92	0.52
1:D:525:LEU:HD22	2:D:600:A1AHO:C27	2.39	0.52
1:C:342:MET:HE2	1:C:417:CYS:HB2	1.92	0.52
1:B:396:MET:HE2	1:B:436:ARG:HA	1.92	0.52
1:D:424:ILE:HD11	1:D:524:HIS:CD2	2.46	0.51
1:A:465:THR:HG23	1:A:468:SER:H	1.76	0.51
1:D:525:LEU:HD22	2:D:600:A1AHO:O5	2.10	0.51
1:C:323:GLU:OE1	1:C:449:LYS:NZ	2.40	0.51
1:A:335:ARG:HG2	1:A:337:PHE:CZ	2.46	0.50
1:C:310:LEU:O	1:C:481:LYS:NZ	2.34	0.50
1:B:538:ASP:O	1:B:542:GLU:HG2	2.11	0.50
1:A:374:ASP:OD1	1:A:471:GLU:OE1	2.30	0.50
1:A:449:LYS:CE	3:A:704:HOH:O	2.59	0.50
1:C:404:PHE:CE1	1:C:410:LEU:HD12	2.46	0.49
1:B:377:HIS:NE2	1:B:460:THR:HB	2.27	0.49
1:A:421:MET:HE2	2:A:600:A1AHO:N1	2.27	0.49
1:B:523:GLU:HG3	1:B:524:HIS:H	1.78	0.49
1:B:401:LYS:NZ	1:B:411:ASP:HB3	2.27	0.49
1:C:459:TYR:CD1	1:D:513:HIS:HB2	2.48	0.49
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.95	0.49
1:A:421:MET:SD	2:A:600:A1AHO:N1	2.86	0.48
1:C:506:GLN:NE2	1:C:506:GLN:HA	2.28	0.48
1:C:410:LEU:HD23	1:C:414:GLN:OE1	2.13	0.48
1:C:380:GLU:OE2	1:C:537:TYR:HA	2.13	0.48
1:B:374:ASP:OD2	1:B:471:GLU:HG3	2.13	0.48
1:A:373:HIS:HD1	1:A:537:TYR:HH	1.59	0.48
1:C:486:LEU:O	1:C:490:MET:HG3	2.14	0.48
1:D:488:HIS:CE1	1:D:492:LYS:HD2	2.50	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:424:ILE:HD12	1:D:424:ILE:N	2.29	0.47
1:B:384:LEU:O	1:B:388:MET:HG3	2.15	0.47
1:A:421:MET:HE3	2:A:600:A1AHO:N1	2.30	0.46
1:B:315:MET:O	1:B:319:LEU:HG	2.15	0.46
1:B:492:LYS:O	1:B:492:LYS:HG2	2.12	0.46
1:B:539:LEU:CB	3:B:733:HOH:O	2.64	0.46
1:D:433:SER:O	1:D:437:MET:HG2	2.15	0.46
1:B:533:VAL:O	1:B:533:VAL:HG12	2.17	0.45
1:D:466:LEU:O	1:D:466:LEU:HD12	2.17	0.45
1:A:370:LEU:HA	1:A:471:GLU:OE2	2.17	0.45
1:A:526:TYR:O	1:A:528:MET:N	2.49	0.45
1:C:508:LEU:HD22	1:D:509:LEU:HD21	1.97	0.45
1:D:310:LEU:O	1:D:481:LYS:CE	2.65	0.45
1:D:363:ARG:NH1	3:D:702:HOH:O	2.32	0.45
1:C:370:LEU:O	1:C:375:GLN:NE2	2.48	0.45
1:C:456:SER:HB2	3:C:712:HOH:O	2.15	0.45
1:C:317:SER:HA	1:C:320:LEU:HB2	1.98	0.44
1:D:435:PHE:HD1	1:D:438:MET:CE	2.31	0.44
1:D:448:LEU:HD11	1:D:507:LEU:HD22	1.99	0.44
1:D:533:VAL:HG12	1:D:533:VAL:O	2.17	0.44
1:C:421:MET:O	1:C:422:VAL:C	2.55	0.44
1:C:484:ASP:OD1	1:D:501:HIS:HE1	2.01	0.44
1:A:472:LYS:HB3	1:A:472:LYS:HE2	1.64	0.44
1:A:539:LEU:HG	1:A:543:MET:CE	2.47	0.44
1:D:434:ARG:O	1:D:438:MET:HG3	2.17	0.44
1:A:354:LEU:HD23	1:A:357:MET:HE3	2.00	0.44
1:A:411:ASP:H	1:A:414:GLN:HE21	1.65	0.44
1:B:358:ILE:HD13	1:B:543:MET:CE	2.47	0.43
1:A:434:ARG:O	1:A:438:MET:HG3	2.18	0.43
1:D:525:LEU:HD22	2:D:600:A1AHO:C26	2.48	0.43
1:A:474:HIS:O	1:A:478:VAL:HG23	2.18	0.43
1:D:409:LEU:C	1:D:410:LEU:HD23	2.38	0.43
1:A:413:ASN:HA	1:A:416:LYS:HE3	2.01	0.43
1:A:335:ARG:HG2	1:A:337:PHE:CE1	2.55	0.42
1:A:448:LEU:HD22	1:A:511:LEU:HD11	2.02	0.42
1:A:490:MET:HB3	1:A:500:GLN:HG2	2.01	0.42
1:A:350:ALA:O	1:A:354:LEU:HG	2.20	0.42
1:B:495:LEU:HD12	1:B:495:LEU:N	2.35	0.41
1:C:477:ARG:HD3	1:C:477:ARG:HA	1.81	0.41
1:A:316:VAL:HG21	1:A:489:LEU:HD21	2.03	0.41
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.84	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:469:LEU:HD22	1:B:469:LEU:N	2.35	0.41
1:A:310:LEU:HG	1:A:314:GLN:HB3	2.02	0.41
1:B:486:LEU:O	1:B:490:MET:HG3	2.20	0.41
1:C:525:LEU:HD22	1:C:525:LEU:O	2.21	0.41
1:D:525:LEU:O	1:D:526:TYR:CB	2.68	0.41
1:A:516:HIS:O	1:A:520:LYS:HG2	2.21	0.41
1:C:418:VAL:CB	1:C:421:MET:SD	3.09	0.41
1:A:404:PHE:CE2	1:A:410:LEU:HD12	2.56	0.40
1:C:389:ILE:HG21	1:C:449:LYS:HG2	2.02	0.40
1:D:362:LYS:HB2	1:D:362:LYS:HE3	1.88	0.40
1:A:335:ARG:HB3	1:A:336:PRO:CA	2.48	0.40
1:B:329:SER:HB2	1:B:408:LEU:HB2	2.03	0.40
1:B:403:LEU:HA	1:B:409:LEU:HD13	2.03	0.40
1:D:474:HIS:O	1:D:478:VAL:HG23	2.21	0.40
1:C:373:HIS:ND1	1:C:537:TYR:OH	2.40	0.40
1:D:498:GLN:HA	1:D:501:HIS:CD2	2.57	0.40
1:B:358:ILE:HD13	1:B:543:MET:HE2	2.04	0.40

All (3) 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:B:498:GLN:NE2	1:B:542:GLU:OE1[1_455]	2.05	0.15
3:C:744:HOH:O	3:D:734:HOH:O[1_545]	2.08	0.12
1:A:481:LYS:HZ2	$1:B:538:ASP:OD1[1_455]$	1.57	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	232/242~(96%)	227~(98%)	4 (2%)	1 (0%)	34	19



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	212/242 (88%)	207 (98%)	5 (2%)	0	100	100
1	С	230/242~(95%)	226~(98%)	4 (2%)	0	100	100
1	D	215/242~(89%)	208~(97%)	6 (3%)	1 (0%)	29	15
All	All	889/968~(92%)	868 (98%)	19 (2%)	2~(0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	538	ASP
1	А	475	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles			
1	А	194/218~(89%)	193 (100%)	1 (0%)		88	86	
1	В	175/218~(80%)	174 (99%)	1 (1%)		86	83	
1	С	187/218~(86%)	186 (100%)	1 (0%)		88	86	
1	D	188/218~(86%)	187 (100%)	1 (0%)		88	86	
All	All	744/872~(85%)	740 (100%)	4 (0%)		88	86	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	525	LEU
1	В	409	LEU
1	С	525	LEU
1	D	466	LEU

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



Mol	Chain	Res	Type
1	А	506	GLN
1	В	413	ASN
1	С	498	GLN
1	С	506	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 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).

Mal	Turne	Chain		Tink	Bo	Bond lengths			Bond angles		
IVIOI	Type	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	A1AHO	D	600	-	35,38,42	1.80	4 (11%)	44,57,63	1.28	4 (9%)	
2	A1AHO	А	600	-	26,28,42	1.78	3 (11%)	32,43,63	2.44	4 (12%)	
2	A1AHO	С	600	-	39,42,42	1.68	4 (10%)	49,63,63	1.04	4 (8%)	
2	A1AHO	В	600	-	39,42,42	1.61	4 (10%)	49,63,63	1.23	6 (12%)	

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.



	1	1	I	1			
Mol	\mathbf{Type}	Chain	Res	Link	Chirals	Torsions	Rings
2	A1AHO	D	600	-	-	7/24/50/56	0/6/5/6
2	A1AHO	А	600	-	-	5/12/38/56	0/5/4/6
2	A1AHO	С	600	-	-	5/28/56/56	0/7/6/6
2	A1AHO	В	600	-	-	10/28/56/56	0/7/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	600	A1AHO	S1-N1	7.52	1.77	1.59
2	D	600	A1AHO	C19-N1	-6.86	1.34	1.47
2	С	600	A1AHO	S1-N1	5.98	1.79	1.67
2	В	600	A1AHO	S1-N1	5.89	1.79	1.67
2	С	600	A1AHO	O6-S1	5.23	1.48	1.43
2	D	600	A1AHO	O6-S1	4.83	1.47	1.43
2	В	600	A1AHO	O6-S1	4.76	1.47	1.43
2	С	600	A1AHO	01-S1	4.74	1.47	1.43
2	В	600	A1AHO	01-S1	4.26	1.47	1.43
2	D	600	A1AHO	S1-N1	4.24	1.76	1.67
2	D	600	A1AHO	01-S1	3.07	1.46	1.43
2	В	600	A1AHO	C23-N1	-2.63	1.41	1.44
2	C	600	A1AHO	C23-N1	-2.53	1.41	1.44
2	А	600	A1AHO	O6-S1	2.33	1.47	1.43
2	A	600	A1AHO	O4-C18	-2.21	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	600	A1AHO	O6-S1-O1	10.45	125.63	119.23
2	А	600	A1AHO	01-S1-N1	-6.68	100.77	107.72
2	D	600	A1AHO	O6-S1-O1	4.83	122.32	119.22
2	D	600	A1AHO	C24-C23-N1	-3.24	115.25	120.02
2	С	600	A1AHO	C17-C12-C11	-2.87	117.20	120.91
2	В	600	A1AHO	C10-C5-C4	-2.86	117.21	120.91
2	D	600	A1AHO	C10-C5-C4	-2.81	117.27	120.91
2	А	600	A1AHO	C10-C5-C4	-2.67	117.46	120.91
2	С	600	A1AHO	C10-C5-C4	-2.51	117.66	120.91
2	В	600	A1AHO	O4-C3-C4	-2.47	98.56	101.99
2	С	600	A1AHO	O4-C3-C2	-2.27	100.17	104.64
2	В	600	A1AHO	C19-N1-C23	2.27	120.61	117.43
2	В	600	A1AHO	O6-S1-O1	2.24	120.66	119.22
2	D	600	A1AHO	O4-C3-C2	-2.23	100.24	104.64
2	B	600	A1AHO	C24-C23-N1	-2.23	116.83	120.16



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
2	С	600	A1AHO	C19-N1-C23	2.19	120.49	117.43
2	А	600	A1AHO	C12-C11-C4	2.13	134.31	128.81
2	В	600	A1AHO	C29-C23-N1	2.11	123.31	120.16

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	600	A1AHO	C18-C1-S1-O1
2	А	600	A1AHO	C2-C1-S1-O1
2	В	600	A1AHO	C20-C19-N1-C23
2	В	600	A1AHO	C20-C19-N1-S1
2	В	600	A1AHO	C18-C1-S1-O1
2	В	600	A1AHO	C18-C1-S1-O6
2	С	600	A1AHO	C19-N1-S1-O1
2	С	600	A1AHO	C23-N1-S1-C1
2	С	600	A1AHO	C23-N1-S1-O1
2	D	600	A1AHO	C19-N1-S1-C1
2	D	600	A1AHO	C19-N1-S1-O1
2	D	600	A1AHO	C23-N1-S1-C1
2	D	600	A1AHO	C23-N1-S1-O1
2	В	600	A1AHO	C24-C23-N1-S1
2	В	600	A1AHO	C29-C23-N1-S1
2	С	600	A1AHO	N1-C19-C20-C22
2	В	600	A1AHO	C11-C4-C5-C6
2	В	600	A1AHO	C11-C4-C5-C10
2	D	600	A1AHO	C24-C23-N1-S1
2	В	600	A1AHO	C2-C1-S1-O1
2	В	600	A1AHO	C2-C1-S1-O6
2	D	600	A1AHO	C29-C23-N1-C19
2	С	600	A1AHO	C19-N1-S1-C1
2	А	600	A1AHO	C18-C1-S1-O6
2	А	600	A1AHO	C18-C11-C12-C13
2	D	600	A1AHO	C24-C23-N1-C19
2	А	600	A1AHO	C2-C1-S1-O6

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes	
2	D	600	A1AHO	4	0	
Continued on most ward						



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	600	A1AHO	5	0
2	С	600	A1AHO	2	0
2	В	600	A1AHO	2	0

Continued from previous page...

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 sufficient must be 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 $>$	#RSR	Z>	2	$OWAB(Å^2)$	Q<0.9
1	А	237/242 (97%)	0.63	25~(10%)	6	6	23, 41, 75, 116	0
1	В	220/242~(90%)	0.87	37~(16%)	1	1	23, 41, 76, 99	0
1	С	233/242 (96%)	0.68	24 (10%)	6	6	25, 44, 73, 89	0
1	D	223/242 (92%)	0.71	27~(12%)	4	4	24, 41, 70, 85	0
All	All	913/968~(94%)	0.72	113 (12%)	4	4	23, 42, 74, 116	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	526	TYR	7.3
1	В	468	SER	6.9
1	В	530	CYS	6.6
1	D	340	ALA	6.2
1	В	528	MET	6.2
1	В	527	SER	5.3
1	С	425[A]	PHE	4.7
1	В	532	ASN	4.7
1	С	494	GLY	4.6
1	D	339	GLU	4.6
1	А	469	LEU	4.6
1	D	511	LEU	4.5
1	С	526	TYR	4.3
1	В	511	LEU	4.2
1	А	532	ASN	4.2
1	A	527	SER	4.2
1	В	525	LEU	4.2
1	В	305	SER	4.0
1	В	510	ILE	4.0
1	А	417	CYS	4.0
1	С	417	CYS	4.0



Mol	Chain	Res	Type	RSRZ
1	В	409	LEU	3.8
1	D	463	SER	3.8
1	А	511	LEU	3.7
1	В	507	LEU	3.7
1	А	418	VAL	3.7
1	С	511	LEU	3.7
1	D	510	ILE	3.7
1	D	532	ASN	3.6
1	В	509	LEU	3.6
1	А	419	GLU	3.6
1	В	508	LEU	3.6
1	С	420	GLY	3.6
1	В	469	LEU	3.5
1	С	509	LEU	3.5
1	В	461	PHE	3.5
1	В	308	LEU	3.4
1	С	310	LEU	3.3
1	А	451	ILE	3.3
1	D	514	ILE	3.3
1	D	509	LEU	3.2
1	D	533	VAL	3.2
1	С	544	LEU	3.2
1	В	415	GLY	3.2
1	А	306	LEU	3.1
1	С	527	SER	3.1
1	С	466	LEU	3.1
1	D	425	PHE	3.1
1	D	308	LEU	3.1
1	D	526	TYR	3.0
1	А	465	THR	3.0
1	A	545	ASP	3.0
1	С	492	LYS	3.0
1	В	342	MET	3.0
1	В	452	ILE	3.0
1	В	514	ILE	3.0
1	D	462	LEU	3.0
1	В	529	LYS	3.0
1	А	546	ALA	3.0
1	D	452	ILE	2.9
1	В	526	TYR	2.9
1	С	415	GLY	2.9
1	С	308	LEU	2.9



Mol	Chain	Res	Type	RSRZ
1	С	437	MET	2.9
1	А	508	LEU	2.9
1	А	531	LYS	2.8
1	В	467	LYS	2.8
1	D	409	LEU	2.8
1	D	507	LEU	2.8
1	А	524	HIS	2.8
1	С	465	THR	2.8
1	В	492	LYS	2.7
1	D	508	LEU	2.7
1	С	421	MET	2.7
1	С	495	LEU	2.7
1	С	508	LEU	2.6
1	А	452	ILE	2.6
1	В	413	ASN	2.6
1	А	420	GLY	2.6
1	В	524	HIS	2.6
1	С	467	LYS	2.6
1	D	412	ARG	2.6
1	В	414	GLN	2.6
1	В	345	LEU	2.6
1	D	505	ALA	2.6
1	С	368	VAL	2.5
1	С	307	ALA	2.4
1	В	512	SER	2.4
1	D	401	LYS	2.4
1	В	533	VAL	2.4
1	D	341	SER	2.4
1	А	497	LEU	2.3
1	В	505	ALA	2.3
1	D	523	GLU	2.3
1	В	544	LEU	2.3
1	A	368	VAL	2.2
1	В	531	LYS	2.2
1	D	382	ALA	2.2
1	А	533	VAL	2.2
1	А	466	LEU	2.2
1	D	415	GLY	2.2
1	С	455	ASN	2.1
1	В	368	VAL	2.1
1	В	496	THR	2.1
1	С	452	ILE	2.1



Mol	Chain	Res	Type	RSRZ
1	D	501	HIS	2.1
1	А	510	ILE	2.1
1	В	411	ASP	2.0
1	D	534	VAL	2.0
1	А	425	PHE	2.0
1	А	455	ASN	2.0
1	В	460	THR	2.0
1	D	343	MET	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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
2	A1AHO	D	600	34/37	0.86	0.17	32,55,81,90	0
2	A1AHO	В	600	37/37	0.87	0.16	24,59,93,102	0
2	A1AHO	С	600	37/37	0.89	0.17	34,53,79,97	0
2	A1AHO	А	600	25/37	0.92	0.11	$25,\!39,\!66,\!75$	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.

