

Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 05:05 pm GMT

PDB ID	:	8B23
Title	:	Time-resolved structure of K+-dependent Na+-PPase from Thermotoga mar-
		itima 600-seconds post reaction initiation with $Na+$
Authors	:	Strauss, J.; Vidilaseris, K.; Goldman, A.
Deposited on	:	2022-09-12
Resolution	:	3.84 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	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.84 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	Whole archive $(\#$ Entries)	Similar resolution $(\#Entries, resolution range(Å))$
R _{free}	130704	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)

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										
			18%										
1	А	735		60%		35%	•						
			16%										
1	В	735		63%		30%	7%						



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10077 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace		
1	Δ	702	Total	С	Ν	0	\mathbf{S}	0	0	0	
1	Л	102	5020	3296	776	923	25	0	0		
1	р	695	Total	С	Ν	0	S	0	1	0	
T	D	080	5043	3308	791	919	25	0	4	0	

 \bullet Molecule 1 is a protein called K(+)-stimulated pyrophosphate-energized sodium pump.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-8	MET	-	initiating methionine	UNP Q9S5X0
А	-7	ARG	-	expression tag	UNP Q9S5X0
А	-6	GLY	-	expression tag	UNP Q9S5X0
А	-5	SER	-	expression tag	UNP Q9S5X0
А	-4	HIS	-	expression tag	UNP Q9S5X0
А	-3	HIS	-	expression tag	UNP Q9S5X0
А	-2	HIS	-	expression tag	UNP Q9S5X0
A	-1	HIS	-	expression tag	UNP Q9S5X0
А	0	HIS	-	expression tag	UNP Q9S5X0
А	1	HIS	-	expression tag	UNP Q9S5X0
А	353	LEU	VAL	engineered mutation	UNP Q9S5X0
A	395	GLY	SER	engineered mutation	UNP Q9S5X0
В	-8	MET	-	initiating methionine	UNP Q9S5X0
В	-7	ARG	-	expression tag	UNP Q9S5X0
В	-6	GLY	-	expression tag	UNP Q9S5X0
В	-5	SER	-	expression tag	UNP Q9S5X0
В	-4	HIS	-	expression tag	UNP Q9S5X0
В	-3	HIS	-	expression tag	UNP Q9S5X0
В	-2	HIS	-	expression tag	UNP Q9S5X0
В	-1	HIS	-	expression tag	UNP Q9S5X0
В	0	HIS	-	expression tag	UNP Q9S5X0
В	1	HIS	-	expression tag	UNP Q9S5X0
В	353	LEU	VAL	engineered mutation	UNP Q9S5X0
В	395	GLY	SER	engineered mutation	UNP Q9S5X0

There are 24 discrepancies between the modelled and reference sequences:





• Molecule 2 is DIPHOSPHATE (three-letter code: DPO) (formula: O₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf			
2	А	1	Total 9	O 7	Р 2	0	0			

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	4	Total Mg 4 4	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total O 1 1	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.



30%

7%

63%

• Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump

MET	GLY	SER	SIH	STH	SIH	HIS	TYR	VAL	ALA	ALA	LEU PHF	F.B.	L9	110	P11	A18		F22	A23	V25	V26	R27 V78	07V	G31		R34	138	<mark>839</mark>	540 Y41	142	V VC	0	L50	I57		162	T66	L67	L68	т7 <mark>0</mark>		T76	A79	-	L82
(183 101	V85	M86	S87	G94	M95	K96 M07	A98		A101	N1 02	V103 B104	V105	A106	E107	A108	R110		G116	P117		K120	V121	A122 Y123	Q124		S127	M129	G130		F136	A137		L141	71.11	Y145	N1 E7	1.158		F169	E4 70	A173		V176 S177	G178	¥179 🖶
A180	G182	C183	S184	1185 1186	A187	M188		G194		T198	K199	M203		L207	V208	K210	T211	E212	L213 N214	L215	P216	0100		N222		V230	D232	N233	D236	V237		01271	D243	11.7T	S247	F248	A251	1252	V253	S254	1256	1257	L258 A259		M262
F263	1265 1265	Y266	V267	GLN	ILE	GLY	ASN	LEU	VAL	H276	q277	T282	1283		L286		P290		F293	L295		L298	L306	Y307	V308	1309 VAT	LYS	LYS	PRU SER	D315	0100		N322	5324 S324	L325	W326	A329		V333	700 V	LOOM	L344	L347	Q348	G349
L350	F355		A359	W363	F364	5365 1366	A300 1367		1370	F371	5372	1374		T384	5385 V386	1300 R.387		T391	1 201	G395	K396	5397	1399 1399	E400	G401	T402	M404	V405	1406 S407	N408	0110	M414	K415	V417	F418	P419	T421	L422		V425	A435	G436	L437 Y438	G439	V440
A441	71.1.1	L445	G446 M4 47	M44/ L448		S456	V45/ D458	S459	Y460	G461	P462	A464	D465	N466	TATO	SER	GLU	MET	CYS	LEU	D477	HA GA	1404	L487	D488	A489	G491	N492	T494		G498	I503	G504	A506	1507	4	L511	S512	L513	F514	Y517	M518	F519	15 <mark>2</mark> 2	S523
P524	D526	1527		V 534 L535	L536	L537 ME20	M539	L540	D541	A542	R543 V544	T545	A546	G547	A548	A552	A553	I 554	T555 VEE6	Y557	F558	VE61	1561 L562	I563		R579 GI M	ALA	ARG	GLU	PRO	GLY	LEU	GLU	TAS	ALA	LYS	r NU D595		R598		700 7	A607	Y613	P614	-
1617	T625	<mark>G626</mark>		r 633 V634	G635	G636	1.638	I639	G640	T641	V642 1643		M647	L648	A649 TRED		G656		W659	N661	A662	K663 Vee A	Y665	L666		N670	K676	G677	P680	H681	r 607		V690	D692	P693	L694	D696	T697	V698	G699 B700	S701	L702	D703 1704	L705	I706
K7 07 1700	60 JT	S710	V7 11	V714	1715	A716	F7 20		H7 24	L725	F726																																		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	83.33Å 111.55Å 106.22Å	Depositor
a, b, c, α , β , γ	90.00° 109.05° 90.00°	Depositor
$Bosolution(\AA)$	100.40 - 3.84	Depositor
Resolution (A)	100.40 - 3.84	EDS
% Data completeness	73.7 (100.40-3.84)	Depositor
(in resolution range)	73.7 (100.40 - 3.84)	EDS
R _{merge}	0.17	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.18 (at 3.89 Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
D D	0.334 , 0.363	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.334 , 0.361	DCC
R_{free} test set	663 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	210.4	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28, 224.9	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10077	wwPDB-VP
Average B, all atoms $(Å^2)$	249.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.02% 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: DPO, MG

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

Mal	Chain	Bond	lengths	Bo	ond angles
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.28	0/5127	0.48	1/7014~(0.0%)
1	В	0.27	0/5148	0.49	0/7013
All	All	0.27	0/10275	0.49	1/14027~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	277	GLN	CA-CB-CG	6.05	126.70	113.40

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	5020	0	4949	220	0
1	В	5043	0	5075	179	0
2	А	9	0	0	0	0
3	А	4	0	0	0	0
4	А	1	0	0	1	0
All	All	10077	0	10024	368	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 18.

All (368) 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:626:GLY:HA3	1:B:720:PHE:CD2	2.12	0.84
1:B:634:VAL:HG21	1:B:720:PHE:HE2	1.44	0.83
1:A:557:TYR:HD1	1:B:415:LYS:HA	1.45	0.78
1:B:68:LEU:HD23	1:B:76:THR:HG22	1.64	0.78
1:A:7:PHE:HB3	1:A:295:LEU:HD13	1.66	0.77
1:B:399:ILE:HA	1:B:680:PRO:HG3	1.65	0.77
1:B:626:GLY:HA3	1:B:720:PHE:HD2	1.47	0.76
1:B:384:THR:O	1:B:661:ASN:ND2	2.18	0.75
1:A:425:VAL:HG13	1:B:546:ALA:HB1	1.68	0.75
1:A:561:TYR:HE2	1:A:614:PRO:HD3	1.52	0.74
1:B:28:LYS:HB2	1:B:104:ARG:HD3	1.70	0.73
1:A:79:ALA:HB1	1:A:179:TYR:HB2	1.70	0.73
1:B:194:GLY:O	1:B:198:THR:HG23	1.87	0.73
1:B:308:VAL:HG21	1:B:324:SER:HB2	1.71	0.73
1:A:626:GLY:HA3	1:A:720:PHE:CD2	2.24	0.72
1:A:636:GLY:HA2	1:A:639:ILE:HD12	1.71	0.72
1:B:394:LEU:HD21	1:B:659:TRP:HD1	1.54	0.71
1:B:282:THR:HA	1:B:347:LEU:HD22	1.70	0.71
1:B:199:LYS:HD2	1:B:696:ASP:HB2	1.72	0.70
1:A:296:VAL:HG21	1:A:339:LEU:HD11	1.71	0.70
1:B:107:GLU:OE1	1:B:110:ARG:NH2	2.25	0.69
1:A:207:LEU:O	1:A:211:THR:N	2.26	0.69
1:B:394:LEU:HD21	1:B:659:TRP:CD1	2.29	0.68
1:A:626:GLY:HA3	1:A:720:PHE:CE2	2.28	0.67
1:B:399:ILE:HG13	1:B:400:GLU:HG3	1.75	0.67
1:A:448:LEU:HD13	1:A:505:SER:HB2	1.76	0.67
1:A:540:LEU:HD22	1:B:535:LEU:HB3	1.77	0.67
1:B:364:PHE:O	1:B:367:ILE:HG13	1.95	0.66
1:A:556:TYR:HH	1:B:556:TYR:HH	1.44	0.65
1:A:717:VAL:HA	1:A:720:PHE:CE1	2.30	0.65
1:A:84:ALA:HA	1:A:186:ILE:HG13	1.76	0.65
1:A:399:ILE:HD11	1:A:671:LEU:HD11	1.78	0.65
1:A:656:GLY:HA3	1:A:695:LYS:HD3	1.77	0.65
1:B:57:ILE:HG12	1:B:189:PHE:HD2	1.61	0.65
1:B:266:TYR:HB3	1:B:277:GLN:HB2	1.78	0.65
1:A:641:THR:HG22	1:A:706:ILE:HG12	1.77	0.65
1:B:94:GLY:HA3	1:B:129:MET:SD	2.37	0.65
1:A:31:GLY:H	1:A:107:GLU:HG3	1.61	0.64



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:340:THR:OG1	1:A:359:ALA:O	2.13	0.64
1:A:440:VAL:HG11	1:A:511:LEU:HD22	1.80	0.63
1:B:634:VAL:HG21	1:B:720:PHE:CE2	2.31	0.63
1:A:344:LEU:HB2	1:A:359:ALA:HB3	1.81	0.63
1:A:340:THR:HG23	1:A:360:ILE:HD13	1.81	0.63
1:B:641:THR:HG22	1:B:706:ILE:HG22	1.79	0.63
1:A:157:ASN:ND2	1:A:161:TYR:OH	2.31	0.63
1:A:222:ASN:HB3	1:A:225:THR:HG23	1.81	0.63
1:A:555:THR:HG23	1:A:702:LEU:HD22	1.81	0.63
1:A:557:TYR:CD1	1:B:415:LYS:HA	2.30	0.63
1:A:539:MET:HE3	1:B:539:MET:HB2	1.82	0.62
1:B:524:PRO:O	1:B:527:ILE:HG12	2.00	0.62
1:B:386:TYR:HA	1:B:391:THR:HB	1.81	0.62
1:A:363:TRP:CE2	1:A:367:ILE:HD11	2.34	0.61
1:A:340:THR:HG21	1:A:363:TRP:HB2	1.82	0.61
1:A:347:LEU:HD12	1:A:359:ALA:HB2	1.83	0.61
1:B:79:ALA:HB1	1:B:179:TYR:HB2	1.83	0.61
1:A:102:ASN:OD1	1:A:103:VAL:N	2.34	0.61
1:A:267:VAL:HB	1:A:274:LEU:HB3	1.82	0.60
1:B:414:MET:O	1:B:417:VAL:HG22	2.01	0.60
1:A:76:THR:HG23	1:A:178:GLY:HA3	1.83	0.60
1:B:556:TYR:CD1	1:B:648:LEU:HD11	2.37	0.60
1:B:265:ILE:HG12	1:B:522:ILE:HD13	1.84	0.60
1:B:254:SER:O	1:B:258:LEU:HG	2.02	0.59
1:B:367:ILE:HA	1:B:370:ILE:HD12	1.83	0.59
1:A:68:LEU:HD13	1:A:76:THR:HG22	1.84	0.59
1:A:399:ILE:HG12	1:A:674:TYR:HE2	1.67	0.59
1:A:645:GLY:HA3	1:A:706:ILE:HD11	1.84	0.59
1:A:394:LEU:HD21	1:A:659:TRP:HD1	1.67	0.59
1:A:666:LEU:HD22	1:A:681:HIS:HD2	1.66	0.59
1:A:703:ASP:OD1	1:A:704:ILE:N	2.36	0.59
1:B:656:GLY:HA3	1:B:695:LYS:HD3	1.83	0.59
1:A:240:LEU:HD22	1:A:458:ASP:HB3	1.85	0.59
1:B:518:MET:HE2	1:B:537:LEU:HB2	1.85	0.59
1:B:216:PRO:HB2	1:B:219:ASP:HB2	1.85	0.58
1:B:337:ALA:HB2	1:B:363:TRP:CZ2	2.38	0.58
1:A:50:LEU:HD21	1:A:92:ILE:HG12	1.83	0.58
1:A:717:VAL:HA	1:A:720:PHE:CD1	2.39	0.58
1:B:716:ALA:O	1:B:720:PHE:HD1	1.85	0.58
1:A:666:LEU:HD22	1:A:681:HIS:CD2	2.39	0.58
1:A:191:ARG:HH21	1:A:243:ASP:HB2	1.69	0.58



	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:208:VAL:HG12	1:A:215:LEU:HB2	1.86	0.57
1:A:724:HIS:ND1	1:A:726:PHE:O	2.35	0.57
1:A:266:TYR:CE2	1:A:353:LEU:HD23	2.39	0.57
1:A:363:TRP:CZ2	1:A:367:ILE:HD11	2.40	0.57
1:B:138:LEU:HD23	1:B:141:LEU:HD12	1.86	0.57
1:A:337:ALA:HB2	1:A:363:TRP:CZ2	2.39	0.57
1:A:409:GLY:HA3	1:A:659:TRP:HE1	1.68	0.57
1:A:82:LEU:O	1:A:86:MET:HG2	2.04	0.57
1:A:157:ASN:OD1	1:A:158:LEU:N	2.38	0.57
1:A:643:LEU:HD11	1:B:548:ALA:HB1	1.86	0.57
1:A:444:ALA:HB2	1:A:508:PHE:HB3	1.86	0.57
1:B:693:PRO:O	1:B:697:THR:HG22	2.05	0.56
1:B:138:LEU:HD12	1:B:298:LEU:HD22	1.87	0.56
1:A:133:VAL:HG13	1:A:245:LEU:HD12	1.86	0.56
1:A:232:ASP:O	1:A:236:ASP:HB2	2.04	0.56
1:A:318:GLN:NE2	1:A:322:ASN:OD1	2.38	0.56
1:B:517:TYR:HB2	1:B:714:VAL:HG22	1.87	0.56
1:A:191:ARG:HD2	1:A:704:ILE:HD12	1.86	0.56
1:B:703:ASP:HA	1:B:706:ILE:HG12	1.86	0.56
1:A:256:ILE:HG23	1:A:287:ILE:HG23	1.87	0.56
1:A:552:ALA:HB1	1:B:647:MET:HG3	1.87	0.56
1:A:80:PHE:HD1	1:A:182:GLY:CA	2.18	0.56
1:A:548:ALA:HB1	1:B:643:LEU:HD11	1.87	0.56
1:B:157:ASN:OD1	1:B:158:LEU:N	2.38	0.56
1:B:237:VAL:HG23	1:B:462:PRO:HG3	1.88	0.56
1:A:195:GLY:HA2	1:A:198:THR:HG22	1.89	0.55
1:B:10:ILE:HD12	1:B:295:LEU:HB3	1.87	0.55
1:A:535:LEU:O	1:B:538:ASN:ND2	2.40	0.55
1:A:622:PRO:HG2	1:A:712:VAL:HG23	1.88	0.55
1:B:102:ASN:OD1	1:B:103:VAL:N	2.39	0.55
1:A:321:LEU:HD22	1:A:457:VAL:HG22	1.87	0.55
1:B:97:MET:HG2	1:B:128:VAL:HB	1.88	0.55
1:B:240:LEU:HD23	1:B:458:ASP:HB3	1.88	0.55
1:A:247:SER:HA	1:A:707:LYS:HE3	1.88	0.55
1:A:490:VAL:O	1:A:494:THR:HG23	2.07	0.55
1:A:266:TYR:HB3	1:A:277:GLN:HB3	1.89	0.55
1:A:361:SER:OG	1:A:362:PRO:HD3	2.06	0.55
1:A:317:PRO:O	1:A:321:LEU:HG	2.07	0.54
1:B:523:SER:H	1:B:526:ASP:HB2	1.71	0.54
1:A:236:ASP:O	1:A:240:LEU:HD23	2.06	0.54
1:B:595:ASP:HB2	1:B:598:ARG:HH11	1.72	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:335:LEU:HA	1:A:338:PHE:HD2	1.73	0.54
1:B:73:THR:HG23	1:B:169:PHE:HZ	1.73	0.54
1:A:10:ILE:HG22	1:A:298:LEU:HD22	1.89	0.54
1:A:540:LEU:HD11	1:B:518:MET:HB3	1.90	0.54
1:B:333:VAL:HG22	1:B:367:ILE:HG22	1.90	0.53
1:B:464:ALA:HB1	1:B:488:ASP:HA	1.89	0.53
1:B:518:MET:CE	1:B:537:LEU:HB2	2.38	0.53
1:A:180:ALA:HB2	1:A:253:VAL:HG21	1.90	0.53
1:B:82:LEU:O	1:B:86:MET:HG2	2.09	0.53
1:B:539:MET:HE3	1:B:545:ILE:HA	1.91	0.53
1:A:333:VAL:HG13	1:A:367:ILE:HG12	1.89	0.53
1:A:546:ALA:HB1	1:B:425:VAL:HG13	1.91	0.53
1:A:556:TYR:CD1	1:A:648:LEU:HD11	2.44	0.52
1:A:4:ALA:HA	1:A:7:PHE:HD2	1.74	0.52
1:A:86:MET:HB3	1:A:136:PHE:HB3	1.91	0.52
1:B:306:LEU:HD12	1:B:309:ILE:HD11	1.92	0.52
1:A:556:TYR:O	1:B:414:MET:HB3	2.09	0.52
1:B:105:VAL:HG13	1:B:118:ALA:HB1	1.92	0.52
1:B:626:GLY:HA3	1:B:720:PHE:CE2	2.44	0.52
1:B:724:HIS:ND1	1:B:726:PHE:O	2.39	0.52
1:A:266:TYR:HE2	1:A:353:LEU:HD23	1.73	0.52
1:A:344:LEU:HD13	1:A:360:ILE:HG12	1.92	0.52
1:A:638:LEU:O	1:A:642:VAL:HG23	2.10	0.52
1:B:10:ILE:HG22	1:B:298:LEU:HD23	1.91	0.52
1:A:258:LEU:HG	1:A:519:PHE:HE2	1.75	0.51
1:A:538:ASN:ND2	1:B:535:LEU:O	2.43	0.51
1:B:666:LEU:HG	1:B:681:HIS:CE1	2.45	0.51
1:A:571:MET:HG2	1:B:400:GLU:OE1	2.10	0.51
1:B:458:ASP:OD1	1:B:498:GLY:HA3	2.10	0.51
1:B:526:ASP:HB3	1:B:534:VAL:HG22	1.93	0.51
1:A:507:ILE:HD11	1:A:646:ALA:HB1	1.92	0.51
1:B:232:ASP:O	1:B:462:PRO:HB3	2.10	0.51
1:B:337:ALA:HB2	1:B:363:TRP:CE2	2.46	0.51
1:A:334:VAL:HG12	1:A:338:PHE:CE2	2.46	0.51
1:A:105:VAL:HG13	1:A:118:ALA:HB1	1.92	0.51
1:A:560:GLY:HA3	1:B:414:MET:HB2	1.93	0.51
1:A:54:THR:HA	1:A:57:ILE:HG12	1.92	0.50
1:B:50:LEU:HD11	1:B:95:MET:SD	2.52	0.50
1:A:73:THR:HB	1:A:75:GLN:OE1	2.11	0.50
1:A:414:MET:HB3	1:B:556:TYR:O	2.12	0.50
1:A:105:VAL:HG21	1:A:122:ALA:HB2	1.93	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:73:THR:HG23	1:A:169:PHE:CE2	2.46	0.50
1:A:384:THR:O	1:A:658:ALA:HA	2.12	0.50
1:A:240:LEU:HD13	1:A:458:ASP:HB2	1.93	0.50
1:A:376:ILE:HG23	1:A:420:PRO:HB3	1.94	0.49
1:B:208:VAL:HG21	1:B:222:ASN:ND2	2.27	0.49
1:B:322:ASN:HB3	1:B:326:TRP:HE1	1.77	0.49
1:B:398:SER:HA	1:B:405:VAL:HG22	1.94	0.49
1:A:561:TYR:CE2	1:A:614:PRO:HD3	2.41	0.49
1:A:109:ALA:HB1	1:A:115:ILE:HG12	1.94	0.49
1:A:80:PHE:HD1	1:A:182:GLY:HA3	1.77	0.49
1:A:415:LYS:HA	1:B:557:TYR:CD1	2.46	0.49
1:B:700:PRO:O	1:B:704:ILE:HG12	2.12	0.49
1:B:350:LEU:HD22	1:B:355:PHE:CD2	2.46	0.49
1:B:507:ILE:O	1:B:511:LEU:HG	2.12	0.49
1:A:80:PHE:CD1	1:A:182:GLY:HA2	2.47	0.49
1:A:634:VAL:HG21	1:A:720:PHE:CE2	2.48	0.49
1:A:690:VAL:O	1:A:693:PRO:HD2	2.13	0.49
1:B:438:TYR:O	1:B:442:ILE:HG12	2.13	0.49
1:A:223:PRO:O	1:A:226:ILE:HG12	2.13	0.48
1:A:536:LEU:HD11	1:B:536:LEU:HG	1.95	0.48
1:B:84:ALA:HA	1:B:186:ILE:HG13	1.94	0.48
1:A:468:GLY:HA2	1:A:484:THR:OG1	2.13	0.48
1:B:676:LYS:HA	1:B:681:HIS:CE1	2.48	0.48
1:A:207:LEU:O	1:A:211:THR:HG23	2.14	0.48
1:B:38:ILE:HA	1:B:41:TYR:HD2	1.78	0.48
1:A:141:LEU:HD22	1:A:252:ILE:HD13	1.96	0.48
1:A:359:ALA:O	1:A:362:PRO:HD2	2.13	0.48
1:B:329:ALA:O	1:B:333:VAL:HG23	2.13	0.48
1:A:340:THR:HG21	1:A:363:TRP:CB	2.43	0.48
1:A:413:GLY:O	1:A:417:VAL:HG23	2.14	0.47
1:A:274:LEU:HD11	1:A:528:GLY:HA2	1.96	0.47
1:B:188:MET:HA	1:B:704:ILE:HG21	1.96	0.47
1:B:322:ASN:O	1:B:326:TRP:CD1	2.68	0.47
1:A:199:LYS:HD2	1:A:696:ASP:HB2	1.97	0.47
1:A:647:MET:HG3	1:B:552:ALA:HB1	1.95	0.47
1:B:103:VAL:O	1:B:107:GLU:HG2	2.14	0.47
1:B:267:VAL:HG12	1:B:276:HIS:HA	1.97	0.47
1:B:547:GLY:O	1:B:637:VAL:HA	2.13	0.47
1:A:361:SER:HA	1:A:364:PHE:HD2	1.79	0.47
1:B:710:SER:O	1:B:714:VAL:HG23	2.14	0.47
1:A:240:LEU:HD12	1:A:241:GLY:N	2.30	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:547:GLY:O	1:A:637:VAL:HA	2.15	0.47
1:A:22:PHE:O	1:A:25:VAL:HG12	2.15	0.47
1:A:686:ILE:O	1:A:690:VAL:HG23	2.15	0.47
1:B:18:ALA:HB2	1:B:131:LEU:HB2	1.97	0.46
1:B:42:ILE:HG23	1:B:230:VAL:HG22	1.97	0.46
1:B:322:ASN:HB3	1:B:326:TRP:NE1	2.30	0.46
1:B:344:LEU:HB2	1:B:359:ALA:HB1	1.97	0.46
1:A:665:TYR:CE1	1:A:670:ASN:HB2	2.51	0.46
1:B:256:ILE:HG23	1:B:287:ILE:HG23	1.95	0.46
1:A:209:GLY:HA2	1:A:215:LEU:N	2.30	0.46
1:A:647:MET:HB3	1:B:556:TYR:CE2	2.50	0.46
1:B:457:VAL:O	1:B:460:TYR:HB3	2.16	0.46
1:A:692:ASP:HA	1:A:695:LYS:HE3	1.97	0.46
1:B:401:GLY:O	1:B:405:VAL:HG23	2.15	0.46
1:B:633:PHE:O	1:B:637:VAL:HG23	2.15	0.46
1:A:477:ASP:HB3	1:A:480:VAL:HG23	1.98	0.46
1:A:622:PRO:O	1:A:720:PHE:HE2	1.98	0.46
1:A:72:THR:HA	1:A:163:ASN:HD21	1.80	0.46
1:A:444:ALA:HB2	1:A:508:PHE:CB	2.46	0.46
1:B:398:SER:HA	1:B:405:VAL:CG2	2.46	0.46
1:A:207:LEU:O	1:A:210:LYS:N	2.46	0.46
1:A:692:ASP:HB2	1:A:693:PRO:HD3	1.97	0.46
1:A:22:PHE:O	1:A:26:VAL:HG23	2.16	0.46
1:A:350:LEU:HD22	1:A:358:GLY:HA2	1.98	0.46
1:B:448:LEU:HD21	1:B:505:SER:HB2	1.97	0.46
1:B:625:THR:HB	1:B:633:PHE:CD2	2.51	0.46
1:A:517:TYR:HB2	1:A:714:VAL:HG22	1.97	0.46
1:A:206:ASP:OD2	1:A:689:THR:HG21	2.16	0.45
1:A:438:TYR:O	1:A:442:ILE:HG12	2.14	0.45
1:B:396:LYS:O	1:B:399:ILE:HG12	2.17	0.45
1:A:649:ALA:HA	1:A:699:GLY:HA3	1.98	0.45
1:A:145:TYR:HD1	1:A:172:PHE:CZ	2.35	0.45
1:A:237:VAL:O	1:A:240:LEU:HG	2.16	0.45
1:A:414:MET:HE1	1:B:563:ILE:HD12	1.97	0.45
1:A:126:GLY:O	1:A:456:SER:HA	2.17	0.45
1:A:556:TYR:CE2	1:B:647:MET:HB3	2.51	0.45
1:B:243:ASP:OD1	1:B:707:LYS:NZ	2.50	0.45
1:A:49:PHE:CD1	1:A:604:SER:HB2	2.51	0.45
1:A:199:LYS:NZ	1:A:696:ASP:OD2	2.42	0.45
1:A:236:ASP:OD2	4:A:901:HOH:O	2.21	0.45
1:A:319:ARG:O	1:A:323:ILE:HG12	2.17	0.45



Interatomic Clash				
Atom-1	Atom-2	distance $(Å)$	overlan (Å)	
1·A·515·ALA·HA	1·B·540·LEU·HD22	1.97	0.45	
1.B.263.PHE.HB2	1:B:283:ILE:HG13	1.01	0.45	
1.A.567.THB.O	1.A.571.MET.HG3	2.16	0.15	
1.A.167.ILE.HG22	$1 \cdot A \cdot 169 \cdot PHE \cdot CD1$	2.51	0.45	
1.B·417·VAL·HA	1.B.650.ILE.HG21	1 99	0.45	
1.A.381.GLU·HA	1.A.384.THB.HG22	1.98	0.45	
1:A:717:VAL:HA	1.A.720.PHE.HE1	1.80	0.19	
1.B.395.GLV.O	1.B.398.SEB.OG	2.24	0.15	
1.A.511.LEU.HG	1.B.545.ILE.HD12	1 97	0.45	
$1 \cdot A \cdot 261 \cdot TYB \cdot HD2$	$1 \cdot A \cdot 519 \cdot PHE \cdot HB3$	1.87	0.44	
1.A.337.ALA.HB2	1.A.363.TRP.CE2	2.52	0.11	
1.A.373.GLV.O	1.A:501.PHE.HE1	2.02	0.11	
1.B.258.LEU.HA	1.B.519.PHE.HD2	1.83	0.11	
1.A.72.THB.HA	1.A.163.ASN.ND2	2.31	0.44	
1.B.258.LEU.O	1.B.262.MET.HG3	2.01	0.11	
$1 \cdot A \cdot 343 \cdot TYB \cdot O$	1:A:347:LEU:HG	2.17	0.11	
1.R.949.1111.0	1.R.26.VAL:HG23	2.11	0.44	
1.A.364.PHE:O	1:A:368:ILE:HG12	2.10	0.11	
1.A.479.GLU.O	1:A:483:ILE:HG12	2.10	0.44	
1.R.558.PHE.CE1	1.R.60.HD.H012	2.11	0.11	
1:A:64:ILE:HD13	1.A.67.LEU.HD12	1 99	0.44	
1.A.514.PHE.O	1.A.518.MET.HG2	2.18	0.11	
1.B.102.ASN.HD22	1.B.466.ASN.HB3	1.83	0.44	
1:A:542:ALA:HA	1:A:545:ILE:HG22	1.00	0.44	
1:B:181:LEU:O	1:B:185:ILE:HG12	2.18	0.44	
1:A:714:VAL:O	1:A:717:VAL:HG12	2.17	0.44	
1:B:86:MET:HB3	1:B:136:PHE:HB3	1.99	0.44	
1:B:266:TYB:O	1:B:277:GLN:N	2.47	0.44	
1:B:555:THR:HG23	1:B:702:LEU:HD22	1.98	0.44	
1:A:203:MET:O	1:A:207:LEU:HG	2.17	0.44	
1:A:530:PRO:HB2	1:A:533:LEU:HD13	1.99	0.44	
1:B:252:ILE:HG13	1:B:445:LEU:HD21	1.99	0.44	
1:B:613:TYR:CE2	1:B:617:ILE:HD11	2.53	0.44	
1:A:556:TYR:CE1	1:A:648:LEU:HD11	2.53	0.43	
1:A:596:TYR:CE2	1:A:600:ILE:HD11	2.52	0.43	
1:B:398:SER:OG	1:B:680:PRO:HB3	2.18	0.43	
1:A:49:PHE:CE1	1:A:604:SER:HB2	2.53	0.43	
1:A:409:GLY:HA3	1:A:659:TRP:NE1	2.32	0.43	
1:A:396:LYS:HA	1:A:399:ILE:HD12	2.00	0.43	
1:B:39:SER:HB2	1:B:103:VAL:HG21	2.01	0.43	
1:B:366:ALA:HB2	1:B:442:ILE:HG22	2.00	0.43	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:236:ASP:O	1:A:462:PRO:HG2	2.19	0.43
1:A:246:GLU:OE2	1:A:707:LYS:HE2	2.18	0.43
1:A:388:TYR:N	1:A:388:TYR:CD1	2.87	0.43
1:B:73:THR:HG23	1:B:169:PHE:CZ	2.50	0.43
1:A:33:GLU:HG2	1:A:34:ARG:N	2.34	0.43
1:A:471:SER:HB2	1:A:480:VAL:HG12	2.00	0.43
1:A:73:THR:HG23	1:A:169:PHE:HE2	1.83	0.43
1:A:359:ALA:C	1:A:362:PRO:HD2	2.39	0.43
1:B:198:THR:HG22	1:B:231:GLY:CA	2.48	0.43
1:B:643:LEU:O	1:B:647:MET:HG2	2.19	0.43
1:A:191:ARG:HD3	1:A:700:PRO:HB2	2.00	0.43
1:A:321:LEU:HD13	1:A:457:VAL:HG13	2.01	0.43
1:A:167:ILE:HD11	1:A:719:ILE:HD11	1.99	0.42
1:A:388:TYR:N	1:A:388:TYR:HD1	2.17	0.42
1:B:203:MET:O	1:B:207:LEU:HG	2.19	0.42
1:A:97:MET:HG2	1:A:128:VAL:HB	1.99	0.42
1:A:622:PRO:HG3	1:A:709:MET:HG3	2.02	0.42
1:A:639:ILE:HG12	1:B:539:MET:HG2	2.01	0.42
1:B:208:VAL:HG21	1:B:222:ASN:HD21	1.83	0.42
1:A:383:TYR:CZ	1:A:419:PRO:HG2	2.54	0.42
1:A:191:ARG:CZ	1:A:700:PRO:HB2	2.50	0.42
1:A:549:LEU:HD11	1:B:511:LEU:HD11	2.01	0.42
1:B:436:GLY:O	1:B:440:VAL:HG23	2.20	0.42
1:B:124:GLN:O	1:B:128:VAL:HG23	2.18	0.42
1:B:503:ILE:O	1:B:507:ILE:HG13	2.19	0.42
1:A:293:PHE:CD2	1:A:445:LEU:HG	2.54	0.42
1:A:622:PRO:HG2	1:A:712:VAL:CG2	2.49	0.42
1:B:665:TYR:CE1	1:B:670:ASN:HB2	2.55	0.42
1:B:129:MET:HG2	1:B:237:VAL:HG13	2.02	0.42
1:B:306:LEU:HA	1:B:309:ILE:HG12	2.02	0.42
1:B:558:PHE:CE2	1:B:562:LEU:HD11	2.55	0.42
1:B:703:ASP:OD1	1:B:704:ILE:N	2.53	0.42
1:A:344:LEU:HD12	1:A:359:ALA:N	2.34	0.42
1:A:306:LEU:O	1:A:310:VAL:HG22	2.20	0.41
1:B:418:PHE:HB3	1:B:419:PRO:HD3	2.01	0.41
1:A:634:VAL:HG21	1:A:720:PHE:CZ	2.55	0.41
1:B:435:ALA:HB3	1:B:439:GLY:HA3	2.01	0.41
1:B:558:PHE:O	1:B:562:LEU:HG	2.20	0.41
1:A:191:ARG:NH2	1:A:239:GLY:O	2.54	0.41
1:B:484:THR:HA	1:B:487:LEU:HG	2.01	0.41
1:B:561:TYR:HD2	1:B:614:PRO:HG3	1.85	0.41



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:24:ALA:HA	1:B:27:ARG:HE	1.85	0.41
1:B:108:ALA:HB1	1:B:117:PRO:HB2	2.01	0.41
1:B:413:GLY:O	1:B:417:VAL:HG13	2.21	0.41
1:B:639:ILE:O	1:B:643:LEU:HG	2.20	0.41
1:B:656:GLY:CA	1:B:695:LYS:HD3	2.48	0.41
1:A:476:LEU:HB3	1:A:480:VAL:HG21	2.03	0.41
1:B:34:ARG:O	1:B:38:ILE:HG12	2.20	0.41
1:B:350:LEU:HD22	1:B:355:PHE:HD2	1.84	0.41
1:A:124:GLN:O	1:A:128:VAL:HG23	2.20	0.41
1:A:643:LEU:HD12	1:B:643:LEU:HD12	2.03	0.41
1:A:698:VAL:O	1:A:702:LEU:HG	2.20	0.41
1:B:199:LYS:CG	1:B:693:PRO:HA	2.50	0.41
1:B:598:ARG:O	1:B:602:ILE:HG12	2.19	0.41
1:A:274:LEU:HD13	1:A:527:ILE:HG22	2.02	0.41
1:A:503:ILE:HD11	1:A:646:ALA:HA	2.02	0.41
1:A:611:MET:O	1:A:614:PRO:HD2	2.21	0.41
1:B:24:ALA:HA	1:B:27:ARG:HH21	1.85	0.41
1:B:373:GLY:HA2	1:B:447:MET:HE3	2.02	0.41
1:A:184:SER:HA	1:A:246:GLU:HG3	2.03	0.41
1:A:553:ALA:HB2	1:B:421:THR:HG21	2.03	0.41
1:A:60:VAL:HG11	1:A:189:PHE:CZ	2.56	0.41
1:A:308:VAL:HG21	1:A:324:SER:HA	2.02	0.41
1:A:421:THR:HG21	1:B:553:ALA:HB2	2.02	0.41
1:A:539:MET:HB2	1:B:537:LEU:HD23	2.03	0.41
1:A:548:ALA:HA	1:A:636:GLY:O	2.21	0.41
1:A:625:THR:HB	1:A:633:PHE:CD2	2.55	0.41
1:A:634:VAL:O	1:A:638:LEU:HG	2.20	0.41
1:A:695:LYS:NZ	1:A:696:ASP:OD2	2.51	0.41
1:B:258:LEU:HD22	1:B:519:PHE:CE2	2.55	0.41
1:A:468:GLY:O	1:A:481:ARG:NH1	2.53	0.41
1:A:506:ALA:HA	1:A:707:LYS:HD3	2.03	0.41
1:B:11:PRO:HG3	1:B:138:LEU:HB2	2.02	0.41
1:B:180:ALA:HB2	1:B:253:VAL:HG21	2.02	0.41
1:A:199:LYS:HG3	1:A:693:PRO:HA	2.03	0.40
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.93	0.40
1:A:522:ILE:HD13	1:A:534:VAL:HG11	2.03	0.40
1:B:371:PHE:O	1:B:374:ILE:HG12	2.22	0.40
1:A:317:PRO:HG2	1:A:490:VAL:HG21	2.04	0.40
1:A:204:ALA:HA	1:A:207:LEU:HD12	2.03	0.40
1:A:435:ALA:HB3	1:A:439:GLY:HA3	2.04	0.40
1:B:62:ILE:O	1:B:66:ILE:HG12	2.22	0.40



continuea from process as pagem				
Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:185:ILE:HD13	1:B:708:ILE:HD11	2.04	0.40	
1:B:207:LEU:O	1:B:211:THR:HG23	2.21	0.40	

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	696/735~(95%)	671~(96%)	25~(4%)	0	100	100
1	В	679/735~(92%)	665~(98%)	14 (2%)	0	100	100
All	All	1375/1470~(94%)	1336 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	496/575~(86%)	494 (100%)	2(0%)	91	95
1	В	513/575~(89%)	513 (100%)	0	100	100
All	All	1009/1150~(88%)	1007 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	388	TYR
1	А	720	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	318	GLN
1	А	322	ASN
1	В	466	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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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 Type Chain	Type	Chain	Dog	Tink	B	ond leng	gths	В	ond ang	les
	Res Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2			
2	DPO	А	801	3	6,8,8	0.65	0	$13,\!13,\!13$	2.10	1 (7%)

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	DPO	А	801	3	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	801	DPO	P2-O4-P1	7.03	156.94	132.83

There are no chirality outliers.

There are no torsion outliers.

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	702/735~(95%)	0.85	132 (18%) 1 1	121, 248, 344, 383	0
1	В	685/735~(93%)	0.71	119 (17%) 1 1	125, 244, 344, 446	0
All	All	1387/1470~(94%)	0.78	251 (18%) 1 1	121, 246, 344, 446	0

All (251) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	526	ASP	10.4
1	А	184	SER	9.3
1	В	255	SER	9.1
1	А	659	TRP	9.1
1	А	127	SER	8.8
1	А	95	MET	8.8
1	В	210	LYS	8.3
1	А	525	SER	8.3
1	А	389	LYS	7.8
1	А	501	PHE	7.6
1	А	91	GLY	7.6
1	В	87	SER	7.3
1	А	243	ASP	7.0
1	А	98	ALA	6.9
1	В	214	ASN	6.6
1	В	42	ILE	6.4
1	А	191	ARG	6.3
1	В	258	LEU	6.3
1	В	123	TYR	6.2
1	В	141	LEU	6.1
1	А	696	ASP	6.1
1	А	286	LEU	6.1
1	A	294	ALA	6.1
1	A	493	THR	6.0



Mol	Chain	Res	Type	RSRZ
1	А	123	TYR	5.9
1	А	548	ALA	5.9
1	А	138	LEU	5.9
1	В	244	LEU	5.7
1	А	392	GLN	5.6
1	В	119	LEU	5.5
1	А	661	ASN	5.5
1	А	235	GLY	5.4
1	В	460	TYR	5.4
1	А	117	PRO	5.4
1	В	199	LYS	5.3
1	А	57	ILE	5.2
1	А	662	ALA	5.2
1	В	562	LEU	5.2
1	А	290	PRO	5.2
1	А	297	GLY	5.1
1	В	184	SER	5.1
1	А	512	SER	5.0
1	А	248	PHE	5.0
1	В	145	TYR	5.0
1	В	236	ASP	5.0
1	А	298	LEU	4.9
1	В	660	ASP	4.8
1	А	126	GLY	4.8
1	В	347	LEU	4.8
1	В	490	VAL	4.8
1	А	500	GLY	4.7
1	A	53	GLU	4.7
1	A	393	PHE	4.7
1	А	542	ALA	4.7
1	A	94	GLY	4.6
1	В	105	VAL	4.6
1	В	209	GLY	4.6
1	А	496	ALA	4.6
1	A	166	GLY	4.6
1	A	449	SER	4.6
1	В	457	VAL	4.6
1	В	286	LEU	4.5
1	В	177	SER	4.5
1	В	248	PHE	4.4
1	А	283	ILE	4.4
1	А	188	MET	4.4



Mol	Chain	Res	Type	RSRZ
1	В	489	ALA	4.4
1	А	258	LEU	4.3
1	А	497	ILE	4.3
1	В	407	SER	4.3
1	А	244	LEU	4.2
1	А	655	SER	4.2
1	В	491	GLY	4.2
1	А	181	LEU	4.1
1	В	691	GLY	4.1
1	В	563	ILE	4.1
1	А	546	ALA	4.1
1	В	661	ASN	4.0
1	В	252	ILE	4.0
1	А	187	ALA	4.0
1	В	122	ALA	4.0
1	В	494	THR	3.9
1	А	511	LEU	3.9
1	А	259	ALA	3.8
1	А	122	ALA	3.8
1	В	294	ALA	3.8
1	В	172	PHE	3.8
1	А	315	ASP	3.8
1	В	690	VAL	3.7
1	В	659	TRP	3.7
1	В	293	PHE	3.7
1	В	203	MET	3.7
1	В	461	GLY	3.6
1	А	700	PRO	3.5
1	В	181	LEU	3.5
1	В	465	ASP	3.5
1	А	636	GLY	3.5
1	В	290	PRO	3.5
1	В	237	VAL	3.5
1	В	543[A]	ARG	3.5
1	В	561	TYR	3.4
1	A	99	THR	3.4
1	A	203	MET	3.4
1	В	405	VAL	3.4
1	A	172	PHE	3.3
1	А	233	ASN	3.3
1	А	241	GLY	3.3
1	В	511	LEU	3.3



Mol	Chain	Res	Type	RSRZ
1	А	423	THR	3.2
1	А	87	SER	3.2
1	В	187	ALA	3.2
1	А	293	PHE	3.2
1	В	138	LEU	3.2
1	А	3	VAL	3.2
1	А	101	ALA	3.1
1	А	658	ALA	3.1
1	А	386	TYR	3.1
1	В	259	ALA	3.1
1	А	503	ILE	3.1
1	В	256	ILE	3.1
1	А	58	PHE	3.1
1	В	458	ASP	3.1
1	А	567	THR	3.1
1	А	314	SER	3.1
1	В	211	THR	3.1
1	В	512	SER	3.1
1	В	212	GLU	3.1
1	В	607	ALA	3.1
1	А	316	ASN	3.0
1	В	142	VAL	3.0
1	В	233	ASN	3.0
1	А	285	ALA	3.0
1	А	639	ILE	3.0
1	А	255	SER	3.0
1	В	421	THR	3.0
1	А	177	SER	3.0
1	А	438	TYR	3.0
1	A	234	VAL	2.9
1	В	283	ILE	2.9
1	В	318	GLN	2.9
1	А	292	PHE	2.9
1	В	173	ALA	2.9
1	A	141	LEU	2.9
1	A	21	ASN	2.9
1	A	271	GLY	2.9
1	В	548	ALA	2.9
1	B	636	GLY	2.9
1	В	639	ILE	2.9
1	A	610	GLN	2.8
1	А	385	SER	2.8



Mol	Chain	Res	Type	RSRZ	
1	В	183	CYS	2.8	
1	А	49	PHE	2.8	
1	В	406	ILE	2.8	
1	В	106	ALA	2.8	
1	А	119	LEU	2.8	
1	В	438	TYR	2.8	
1	А	42	ILE	2.8	
1	А	563	ILE	2.8	
1	В	180	ALA	2.8	
1	А	549	LEU	2.8	
1	А	450	PHE	2.7	
1	В	493	THR	2.7	
1	А	519	PHE	2.7	
1	А	155	VAL	2.7	
1	А	640	GLY	2.7	
1	А	564	SER	2.7	
1	В	348[A]	GLN	2.6	
1	В	40	SER	2.6	
1	В	121	VAL	2.6	
1	А	508	PHE	2.6	
1	В	422	LEU	2.6	
1	В	664	LYS	2.6	
1	В	247	SER	2.6	
1	В	254	SER	2.5	
1	В	710 SER		2.5	
1	В	282	THR	2.5	
1	А	702	LEU	2.5	
1	А	199	LYS	2.5	
1	В	188	MET	2.5	
1	В	251	ALA	2.5	
1	A	102	ASN	2.5	
1	А	185	ILE	2.5	
1	В	523	SER	2.5	
1	А	690	VAL	2.4	
1	В	198	THR	2.4	
1	В	104	ARG	2.4	
1	В	31	GLY	2.4	
1	А	371	PHE	2.4	
1	В	179	TYR	2.4	
1	В	541[A]	ASP	2.4	
1	В	116	GLY	2.4	
1	А	93	VAL	2.4	

Continued from previous page...



Mol	Chain	Res	Type	RSRZ	
1	В	101	ALA	2.4	
1	А	396	LYS	2.4	
1	А	7	PHE	2.4	
1	В	418	PHE	2.3	
1	В	711	VAL	2.3	
1	А	183	CYS	2.3	
1	А	695	LYS	2.3	
1	А	180	ALA	2.3	
1	В	46	ALA	2.3	
1	А	694	LEU	2.3	
1	В	387	ARG	2.3	
1	В	514	PHE	2.3	
1	A	522	ILE	2.3	
1	В	425	VAL	2.3	
1	В	488	ASP	2.3	
1	А	405	VAL	2.2	
1	В	403	GLY	2.2	
1	А	445	LEU	2.2	
1	А	447	MET	2.2	
1	В	127	SER	2.2	
1	В	408	ASN	2.2	
1	А	486	HIS	2.2	
1	А	502	ALA	2.2	
1	А	505	SER	2.2	
1	А	287	ILE	2.2	
1	А	236	ASP	2.2	
1	В	663	LYS	2.2	
1	В	542	ALA	2.2	
1	А	660	ASP	2.2	
1	В	544	VAL	2.2	
1	A	194	GLY	2.2	
1	В	257	ILE	2.2	
1	В	207	LEU	2.2	
1	A	494	THR	2.2	
1	A	499	LYS	2.2	
1	В	401	GLY	2.1	
1	A	131	LEU	2.1	
1	В	98	ALA	2.1	
1	A	295	LEU	2.1	
1	В	464	ALA	2.1	
1	А	116	GLY	2.1	
1	В	677	GLY	2.1	



8B23

Mol	Chain	in Res Type		RSRZ
1	В	687	GLY	2.1
1	А	96	LYS	2.1
1	А	289	TYR	2.1
1	А	448	LEU	2.1
1	А	541	ASP	2.1
1	В	525	SER	2.1
1	В	694	LEU	2.1
1	А	137	ALA	2.0
1	В	698	VAL	2.0
1	А	571	MET	2.0
1	В	510	ALA	2.0
1	А	457	VAL	2.0
1	В	456	SER	2.0
1	А	453	THR	2.0
1	A	559	SER	2.0
1	В	692	ASP	2.0
1	В	176	VAL	2.0

Continued from previous page...

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	MG	А	805	1/1	0.41	0.22	258,258,258,258	0
3	MG	А	802	1/1	0.46	0.20	266,266,266,266	0
3	MG	А	803	1/1	0.76	0.11	285,285,285,285	0
2	DPO	А	801	9/9	0.87	0.13	274,274,274,274	0
3	MG	А	804	1/1	0.92	0.15	276,276,276,276	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.

