

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

#### Mar 25, 2024 - 03:27 pm GMT

PDB ID	:	80JZ
Title	:	Arabidopsis thaliana Phosphoenolpyruvate carboxylase 1 (PPC1) G678S mu-
		tant
Authors	:	Loris, R.; Haesaerts, S.; Larsen, P.B.
Deposited on	:	2023-03-25
Resolution	:	3.25  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The 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
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 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
D	120704	
$R_{free}$	130704	1619(3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	974	% 65%	25%	•	7%
1	В	974	66%	23%	•	9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	А	1001	-	-	Х	-



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14457 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		A	toms			ZeroOcc	AltConf	Trace
1	А	906	Total 7268	C 4615	N 1273	O 1351	S 29	0	3	0
1	В	890	Total 7144	C 4534	N 1245	0 1336	S 29	0	0	0

• Molecule 1 is a protein called Phosphoenolpyruvate carboxylase 1.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-6	MET	-	initiating methionine	UNP Q9MAH0
А	-5	HIS	-	expression tag	UNP Q9MAH0
А	-4	HIS	-	expression tag	UNP Q9MAH0
А	-3	HIS	-	expression tag	UNP Q9MAH0
А	-2	HIS	-	expression tag	UNP Q9MAH0
А	-1	HIS	-	expression tag	UNP Q9MAH0
А	0	HIS	-	expression tag	UNP Q9MAH0
А	678	SER	GLY	engineered mutation	UNP Q9MAH0
В	-6	MET	-	initiating methionine	UNP Q9MAH0
В	-5	HIS	-	expression tag	UNP Q9MAH0
В	-4	HIS	-	expression tag	UNP Q9MAH0
В	-3	HIS	-	expression tag	UNP Q9MAH0
В	-2	HIS	-	expression tag	UNP Q9MAH0
В	-1	HIS	-	expression tag	UNP Q9MAH0
В	0	HIS	-	expression tag	UNP Q9MAH0
В	678	SER	GLY	engineered mutation	UNP Q9MAH0

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	35	Total O   35 35	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.



23%

• Molecule 1: Phosphoenolpyruvate carboxylase 1

10%

66%

Chain B:

MET HIS	SIH	SIH	HIS	MET	ASN	ARG LYS	TEU	GLU	MET	ALA SER	ILE	VAL	SIH	LEU ARG	GLN	VAL	PRO	GLY	VAL	GLU	ASP	LYS	LEU VAL	GLU	Y 33 D34	A35 1.36	L37	D39	R40 F41	1	L40 H49	D52	L53 R54	L60	Y61	E66
0 U	K70	E72	K75	E.70		G80 S81	V82	L83	L86	<mark>G89</mark>	D90	N93	194 •	A95 K96	A97	20	M101	<b>F102</b>	A108	0112	L V	R115 R116	R117 • R118 •	1119 •	K120 K121	LEU	LYS	ASP	PHE VAL	ASP	SER	SER ALA	THR THR	GLU S137	D138 L139	E140
E141	F143	K144 K145	L146	D149	0017	S153	E155	E156 1157	F158	L161	E E	1165 V166	D167	L168 V169	01 11 12	A172 H173	P174	9/11	S181	L182 L183		L193	L196		1201 T202	D205		F221 R222	E225		07 7N	M237	G240 M241	F244	H245 E246	T247
1248	K250	P253	L256	R257	T261	A262 1.263	K264	N265	G267	1268 E269	500 500	171 C	A276	P277 L278	1279	4280 F281	S282	M285		K289	R294	D302	1.306	A307	K308 M309	M310	Y315	F316 N317	Q318 I319	E320	1321	F324	M328 W329	R330 • C331	N332	R336
N3AF		K348 D349	A350	K352	W358	K359	T363	T364 E365	0 1 1 1	L3/8	R384	L388	L389	H393	90011 1	0650	E399	N404	L405	E406 Q407	F408	L409 E410	P411	Y416	R417 S418	A428	L C C	r 435 L436	R437	S445	D450	I451 R452	Q453 E454	R457	D460	V461
L462		L409	R475 E476	W477 c/70		R481	L490	K493	R494	L496	F497	L501	P502	K503 T504	E505	1507 I507		0190	T513	I517		1528	8531	L545	E548	K552	<b>Q553</b>	L555 L555	V558	с <mark>у</mark> ЦЦ	E302 K563	L564	L567	W582	R586 1587	
K590	E592	V 593 M 594	D599	Lena Lena	000	R606	S608	A609 A610	W611	4012 L613	Y614	GION	E618	V621		K630 L631	T632	M633 F634		6639 6639	T640	V 041 G 642	P656	P657	D658 T659	R665		deco Ge70	E671 V672		c/oh	S678	0688	T691 A692	A 693 T 694	L695
MGOO	R700	P702	I703	P705	R710	A711 1.712	L713	D714 E715	M716	V719	A720	E723	Y724	R725 S726	V727	V/28 F729		K/33	E736	Y /37 F738	R739	L/40 A741	E744	L745	E/46	G753 S754	R755	SER	LYS ARG	LYS	SER	GLY <mark>G764</mark>	I765	S767 L768	1771	P772
W773	F775	A777	T778 0779	T780	F782	V786	W7.87	L788 G789	F7 90	6/ 91 S792	A793	L/ 94 R795	H7 96	V797 I798	E7 99	D801	V802	K803	L808	u809 D810	M811	1812	W815	F817	F818	T821 1822	D823	L824 1825	E826 • M827	V828 E920	LOZU	L843 L844	E848	L849	E861	K865
<b>T866</b>	<b>1</b> 869	K874	ASP LEU	LEU	GLY	ASP PRO	TYR	LEU	<b>Q885</b> D885	L887	R888	L8890		1894 T895	T896	K906	R907	1908 R909	D910	1164	T916	ARG	PRO HTS	ILE	LYS	GLU TLE	ALA	GLU SER	SER K930	P931	K933	E934 L935	Y944	L948	L952	I953
L954 тобб		6967																																		



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	128.27Å 160.28Å 141.30Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	49.32 - 3.25	Depositor
Resolution (A)	49.32 - 3.25	EDS
% Data completeness	99.5 (49.32-3.25)	Depositor
(in resolution range)	99.5(49.32 - 3.25)	EDS
$R_{merge}$	0.24	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.04 (at 3.25 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
B B.	0.220 , $0.261$	Depositor
$n, n_{free}$	0.224 , $0.263$	DCC
$R_{free}$ test set	2322 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	111.3	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28 , 75.3	EDS
L-test for $twinning^2$	$ < L >=0.44, < L^2>=0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14457	wwPDB-VP
Average B, all atoms $(Å^2)$	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.53% 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: PO4

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

Mal	Chain	Bond	lengths	Bond angles						
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5					
1	А	0.39	0/7435	0.58	3/10068~(0.0%)					
1	В	0.29	0/7297	0.46	0/9879					
All	All	0.34	0/14732	0.53	3/19947~(0.0%)					

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	889	LEU	CA-CB-CG	5.72	128.47	115.30
1	А	768	LEU	CA-CB-CG	5.63	128.25	115.30
1	А	849	LEU	CA-CB-CG	5.11	127.04	115.30

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	7268	0	7202	167	0
1	В	7144	0	7086	147	0
2	А	5	0	0	2	0
2	В	5	0	0	1	0
3	А	35	0	0	2	0
All	All	14457	0	14288	313	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 11.

All (313) 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:A:173:HIS:ND1	1:A:669:GLN:OE1	2.00	0.94
1:B:173:HIS:ND1	1:B:669:GLN:OE1	2.10	0.85
1:B:404:ASN:HB2	1:B:407:GLN:HB2	1.58	0.85
1:A:618:GLU:OE1	1:A:710:ARG:NH2	2.13	0.81
1:B:172:ALA:HB2	1:B:285:MET:HG3	1.64	0.80
1:A:638:GLY:HA2	1:A:669:GLN:HG3	1.64	0.80
1:B:332:ASN:HD21	1:B:418:SER:HA	1.48	0.78
1:B:306:LEU:HD22	1:B:389:LEU:HD11	1.68	0.76
1:A:332:ASN:HD21	1:A:418:SER:HA	1.50	0.75
1:A:158:PHE:HB2	1:A:268:ILE:HD13	1.69	0.74
1:A:528:TYR:HB2	1:A:555:LEU:HD13	1.69	0.73
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.71	0.72
1:B:460:ASP:OD1	1:B:475:ARG:NH1	2.22	0.72
1:A:451:ILE:HG13	1:A:517:ILE:HD11	1.71	0.72
1:A:345:ASN:OD1	1:A:345:ASN:N	2.22	0.71
1:B:345:ASN:N	1:B:345:ASN:OD1	2.22	0.71
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.71	0.71
1:A:332:ASN:ND2	1:A:418:SER:HA	2.07	0.69
1:B:702:PRO:HB3	1:B:816:PRO:HG2	1.76	0.68
1:A:723:GLU:HG2	1:A:789:GLY:HA2	1.74	0.68
1:B:158:PHE:HB2	1:B:268:ILE:HD13	1.76	0.68
1:B:175:THR:HG23	1:B:671:GLU:H	1.59	0.68
1:A:844:LEU:HD22	1:A:909:ARG:HH21	1.58	0.67
1:B:169:VAL:HB	1:B:282:SER:HB2	1.77	0.67
1:A:772:PRO:HA	1:A:775:PHE:HB3	1.76	0.67
1:A:306:LEU:O	1:A:310:MET:HG3	1.94	0.67
1:A:517:ILE:HD13	1:A:555:LEU:HD21	1.78	0.66
1:A:497:PHE:HD1	1:A:497:PHE:H	1.44	0.66
1:A:716:MET:HG3	1:A:793:ALA:HB1	1.78	0.66
1:A:450:ASP:OD2	1:A:665:ARG:NH2	2.29	0.65
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.78	0.65
1:B:772:PRO:HA	1:B:775:PHE:HB3	1.79	0.65
1:A:755:ARG:HD3	1:A:769:ARG:NH2	2.12	0.64
1:A:34:ASP:O	1:A:38:LEU:HB2	1.97	0.64
1:A:175:THR:HG23	1:A:671:GLU:H	1.60	0.64
1:B:384:ARG:HD2	1:B:396:VAL:HB	1.80	0.63
1:B:638:GLY:HA2	1:B:669:GLN:HG3	1.79	0.63



A + 1	At arra 0	Interatomic	Clash	
Atom-1	Atom-1 Atom-2		overlap (Å)	
1:A:641:VAL:HG21	1:A:828:VAL:HG21	1.78	0.63	
1:B:739:ARG:NH1	1:B:744:GLU:OE1	2.32	0.63	
1:A:746:GLU:HG3	1:A:952:LEU:HD21	1.81	0.62	
1:B:843:LEU:HD22	1:B:906:LYS:HD2	1.82	0.62	
1:B:253:PRO:O	1:B:257:ARG:HG3	1.99	0.62	
1:B:656:PRO:HG2	1:B:659:THR:HG21	1.81	0.62	
1:A:908:ILE:HD12	1:A:944:TYR:CD2	2.35	0.61	
1:B:593:VAL:HG12	1:B:631:LEU:HD11	1.82	0.61	
1:B:888:ARG:O	1:B:890:ARG:N	2.34	0.61	
1:A:315:TYR:HB3	1:A:378:LEU:HD21	1.83	0.61	
1:A:106:ASN:OD1	1:A:890:ARG:NH2	2.34	0.60	
1:A:908:ILE:HD11	1:A:948:LEU:HB3	1.82	0.60	
1:A:228:ARG:HH12	1:A:938:LEU:HB3	1.67	0.59	
1:A:449:LEU:O	1:A:526:GLY:N	2.27	0.59	
1:A:884:LYS:HA	1:A:887:LEU:HD23	1.83	0.59	
1:B:908:ILE:HD11	1:B:948:LEU:HB3	1.84	0.59	
1:A:252:VAL:HG13	1:A:279:ILE:HD11	1.84	0.59	
1:A:318:GLN:HB3	1:A:435:PHE:HE1	1.66	0.58	
1:B:332:ASN:ND2	1:B:418:SER:HA	2.16	0.58	
1:A:739:ARG:NH1	1:A:744:GLU:OE1	2.37	0.57	
1:A:593:VAL:HG12	1:A:631:LEU:HD11	1.86	0.57	
1:B:181:SER:OG	2:B:1001:PO4:O1	2.17	0.57	
1:B:610:ALA:HA	1:B:613:LEU:HD12	1.86	0.57	
1:A:416:TYR:CD2	1:A:428:ALA:HB1	2.39	0.57	
1:A:243:TYR:OH	1:A:674:GLU:HG2	2.04	0.57	
1:B:318:GLN:HB3	1:B:435:PHE:HE1	1.70	0.57	
1:A:48:LEU:HD22	1:A:222:ARG:NH1	2.20	0.56	
1:A:201:ILE:H	1:A:201:ILE:HD13	1.71	0.56	
1:A:416:TYR:OH	1:A:429:ASP:OD1	2.17	0.56	
1:B:306:LEU:O	1:B:310:MET:HG3	2.05	0.56	
1:B:528:TYR:HB2	1:B:555:LEU:HD13	1.88	0.56	
1:A:638:GLY:HA2	1:A:669:GLN:CG	2.34	0.56	
1:B:611:TRP:CZ2	1:B:615:LYS:HE3	2.40	0.56	
1:A:37:LEU:HD21	1:A:193:LEU:HD21	1.88	0.56	
1:A:237:MET:O	1:A:241:MET:HG2	2.06	0.55	
1:B:844:LEU:HD22	1:B:909:ARG:HH21	1.72	0.55	
1:A:237:MET:HG2	1:A:303:VAL:HG12	1.87	0.55	
1:A:794:ILE:O	1:A:798:ILE:HG12	2.07	0.54	
1:A:262:ALA:O	1:A:266:ILE:HG12	2.07	0.54	
1:B:478:SER:H	1:B:481:ARG:NH1	2.04	0.54	
1:A:167:ASP:HB3	1:A:665:ARG:HG3	1.88	0.54	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:915:VAL:N	1:A:943:GLU:O	2.36	0.54
1:A:728:VAL:HG23	1:A:729:PHE:CD2	2.43	0.54
1:B:477:TRP:CG	1:B:481:ARG:HD2	2.43	0.54
1:B:501:LEU:HD12	1:B:502:PRO:HD2	1.90	0.53
1:A:406:GLU:HB3	1:A:409:LEU:HD12	1.89	0.53
1:B:315:TYR:HB3	1:B:378:LEU:HD21	1.90	0.53
1:A:602:LYS:NZ	1:A:768:LEU:O	2.33	0.53
1:B:621:VAL:HG21	1:B:659:THR:HG22	1.91	0.53
1:A:582:TRP:O	1:A:586:ARG:HD3	2.08	0.53
1:B:824:LEU:O	1:B:828:VAL:HG23	2.08	0.53
1:B:582:TRP:O	1:B:586:ARG:HD3	2.09	0.53
1:A:302:ASP:O	1:A:306:LEU:HB2	2.09	0.52
1:B:513:THR:O	1:B:517:ILE:HG13	2.10	0.52
1:B:728:VAL:HG23	1:B:729:PHE:CD2	2.45	0.52
1:A:656:PRO:HG2	1:A:659:THR:HG21	1.92	0.52
1:B:237:MET:O	1:B:241:MET:HG2	2.10	0.52
1:A:527:ALA:HB2	1:A:556:ARG:CZ	2.39	0.52
1:B:716:MET:SD	1:B:797:VAL:HG21	2.49	0.52
1:A:169:VAL:HB	1:A:282:SER:HB2	1.92	0.52
1:B:497:PHE:HD1	1:B:497:PHE:H	1.58	0.52
1:A:404:ASN:HB2	1:A:407:GLN:HB2	1.92	0.52
1:B:308:ARG:HG3	1:B:445:SER:HB3	1.91	0.52
1:B:454:GLU:HA	1:B:531:SER:HB2	1.91	0.51
1:A:165:THR:HG22	1:A:663:SER:HA	1.91	0.51
1:A:716:MET:CG	1:A:793:ALA:HB1	2.41	0.51
1:A:249:TRP:HE1	1:A:318:GLN:HE22	1.59	0.51
1:A:733:ARG:CZ	1:A:849:LEU:HD13	2.40	0.51
1:B:638:GLY:HA2	1:B:669:GLN:CG	2.39	0.51
1:B:724:TYR:CD1	1:B:788:LEU:HD23	2.46	0.51
1:A:641:VAL:HG21	1:A:828:VAL:CG2	2.40	0.51
1:A:786:VAL:HG11	1:A:828:VAL:HG21	1.93	0.51
1:B:201:ILE:HD13	1:B:201:ILE:H	1.75	0.51
1:B:642:GLY:HA3	1:B:774:ILE:HD12	1.92	0.51
1:B:794:ILE:O	1:B:798:ILE:HG12	2.10	0.51
1:B:887:LEU:HD23	1:B:887:LEU:H	1.76	0.51
1:A:83:LEU:HD12	1:A:899:VAL:HG12	1.92	0.51
1:A:49:HIS:HB3	1:A:53:LEU:HD23	1.92	0.50
1:B:33:TYR:HE1	1:B:36:LEU:HD22	1.75	0.50
1:A:846:SER:HB3	3:A:1123:HOH:O	2.12	0.50
1:B:723:GLU:HG2	1:B:789:GLY:HA2	1.93	0.50
1:B:161:LEU:HD13	1:B:695:LEU:HD22	1.92	0.50



<b>A</b> t a sec <b>1</b>	<b>A t</b> area <b>D</b>	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:641:VAL:HG21	1:B:828:VAL:HG21	1.93	0.50	
1:A:607:LEU:HB2	1:A:790:PHE:CE1	2.47	0.50	
1:B:37:LEU:HD11	1:B:108:ALA:HB2	1.94	0.49	
1:B:716:MET:HG3	1:B:793:ALA:HB1	1.93	0.49	
1:A:843:LEU:HD22	1:A:906:LYS:HD2	1.94	0.49	
1:B:861:GLU:HG3	1:B:865:LYS:HE3	1.95	0.49	
1:B:60:LEU:HD21	1:B:83:LEU:HD21	1.94	0.49	
1:A:202:THR:O	1:A:205:ASP:N	2.45	0.49	
1:B:501:LEU:O	1:B:503:LYS:HG3	2.13	0.49	
1:A:58:GLN:O	1:A:62:GLU:HG3	2.13	0.49	
1:A:244:PHE:HA	1:A:248:ILE:HB	1.94	0.49	
1:B:60:LEU:HG	1:B:79:LEU:HD21	1.94	0.49	
1:A:712:LEU:HG	1:A:716:MET:HE2	1.95	0.48	
1:A:343:HIS:HA	1:A:346:SER:HB2	1.94	0.48	
1:A:558:VAL:HG23	1:A:593:VAL:HA	1.94	0.48	
1:A:112:GLN:O	1:A:116:ARG:HB2	2.14	0.48	
1:A:150:LEU:HD11	1:A:700:ARG:HB2	1.96	0.48	
1:A:336:ARG:NH2	1:A:366:PRO:HG3	2.29	0.48	
1:B:240:GLY:HA3	1:B:285:MET:CE	2.44	0.47	
1:A:40:ARG:O	1:A:44:ILE:HG13	2.13	0.47	
1:A:457:ARG:NE	1:A:506:GLU:HB3	2.29	0.47	
1:B:791:GLY:HA2	1:B:866:LEU:HD12	1.96	0.47	
1:A:172:ALA:HB2	1:A:285:MET:HG3	1.95	0.47	
1:A:452:ARG:HG3	1:A:529:ILE:HB	1.96	0.47	
1:A:460:ASP:OD1	1:A:475:ARG:NH1	2.46	0.47	
1:A:174:PRO:O	1:A:747:TYR:OH	2.33	0.47	
1:A:497:PHE:N	1:A:497:PHE:CD1	2.83	0.47	
1:B:594:MET:HA	1:B:634:PHE:HB3	1.96	0.47	
1:B:563:LYS:NZ	1:B:766:GLU:OE2	2.48	0.47	
1:B:618:GLU:OE1	1:B:710:ARG:NH2	2.48	0.47	
1:B:952:LEU:O	1:B:955:THR:OG1	2.24	0.47	
1:A:294:ARG:HD3	1:A:754:SER:O	2.14	0.47	
1:B:150:LEU:HD11	1:B:700:ARG:HD3	1.97	0.47	
1:A:298:GLU:OE1	1:A:301[A]:ARG:NH1	2.48	0.47	
1:A:501:LEU:HD12	1:A:502:PRO:HD2	1.97	0.47	
1:A:618:GLU:CD	1:A:710:ARG:HH22	2.16	0.47	
1:B:112:GLN:O	1:B:116:ARG:HB2	2.15	0.47	
1:A:607:LEU:HB2	1:A:790:PHE:CZ	2.50	0.46	
1:B:587:ILE:HD13	1:B:587:ILE:HA	1.76	0.46	
1:A:724:TYR:CE2	1:A:728:VAL:HG21	2.50	0.46	
1:A:844:LEU:HD13	1:A:909:ARG:NH2	2.31	0.46	



<b>A 1 1</b>	<b>A t</b> area <b>D</b>	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:621:VAL:HG21	1:A:659:THR:HG22	1.98	0.46	
1:A:90:ASP:O	1:A:94:ILE:HG12	2.16	0.46	
1:A:388:LEU:HD12	1:A:388:LEU:HA	1.79	0.46	
1:B:497:PHE:HE1	1:B:548:GLU:HG3	1.81	0.46	
1:A:218:GLN:O	1:A:222:ARG:HB2	2.16	0.46	
1:B:90:ASP:O	1:B:94:ILE:HG12	2.15	0.46	
1:B:256:LEU:HB3	1:B:437:ARG:CZ	2.46	0.46	
1:B:890:ARG:O	1:B:894:ILE:HG13	2.15	0.46	
1:A:399:GLU:CD	1:A:399:GLU:H	2.18	0.46	
1:A:87:ASP:HB3	1:A:88:PRO:HD2	1.97	0.46	
1:B:78:GLU:O	1:B:81:SER:OG	2.34	0.46	
1:B:336:ARG:NH2	1:B:363:THR:O	2.48	0.46	
1:B:611:TRP:CE2	1:B:615:LYS:HE3	2.51	0.46	
1:B:739:ARG:HB3	1:B:745:LEU:HD11	1.97	0.46	
1:A:501:LEU:O	1:A:503:LYS:HG3	2.15	0.46	
1:B:410:GLU:HB3	1:B:411:PRO:HD3	1.97	0.45	
1:B:506:GLU:O	1:B:510:VAL:HG12	2.16	0.45	
1:B:558:VAL:HG23	1:B:593:VAL:HA	1.98	0.45	
1:A:308:ARG:NH2	1:A:523:ASP:OD1	2.49	0.45	
1:A:38:LEU:HD12	1:A:38:LEU:HA	1.76	0.45	
1:A:442:PHE:HB3	1:A:446:LEU:HD23	1.98	0.45	
1:A:848:GLU:O	1:A:851:PRO:HD2	2.17	0.45	
1:B:237:MET:HB2	1:B:237:MET:HE2	1.87	0.45	
1:B:746:GLU:HG3	1:B:952:LEU:HD21	1.98	0.45	
1:A:234:GLN:NE2	1:A:299:VAL:HG22	2.31	0.45	
1:A:326:MET:HG3	1:A:371:LEU:HD11	1.98	0.45	
1:A:244:PHE:C	1:A:246:GLU:H	2.20	0.45	
1:A:416:TYR:CE2	1:A:428:ALA:HB1	2.52	0.45	
1:A:314:MET:HB3	1:A:314:MET:HE2	1.85	0.45	
1:A:918:ARG:NE	3:A:1101:HOH:O	2.19	0.45	
1:A:945:ALA:HB1	1:A:946:PRO:HD2	1.99	0.45	
1:A:305:LEU:HD13	1:A:305:LEU:HA	1.83	0.45	
1:A:606[A]:ARG:HA	1:A:606[A]:ARG:HD2	1.88	0.45	
1:B:405:LEU:HD12	1:B:405:LEU:H	1.82	0.45	
1:B:450:ASP:OD2	1:B:665:ARG:NH2	2.50	0.45	
1:B:552:LYS:HG3	1:B:553:GLN:OE1	2.17	0.45	
1:B:724:TYR:O	1:B:728:VAL:HG22	2.17	0.45	
1:A:301[B]:ARG:HA	1:A:520:LEU:HD11	1.98	0.45	
1:A:80:GLY:O	1:A:84:THR:HG23	2.17	0.44	
1:A:237:MET:HE3	1:A:303:VAL:HB	1.99	0.44	
1:A:301[A]:ARG:HA	1:A:520:LEU:HD11	1.97	0.44	



A 4 1	A t area 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:61:TYR:HE1	1:B:889:LEU:HD11	1.82	0.44	
1:B:139:LEU:N	1:B:688:GLN:OE1	2.50	0.44	
1:B:712:LEU:HD11	1:B:797:VAL:HG13	1.99	0.44	
1:A:180:ARG:N	2:A:1001:PO4:O4	2.50	0.44	
1:A:480:GLU:H	1:A:480:GLU:HG2	1.47	0.44	
1:A:723:GLU:O	1:A:726:SER:OG	2.28	0.44	
1:A:506:GLU:O	1:A:510:VAL:HG12	2.18	0.44	
1:B:89:GLY:O	1:B:93:VAL:HG23	2.18	0.44	
1:A:338:ARG:O	1:A:342:VAL:HG23	2.17	0.44	
1:A:490:LEU:HB3	1:A:582:TRP:CZ2	2.52	0.44	
1:A:495:PRO:O	1:B:494:ARG:NE	2.46	0.44	
1:A:733:ARG:NH1	1:A:849:LEU:HD13	2.32	0.44	
1:B:244:PHE:C	1:B:246:GLU:H	2.20	0.44	
1:B:723:GLU:O	1:B:726:SER:OG	2.35	0.44	
1:A:755:ARG:HD3	1:A:769:ARG:CZ	2.48	0.44	
1:B:457:ARG:NE	1:B:506:GLU:HB3	2.33	0.44	
1:B:615:LYS:NZ	1:B:714:ASP:OD1	2.34	0.44	
1:B:52:ASP:OD1	1:B:52:ASP:N	2.51	0.44	
1:B:416:TYR:CD2	1:B:428:ALA:HB1	2.53	0.43	
1:A:463:ASP:HB2	1:A:475:ARG:HG3	1.99	0.43	
1:B:587:ILE:HD12	1:B:590:LYS:O	2.18	0.43	
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.80	0.43	
1:A:252:VAL:HG11	1:A:441:THR:HG21	1.99	0.43	
1:A:252:VAL:HB	1:A:253:PRO:HD3	2.01	0.43	
1:B:157:ILE:O	1:B:161:LEU:HB2	2.18	0.43	
1:B:202:THR:O	1:B:205:ASP:N	2.50	0.43	
1:B:350:ALA:HB1	1:B:352:LYS:HG3	2.00	0.43	
1:A:583:TYR:CZ	1:A:587:ILE:HG12	2.54	0.43	
1:B:66:GLU:HB2	1:B:75:LYS:HE2	2.01	0.43	
1:B:168:LEU:O	1:B:281:PHE:HA	2.18	0.43	
1:B:463:ASP:HB2	1:B:475:ARG:HG3	2.00	0.43	
1:A:283:SER:O	1:A:449:LEU:HD12	2.17	0.43	
1:B:477:TRP:HA	1:B:481:ARG:NH1	2.34	0.43	
1:B:590:LYS:HG2	1:B:630:LYS:HE2	2.00	0.43	
1:B:821:THR:O	1:B:825:ILE:HG12	2.17	0.43	
1:B:167:ASP:HB3	1:B:665:ARG:HG3	2.01	0.43	
1:B:169:VAL:HA	1:B:282:SER:O	2.19	0.43	
1:B:365:GLU:H	1:B:365:GLU:HG2	1.71	0.43	
1:A:454:GLU:HA	1:A:531:SER:HB2	2.00	0.42	
1:B:157:ILE:HG23	1:B:695:LEU:HD21	2.00	0.42	
1:B:496:LEU:HB3	1:B:497:PHE:H	1.68	0.42	



	A t area 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:724:TYR:HD1	1:A:788:LEU:HB3	1.84	0.42	
1:A:834:PRO:HG3	1:A:860:PHE:CE1	2.55	0.42	
1:A:857:ARG:O	1:A:860:PHE:HB3	2.20	0.42	
1:B:244:PHE:HA	1:B:248:ILE:HB	2.00	0.42	
1:B:451:ILE:HG13	1:B:517:ILE:HD11	2.01	0.42	
1:B:510:VAL:O	1:B:513:THR:OG1	2.29	0.42	
1:B:528:TYR:HB2	1:B:555:LEU:CD1	2.49	0.42	
1:A:234:GLN:HE22	1:A:299:VAL:HG22	1.83	0.42	
1:B:603:ASP:OD1	1:B:603:ASP:N	2.43	0.42	
1:B:786:VAL:HG11	1:B:828:VAL:HG11	2.01	0.42	
1:A:520:LEU:HD23	1:A:520:LEU:HA	1.84	0.42	
1:B:497:PHE:CD1	1:B:497:PHE:N	2.87	0.42	
1:B:733:ARG:NH2	1:B:736:GLU:OE2	2.52	0.42	
1:A:139:LEU:HD11	1:A:259:VAL:HG22	2.01	0.42	
1:B:294:ARG:HD3	1:B:754:SER:O	2.19	0.42	
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.70	0.42	
1:A:716:MET:SD	1:A:797:VAL:HG21	2.58	0.42	
1:B:562:GLU:HG2	1:B:599:ASP:HB2	2.02	0.42	
1:A:86:LEU:HD13	1:A:94:ILE:HG13	2.01	0.42	
1:A:179:ARG:HB2	2:A:1001:PO4:O4	2.19	0.42	
1:A:497:PHE:HE1	1:A:548:GLU:HG3	1.85	0.42	
1:B:96:LYS:HE2	1:B:225:GLU:OE2	2.20	0.42	
1:A:169:VAL:HA	1:A:282:SER:O	2.19	0.42	
1:A:768:LEU:HD13	1:A:769:ARG:O	2.20	0.42	
1:B:273:PRO:HB2	1:B:276:ALA:HB2	2.01	0.42	
1:B:302:ASP:O	1:B:306:LEU:HB2	2.20	0.42	
1:A:496:LEU:HB3	1:A:497:PHE:H	1.64	0.42	
1:B:48:LEU:HD22	1:B:222:ARG:NH1	2.35	0.41	
1:A:611:TRP:CZ2	1:A:615:LYS:HD3	2.55	0.41	
1:B:153:SER:OG	1:B:156:GLU:HG3	2.20	0.41	
1:B:406:GLU:HA	1:B:409:LEU:HB2	2.02	0.41	
1:A:76:LEU:HB3	1:A:839:LEU:HD22	2.02	0.41	
1:A:242:SER:HA	1:A:245:HIS:NE2	2.36	0.41	
1:B:591:GLN:NE2	1:B:592:GLU:O	2.48	0.41	
1:A:462:LEU:O	1:A:466:THR:HG23	2.20	0.41	
1:A:784:LEU:HB3	1:A:785:PRO:HD3	2.02	0.41	
1:B:86:LEU:HD13	1:B:94:ILE:HG13	2.03	0.41	
1:B:289:ARG:HG2	1:B:452:ARG:O	2.20	0.41	
1:A:60:LEU:HD21	1:A:83:LEU:HD21	2.02	0.41	
1:A:402:PHE:CZ	1:A:408:PHE:HA	2.56	0.41	
1:A:724:TYR:CD1	1:A:788:LEU:HD23	2.55	0.41	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:614:TYR:CZ	1:B:656:PRO:HB3	2.56	0.41
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.90	0.41
1:A:490:LEU:HD13	1:A:582:TRP:CZ3	2.56	0.41
1:B:245:HIS:H	1:B:245:HIS:CD2	2.38	0.41
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.90	0.41
1:B:724:TYR:CE2	1:B:728:VAL:HG21	2.56	0.41
1:A:52:ASP:OD1	1:A:52:ASP:N	2.54	0.41
1:A:274:TYR:OH	1:A:413:GLU:OE2	2.35	0.41
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.91	0.41
1:A:530:ILE:HD13	1:A:530:ILE:HG21	1.80	0.41
1:A:657:PRO:HB3	1:A:702:PRO:HD2	2.02	0.41
1:A:703:ILE:HD12	1:A:814:HIS:O	2.20	0.41
1:A:917:LEU:H	1:A:917:LEU:HG	1.79	0.41
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.95	0.41
1:B:672:VAL:HA	1:B:675:GLN:HB2	2.03	0.41
1:B:408:PHE:O	1:B:411:PRO:HD2	2.21	0.41
1:B:777:TRP:HA	1:B:780:THR:HG22	2.02	0.41
1:A:115:TYR:O	1:A:119:ILE:HG22	2.21	0.40
1:A:587:ILE:HD13	1:A:587:ILE:HA	1.74	0.40
1:B:98:PHE:CZ	1:B:896:THR:HG21	2.56	0.40
1:B:174:PRO:HB3	1:B:753:GLY:HA3	2.03	0.40
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.93	0.40
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.81	0.40
1:B:201:ILE:O	1:B:201:ILE:HG12	2.20	0.40
1:A:168:LEU:O	1:A:281:PHE:HA	2.21	0.40
1:A:546:GLN:OE1	1:A:555:LEU:N	2.53	0.40
1:A:712:LEU:O	1:A:716:MET:HB2	2.21	0.40
1:A:798:ILE:HG12	1:A:798:ILE:H	1.69	0.40
1:B:621:VAL:HG21	1:B:659:THR:HA	2.02	0.40
1:B:801:ASP:OD2	1:B:803:ARG:NH2	2.55	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	899/974~(92%)	849 (94%)	44 (5%)	6 (1%)	22	58
1	В	880/974~(90%)	832 (94%)	43~(5%)	5(1%)	25	61
All	All	1779/1948~(91%)	1681 (94%)	87 (5%)	11 (1%)	25	61

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

All (11) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	670	GLY
1	А	918	ARG
1	А	919	PRO
1	В	670	GLY
1	В	889	LEU
1	А	848	GLU
1	А	911	PRO
1	В	848	GLU
1	В	888	ARG
1	В	911	PRO
1	А	119	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	779/850~(92%)	713~(92%)	66~(8%)	10	36	
1	В	769/850~(90%)	710~(92%)	59~(8%)	13	41	
All	All	1548/1700~(91%)	1423~(92%)	125~(8%)	11	39	

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	33	TYR
1	А	54	ARG



Mol	Chain	Res	Type
1	А	71	HIS
1	А	79	LEU
1	А	102	LEU
1	А	116	ARG
1	А	117	ARG
1	А	149	ASP
1	А	165	THR
1	А	169	VAL
1	А	175	THR
1	А	182	LEU
1	А	196	LEU
1	А	201	ILE
1	А	228	ARG
1	А	237	MET
1	А	256	LEU
1	А	269	GLU
1	А	279	ILE
1	А	306	LEU
1	А	308	ARG
1	А	318	GLN
1	А	319	ILE
1	А	324	PHE
1	А	328	MET
1	А	332	ASN
1	А	345	ASN
1	А	348	LYS
1	А	349	ASP
1	А	358	TRP
1	А	359	LYS
1	А	365	GLU
1	А	384	ARG
1	А	388	LEU
1	А	393	HIS
1	А	406	GLU
1	A	469	LEU
1	A	480	GLU
1	А	497	PHE
1	A	504	THR
1	А	509	ASP
1	А	510	VAL
1	А	552	LYS
1	А	555	LEU



Mol	Chain	Res	Type
1	А	558	VAL
1	А	567	LEU
1	А	587	ILE
1	А	632	THR
1	А	634	PHE
1	А	658	ASP
1	А	665	ARG
1	А	688	GLN
1	А	713	LEU
1	А	716	MET
1	А	723	GLU
1	А	767	SER
1	А	768	LEU
1	А	771	ILE
1	А	798	ILE
1	А	799	GLU
1	А	849	LEU
1	А	882	TYR
1	А	887	LEU
1	А	889	LEU
1	А	917	LEU
1	А	954	LEU
1	В	33	TYR
1	В	34	ASP
1	В	54	ARG
1	В	71	HIS
1	В	102	LEU
1	В	116	ARG
1	В	149	ASP
1	В	165	THR
1	В	169	VAL
1	В	182	LEU
1	В	196	LEU
1	B	201	ILE
1	В	228	ARG
1	В	237	MET
1	В	256	LEU
1	B	269	GLU
1	В	278	LEU
1	В	279	ILE
1	В	306	LEU
1	В	308	ARG



Mol	Chain	Res	Type
1	В	319	ILE
1	В	324	PHE
1	В	328	MET
1	В	332	ASN
1	В	345	ASN
1	В	348	LYS
1	В	349	ASP
1	В	358	TRP
1	В	359	LYS
1	В	365	GLU
1	В	378	LEU
1	В	384	ARG
1	В	388	LEU
1	В	393	HIS
1	В	399	GLU
1	В	406	GLU
1	В	469	LEU
1	В	493	LYS
1	В	497	PHE
1	В	504	THR
1	В	510	VAL
1	В	552	LYS
1	В	555	LEU
1	В	558	VAL
1	В	567	LEU
1	В	587	ILE
1	В	632	THR
1	В	658	ASP
1	В	688	GLN
1	В	716	MET
1	В	723	GLU
1	В	767	SER
1	В	768	LEU
1	В	771	ILE
1	В	798	ILE
1	В	799	GLU
1	В	849	LEU
1	В	887	LEU
1	В	954	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	112	GLN
1	В	332	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)

2 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 True		Chain	Dec	Dec Link	Tinle	Bond lengths		Bond angles		
1VIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	PO4	В	1001	-	$4,\!4,\!4$	0.98	0	$6,\!6,\!6$	0.45	0
2	PO4	А	1001	-	4,4,4	1.27	0	$6,\!6,\!6$	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1001	PO4	1	0
2	А	1001	PO4	2	0

## 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	906/974~(93%)	-0.12	12 (1%) 77 68	58, 95, 156, 252	0
1	В	890/974~(91%)	0.51	101 (11%) 5 4	91, 168, 241, 297	0
All	All	1796/1948~(92%)	0.19	113 (6%) 20 13	58, 126, 227, 297	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	815	TRP	8.9
1	В	790	PHE	7.4
1	В	607	LEU	6.9
1	В	794	ILE	6.4
1	В	197	TYR	6.3
1	В	916	THR	6.2
1	В	608	SER	6.0
1	В	705	PRO	5.9
1	В	818	PHE	5.9
1	В	118	ARG	5.5
1	В	245	HIS	5.0
1	В	869	GLN	4.8
1	В	823	ASP	4.7
1	В	793	ALA	4.6
1	В	143	PHE	4.4
1	В	246	GLU	4.4
1	В	716	MET	4.3
1	В	611	TRP	4.0
1	В	692	ALA	4.0
1	В	266	ILE	3.9
1	В	782	PHE	3.8
1	В	809	GLN	3.7
1	В	49	HIS	3.7
1	В	638	GLY	3.7



80JZ
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Mol	Chain	Res	Type	RSRZ
1	В	829	PHE	3.6
1	В	564	LEU	3.6
1	В	603	ASP	3.5
1	В	101	MET	3.5
1	В	678	SER	3.4
1	В	193	LEU	3.4
1	В	116	ARG	3.4
1	В	181	SER	3.3
1	В	221	PHE	3.2
1	А	197	TYR	3.2
1	В	261	THR	3.1
1	В	779	GLN	3.1
1	В	606	ARG	3.1
1	В	719	VAL	3.1
1	В	263	LEU	3.1
1	В	247	THR	3.0
1	В	196	LEU	3.0
1	В	330	ARG	3.0
1	В	268	ILE	3.0
1	А	136	GLU	3.0
1	В	703	ILE	3.0
1	В	765	ILE	3.0
1	В	822	ILE	3.0
1	В	144	LYS	3.0
1	В	38	LEU	2.9
1	В	826	GLU	2.9
1	В	812	TYR	2.9
1	А	350	ALA	2.9
1	В	146	LEU	2.9
1	В	737	TYR	2.9
1	В	720	ALA	2.9
1	В	278	LEU	2.9
1	В	932	ALA	2.9
1	В	98	PHE	2.8
1	В	250	LYS	2.7
1	В	329	TRP	2.6
1	В	490	LEU	2.6
1	В	37	LEU	2.6
1	В	72	GLU	2.6
1	В	153	SER	2.6
1	А	709	TRP	2.5
1	В	137	SER	2.5



Mol	Chain	Res	Type	RSRZ	
1	A	317	ASN	2.5	
1	В	117	ARG	2.5	
1	В	161	LEU	2.5	
1	В	350	ALA	2.5	
1	А	78	GLU	2.5	
1	В	795	ARG	2.5	
1	В	317	ASN	2.5	
1	В	154	PRO	2.4	
1	В	93	VAL	2.4	
1	В	139	LEU	2.4	
1	В	728	VAL	2.4	
1	В	712	LEU	2.4	
1	В	933	LYS	2.4	
1	В	142	THR	2.4	
1	В	688	GLN	2.4	
1	В	41	PHE	2.4	
1	В	811	MET	2.4	
1	В	119	ILE	2.3	
1	В	741	ALA	2.3	
1	В	691	THR	2.3	
1	А	703	ILE	2.3	
1	А	761	PRO	2.3	
1	В	816	PRO	2.3	
1	В	727	VAL	2.3	
1	В	954	LEU	2.2	
1	В	69	GLY	2.2	
1	В	265	ASN	2.2	
1	В	808	LEU	2.2	
1	В	321	ASP	2.2	
1	А	352	LYS	2.2	
1	В	141	GLU	2.2	
1	В	791	GLY	2.2	
1	В	39	ASP	2.2	
1	A	497	PHE	2.2	
1	B	699	MET	2.2	
1	В	670	GLY	2.2	
1	В	935	LEU	2.2	
1	В	934	GLU	2.2	
1	В	70	LYS	2.2	
1	A	193	LEU	2.1	
1	В	639	GLY	2.1	
1	В	694	THR	2.1	



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Mol	Chain	Res	Type	RSRZ
1	В	94	ILE	2.1
1	А	88	PRO	2.1
1	В	158	PHE	2.1
1	В	944	TYR	2.0
1	В	115	TYR	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	$B-factors(Å^2)$	Q<0.9
2	PO4	В	1001	5/5	0.91	0.74	181,185,189,199	0
2	PO4	А	1001	5/5	0.92	0.35	121,126,131,134	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

