

Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 05:23 AM EDT

Title : Crystal structure of the photosynthetic phosphoenolpyruvate can	rboxylase
isoenzyme from maize in complex with Gly	
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Deposited on : 2017-05-25	
Resolution : $3.30 \text{ Å}(\text{reported})$	

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

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

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	970	% 73%	20%	• 5%
1	В	970	74%	20%	• 5%
1	С	970	% 7 5%	19%	• 5%
1	D	970	% 	18%	• 5%

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	GLY	В	1001	-	Х	-	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29339 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	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	018	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	Л	910	7318	4646	1275	1367	30	0	0	0
1	В	017	Total	С	Ν	Ο	S	0	0	0
1	D	911	7309	4640	1274	1365	30	0	0	U
1	С	018	Total	С	Ν	Ο	S	0	0	0
1		918	7318	4645	1275	1368	30	0		0
1	а	018	Total	С	Ν	Ο	S	0	0	0
I D	918	7317	4646	1275	1366	30	0	0	U	

• Molecule 1 is a protein called Phosphoenolpyruvate carboxylase.

• Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



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



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Mol	Chain	Residues	A	ton	\mathbf{ns}		ZeroOcc	AltConf
2	В	1	Total 5	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	N 1	0 2	0	0
2	С	1	Total 5	C 2	N 1	O 2	0	0
2	D	1	Total 5	С 2	N 1	O 2	0	0

• Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	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: Phosphoenolpyruvate carboxylase

 \bullet Molecule 1: Phosphoenolpyruvate carboxylase

Chain B: 20% • 5% 74%













4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	156.95Å 167.24Å 242.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	57.08 - 3.30	Depositor
Resolution (A)	57.08 - 3.30	EDS
% Data completeness	93.2 (57.08-3.30)	Depositor
(in resolution range)	93.3 (57.08-3.30)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.87 (at 3.33 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
B B.	0.210 , 0.253	Depositor
II, II free	0.212 , 0.251	DCC
R_{free} test set	4518 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 29.3	EDS
L-test for $twinning^2$	$ < L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29339	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 38.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4006e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: ACT

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.34	0/7473	0.51	0/10119	
1	В	0.35	0/7464	0.53	0/10108	
1	С	0.33	0/7473	0.50	0/10120	
1	D	0.33	0/7472	0.50	0/10119	
All	All	0.34	0/29882	0.51	0/40466	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	7318	0	7314	114	0
1	В	7309	0	7303	114	0
1	С	7318	0	7309	100	0
1	D	7317	0	7314	98	0
2	А	5	0	2	1	0
2	В	10	0	4	1	0
2	С	5	0	2	1	0
2	D	5	0	2	0	0
3	A	12	0	9	2	0



pagen						
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	12	0	9	0	0
3	С	16	0	12	0	0
3	D	12	0	9	1	0
All	All	29339	0	29289	414	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 7.

All (414) 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:388:ARG:HH12	1:B:402:ALA:HA	1.39	0.88
1:D:743:ARG:HH22	1:D:762:LYS:HE3	1.43	0.82
1:B:386:ARG:NH1	1:B:387:GLU:OE1	2.17	0.77
1:C:362:TRP:NE1	1:C:380:ASP:OD2	2.19	0.75
1:B:568:LEU:HD22	1:B:608:ALA:HB2	1.67	0.74
1:A:465:VAL:HG22	1:A:511:ILE:HG23	1.69	0.74
1:B:276:LEU:HD12	1:B:277:PRO:HD2	1.71	0.72
1:C:720:MET:HB3	1:C:797:ALA:HB1	1.70	0.72
1:D:88:THR:HB	1:D:919:VAL:HG21	1.72	0.72
1:C:487:GLN:OE1	1:C:580:ARG:NH1	2.24	0.71
1:B:465:VAL:HG22	1:B:511:ILE:HG23	1.72	0.70
1:C:568:LEU:HD22	1:C:608:ALA:HB2	1.73	0.69
1:B:812:LEU:HA	1:B:815:MET:HE3	1.76	0.68
1:C:88:THR:HB	1:C:919:VAL:HG11	1.75	0.66
1:A:293:ARG:NH2	1:A:304:THR:OG1	2.27	0.66
1:D:312:ARG:HH21	1:D:528:SER:HB3	1.60	0.66
1:C:41:LEU:HD12	1:C:112:ALA:HB2	1.79	0.65
1:A:192:ARG:NH1	1:A:220:GLU:OE1	2.30	0.65
1:A:103:LEU:HD13	1:A:961:GLY:HA2	1.78	0.65
1:D:259:PHE:HE1	1:D:692:GLN:HE21	1.45	0.64
1:A:937:GLY:HA2	1:A:940:LYS:HD2	1.79	0.64
1:C:40:LEU:HG	1:C:44:ARG:HH21	1.62	0.63
1:D:171:ASP:HB3	1:D:669:ARG:HG2	1.80	0.63
1:A:720:MET:HB3	1:A:797:ALA:HB1	1.81	0.63
1:D:288:TRP:CD1	1:D:454:ASP:HB2	2.35	0.62
1:D:564:LEU:HD13	1:D:598:MET:HG2	1.80	0.62
1:D:659:GLN:HA	3:D:1004:ACT:H1	1.81	0.62
1:C:293:ARG:NH2	1:C:304:THR:OG1	2.32	0.61
1:C:178:PRO:O	1:C:751:TYR:OH	2.17	0.61
1:A:606:LYS:HG3	1:A:777:TRP:CD1	2.36	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:206:THR:HB	1:C:209:ASP:H	1.67	0.60
1:B:505:LEU:HD12	1:B:506:PRO:HD2	1.83	0.60
1:D:336:ASN:HD22	1:D:422:SER:HA	1.66	0.60
1:A:361:PHE:HD2	1:A:379:ARG:HH12	1.49	0.60
1:B:501:LEU:HD12	1:B:502:PRO:HD2	1.84	0.60
1:A:706:PRO:HB3	1:A:820:PRO:HG2	1.84	0.59
1:C:276:LEU:HD12	1:C:277:PRO:HD2	1.84	0.59
1:A:499:PRO:HB2	1:C:499:PRO:HB2	1.84	0.59
1:C:743:ARG:NH1	1:C:748:GLU:OE2	2.35	0.59
1:D:428:ASP:HB3	1:D:431:ILE:HD12	1.82	0.59
1:A:241:MET:HG3	1:A:307:VAL:HG13	1.84	0.59
1:A:764:ARG:HG3	1:A:765:PRO:HD2	1.84	0.59
1:A:657:LEU:HG	1:A:820:PRO:HB3	1.86	0.58
1:A:428:ASP:HB3	1:A:431:ILE:HD12	1.84	0.58
1:B:173:VAL:HG22	1:B:286:SER:HB2	1.84	0.58
1:D:790:VAL:HG11	1:D:832:VAL:HG21	1.85	0.58
1:B:487:GLN:OE1	1:B:580:ARG:NH1	2.36	0.58
1:B:103:LEU:HD13	1:B:961:GLY:HA2	1.86	0.58
1:A:171:ASP:HB3	1:A:669:ARG:HG2	1.85	0.57
1:C:421:LYS:NZ	1:C:425:ASP:OD2	2.35	0.57
1:C:597:VAL:HG12	1:C:635:LEU:HD11	1.87	0.57
1:C:355:THR:HG22	1:C:357:TYR:HB3	1.86	0.57
1:D:568:LEU:HD12	1:D:616:GLN:HG2	1.86	0.57
1:B:248:ILE:HA	1:B:252:VAL:HB	1.87	0.57
1:C:115:VAL:HG21	1:C:197:LEU:HD23	1.86	0.57
1:D:63:GLU:OE1	1:D:86:LYS:NZ	2.34	0.57
1:D:147:LEU:HB3	1:D:270:ILE:HD13	1.87	0.57
1:B:88:THR:HB	1:B:919:VAL:HG21	1.85	0.57
1:C:604:SER:HB3	1:C:613:ALA:HB1	1.87	0.57
1:A:49:LEU:HD11	1:A:57:LEU:HD22	1.87	0.57
1:B:770:THR:HG23	1:B:771:THR:HG23	1.87	0.56
1:B:727:GLU:OE2	1:B:863:LYS:NZ	2.38	0.56
1:C:550:GLN:OE1	1:C:559:LEU:N	2.38	0.56
1:C:248:ILE:HA	1:C:252:VAL:HB	1.88	0.56
1:C:312:ARG:HH21	1:C:528:SER:HB3	1.70	0.56
1:A:767:GLY:O	1:A:770:THR:HG22	2.05	0.56
1:B:184:ARG:O	1:B:188:GLN:HG3	2.06	0.56
1:C:110:ASN:O	1:C:114:GLU:HG3	2.06	0.56
1:D:96:ILE:HG21	1:D:938:LEU:HD21	1.87	0.55
1:D:725:THR:HG22	1:D:729:ARG:HD2	1.86	0.55
1:A:288:TRP:CD1	1:A:454:ASP:HB2	2.42	0.55



	a do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:334:ARG:NH1	1:B:928:GLU:OE2	2.38	0.55
1:D:388:ARG:HH12	1:D:402:ALA:HA	1.71	0.55
1:A:52:LEU:HD13	1:A:226:ARG:NH1	2.21	0.55
1:C:101:SER:O	1:C:105:MET:HG3	2.06	0.55
1:A:88:THR:HB	1:A:919:VAL:HG21	1.89	0.55
1:B:930:ALA:HB3	1:B:931:ASP:HA	1.88	0.55
1:A:178:PRO:O	1:A:751:TYR:OH	2.24	0.55
1:C:241:MET:O	1:C:245:MET:HG2	2.06	0.55
1:D:67:VAL:HG11	1:D:83:LEU:HB2	1.89	0.55
1:D:121:ARG:NH1	1:D:689:GLN:OE1	2.41	0.54
1:B:550:GLN:OE1	1:B:559:LEU:N	2.40	0.54
1:A:652:THR:HB	1:A:693:ARG:HD3	1.90	0.54
1:B:288:TRP:CD1	1:B:454:ASP:HB2	2.42	0.54
1:A:730:SER:HA	1:A:734:LYS:HE3	1.88	0.54
1:B:499:PRO:HB2	1:D:499:PRO:HB2	1.88	0.54
1:A:727:GLU:OE2	1:A:863:LYS:NZ	2.40	0.54
1:D:501:LEU:HD12	1:D:502:PRO:HD2	1.90	0.54
1:C:196:CYS:O	1:C:200:LEU:HB2	2.08	0.53
1:A:602:SER:HB2	3:A:1002:ACT:H1	1.90	0.53
1:A:189:LYS:HG2	1:A:192:ARG:HH12	1.73	0.53
1:A:743:ARG:NH1	1:A:748:GLU:OE2	2.41	0.53
1:C:165:LEU:HD12	1:C:267:LEU:HD21	1.91	0.53
1:A:568:LEU:HD12	1:A:616:GLN:HG2	1.91	0.53
1:B:171:ASP:HB3	1:B:669:ARG:HG2	1.90	0.53
1:C:184:ARG:O	1:C:188:GLN:HG3	2.09	0.52
1:A:621:GLN:HG2	1:A:637:LEU:HD13	1.92	0.52
1:C:70:ASP:HB3	1:C:79:LYS:HE3	1.91	0.52
1:A:149:ARG:NH1	1:A:700:GLU:OE1	2.42	0.52
1:A:742:PHE:CZ	1:A:748:GLU:HG3	2.43	0.52
1:A:872:LEU:HD21	1:A:880:ILE:HD12	1.91	0.52
1:B:312:ARG:HH21	1:B:528:SER:HB3	1.74	0.52
1:B:716:LEU:HD23	1:B:815:MET:HE2	1.92	0.52
1:C:141:SER:OG	1:C:149:ARG:NH2	2.41	0.52
1:B:214:ASP:O	1:B:218:GLN:HG2	2.09	0.52
1:C:142:ASP:HB2	1:C:692:GLN:OE1	2.09	0.52
1:A:550:GLN:OE1	1:A:559:LEU:N	2.42	0.52
1:B:336:ASN:HD22	1:B:422:SER:HB2	1.75	0.52
1:B:249:HIS:CD2	1:B:318:LEU:HD21	2.44	0.52
1:D:904:PHE:O	1:D:908:THR:OG1	2.18	0.51
1:C:241:MET:HG3	1:C:307:VAL:HG13	1.92	0.51
1:C:465:VAL:HG22	1:C:511:ILE:HG23	1.91	0.51



	i ageni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:615:TRP:CZ2	1:B:619:ARG:HD2	2.46	0.51
1:D:113:GLU:O	1:D:117:ILE:HG12	2.11	0.51
1:B:498:ARG:HD2	1:D:473:LEU:HD13	1.92	0.51
1:A:568:LEU:HD22	1:A:608:ALA:HB2	1.93	0.51
1:D:388:ARG:NH1	1:D:401:SER:O	2.43	0.51
1:A:276:LEU:HD12	1:A:277:PRO:HD2	1.92	0.51
1:B:652:THR:HB	1:B:693:ARG:HD3	1.93	0.51
1:C:433:ASP:HA	1:C:437:LEU:HB2	1.92	0.51
1:B:333:TRP:CZ3	1:B:334:ARG:HG2	2.45	0.51
1:B:52:LEU:HD13	1:B:226:ARG:HH11	1.76	0.50
1:B:566:GLU:HG2	1:B:603:ASP:HB2	1.92	0.50
1:B:732:VAL:HG23	1:B:733:VAL:HG23	1.92	0.50
1:A:595:GLN:NE2	1:A:596:GLN:O	2.43	0.50
1:D:489:TRP:O	1:D:492:SER:OG	2.25	0.50
1:C:226:ARG:NE	1:D:428:ASP:OD1	2.43	0.50
1:A:237:PRO:HB2	1:A:303:VAL:HG11	1.94	0.50
1:B:102:ILE:HG21	1:B:901:LEU:HG	1.94	0.50
1:D:184:ARG:O	1:D:188:GLN:HG3	2.12	0.50
1:D:241:MET:O	1:D:245:MET:HG2	2.11	0.50
1:D:248:ILE:HA	1:D:252:VAL:HB	1.93	0.50
1:C:606:LYS:HG3	1:C:777:TRP:CD1	2.47	0.50
1:C:168:GLN:HG3	1:C:666:GLY:HA2	1.93	0.50
1:D:910:LYS:HE2	1:D:917:PHE:CD1	2.46	0.50
1:A:467:ASP:OD1	1:A:477:SER:OG	2.26	0.50
1:C:710:LYS:NZ	1:C:814:GLU:OE1	2.45	0.50
1:A:52:LEU:HD13	1:A:226:ARG:HH11	1.77	0.49
1:A:812:LEU:HA	1:A:815:MET:HE2	1.94	0.49
1:B:196:CYS:O	1:B:200:LEU:HB2	2.12	0.49
1:C:446:PHE:HB3	1:C:450:LEU:HD12	1.94	0.49
1:D:761:ALA:HB1	1:D:776:PRO:HG3	1.93	0.49
1:A:168:GLN:HG3	1:A:666:GLY:HA2	1.94	0.49
1:A:747:PRO:HB3	1:A:909:LEU:HD11	1.94	0.49
1:A:102:ILE:HG21	1:A:901:LEU:HG	1.94	0.49
1:B:326:LEU:HD21	1:B:436:LEU:HD13	1.94	0.49
1:D:276:LEU:HD12	1:D:277:PRO:HD2	1.93	0.49
1:C:171:ASP:HB3	1:C:669:ARG:HG2	1.95	0.49
1:A:241:MET:O	1:A:245:MET:HG2	2.13	0.49
1:B:680:CYS:HB3	1:B:690:THR:HG21	1.94	0.49
1:C:591:ILE:HB	1:C:594:LYS:O	2.13	0.49
1:D:277:PRO:HG2	1:D:280:VAL:HG23	1.94	0.49
1:D:337:ASP:O	1:D:341:VAL:HG23	2.13	0.49



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:184:ARG:O	1:A:188:GLN:HG3	2.13	0.49
1:D:386:ARG:NH1	1:D:387:GLU:OE2	2.46	0.49
1:A:388:ARG:NH1	1:A:401:SER:O	2.45	0.49
1:C:568:LEU:HD12	1:C:616:GLN:HG2	1.95	0.49
1:A:357:TYR:HD2	1:A:358:TYR:N	2.11	0.48
1:B:483:GLU:OE1	1:B:541:SER:HB3	2.13	0.48
1:A:248:ILE:HA	1:A:252:VAL:HB	1.95	0.48
1:A:948:PRO:HB2	1:A:951:LEU:HD12	1.96	0.48
1:B:564:LEU:HD13	1:B:598:MET:HG2	1.96	0.48
1:B:706:PRO:HB3	1:B:820:PRO:HG2	1.94	0.48
1:C:922:GLN:HB3	1:C:923:PRO:HD2	1.95	0.48
1:D:178:PRO:O	1:D:751:TYR:OH	2.31	0.48
1:A:854:LYS:N	1:A:855:PRO:HD2	2.28	0.48
1:B:113:GLU:O	1:B:117:ILE:HG12	2.14	0.48
1:D:110:ASN:O	1:D:114:GLU:HG3	2.14	0.48
1:D:894:ARG:HG2	1:D:898:ILE:HD11	1.94	0.48
1:B:742:PHE:CZ	1:B:748:GLU:HG3	2.48	0.48
1:A:122:ARG:NH1	1:B:204:ASP:OD2	2.45	0.47
1:C:652:THR:HB	1:C:693:ARG:HD3	1.96	0.47
1:D:595:GLN:NE2	1:D:596:GLN:O	2.47	0.47
1:C:888:LYS:O	1:C:892:VAL:HG23	2.13	0.47
1:D:641:ARG:HH12	1:D:659:GLN:NE2	2.12	0.47
1:B:719:GLU:O	1:B:723:VAL:HG23	2.15	0.47
1:B:767:GLY:O	1:B:770:THR:HG22	2.13	0.47
1:B:743:ARG:NH1	1:B:748:GLU:OE2	2.47	0.47
1:D:173:VAL:HG22	1:D:286:SER:HB2	1.96	0.47
1:B:83:LEU:HD23	1:B:903:VAL:HG21	1.97	0.47
1:B:502:PRO:HG2	1:B:505:LEU:HB2	1.97	0.47
1:C:868:GLN:NE2	1:C:880:ILE:HD12	2.29	0.47
1:A:525:PRO:O	1:A:528:SER:OG	2.33	0.47
1:C:162:PHE:CE2	1:C:166:LYS:HD2	2.50	0.47
1:C:288:TRP:CD1	1:C:454:ASP:HB2	2.50	0.47
1:D:770:THR:HG23	1:D:771:THR:HG23	1.96	0.47
1:A:70:ASP:HB3	1:A:79:LYS:HE3	1.97	0.47
1:A:144:GLU:CD	1:A:269:ASN:HD22	2.18	0.47
1:A:293:ARG:HG2	1:A:456:ARG:O	2.15	0.47
1:B:41:LEU:HD21	1:B:197:LEU:HD13	1.97	0.47
1:B:655:ALA:O	1:B:659:GLN:HG3	2.14	0.47
1:A:750:GLU:HG3	1:A:955:LEU:HD21	1.97	0.47
1:C:464:ASP:OD1	1:C:479:ARG:NH2	2.45	0.47
1:A:267:LEU:O	1:A:272:ILE:HB	2.15	0.47



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:388:ARG:HH12	1:A:402:ALA:HA	1.80	0.47
1:A:826:LEU:HB3	1:A:871:LEU:HD11	1.97	0.47
1:B:618:TYR:CD2	1:B:660:PRO:HD3	2.50	0.47
1:B:720:MET:HB3	1:B:797:ALA:HB1	1.96	0.47
1:A:86:LYS:O	1:A:922:GLN:NE2	2.48	0.46
1:D:606:LYS:HG3	1:D:777:TRP:CD1	2.50	0.46
1:D:142:ASP:HB2	1:D:692:GLN:OE1	2.15	0.46
1:C:41:LEU:HD11	1:C:197:LEU:HD22	1.97	0.46
1:C:86:LYS:O	1:C:922:GLN:NE2	2.48	0.46
1:C:388:ARG:HH12	1:C:402:ALA:HA	1.80	0.46
1:C:449:SER:O	1:C:451:VAL:N	2.44	0.46
1:D:196:CYS:O	1:D:200:LEU:HB2	2.15	0.46
1:B:121:ARG:NH2	1:B:693:ARG:HH22	2.14	0.46
1:A:845:ASP:HA	1:A:849:VAL:HG23	1.97	0.46
1:B:568:LEU:HD12	1:B:616:GLN:HG2	1.97	0.46
1:A:60:PHE:CE2	1:A:90:LEU:HD11	2.50	0.46
1:A:885:PRO:O	1:A:887:LEU:N	2.49	0.46
1:B:178:PRO:O	1:B:751:TYR:OH	2.33	0.46
1:A:102:ILE:O	1:A:106:LEU:HB2	2.16	0.46
1:A:732:VAL:HG23	1:A:733:VAL:HG23	1.98	0.46
1:C:259:PHE:HA	1:C:688:PHE:HE1	1.81	0.46
1:A:254:LYS:O	1:A:257:PRO:HD2	2.15	0.46
1:B:861:ARG:O	1:B:865:VAL:HG23	2.16	0.46
1:D:781:TRP:HA	1:D:784:THR:HG22	1.98	0.46
1:A:446:PHE:HB3	1:A:450:LEU:HA	1.98	0.45
1:D:505:LEU:HD12	1:D:506:PRO:HD2	1.98	0.45
1:B:406:PHE:HD1	1:B:411:GLU:HG2	1.81	0.45
1:B:617:LEU:O	1:B:621:GLN:HG3	2.17	0.45
1:B:241:MET:O	1:B:245:MET:HG2	2.15	0.45
1:A:121:ARG:NH2	1:A:693:ARG:HH22	2.14	0.45
1:B:811:VAL:HG12	1:B:815:MET:HE2	1.99	0.45
1:C:53:HIS:HD1	1:C:926:SER:HG	1.64	0.45
1:D:446:PHE:HB3	1:D:450:LEU:HD12	1.99	0.45
1:B:52:LEU:HD13	1:B:226:ARG:NH1	2.32	0.45
1:A:730:SER:HA	1:A:734:LYS:HB2	1.97	0.45
1:C:40:LEU:HG	1:C:44:ARG:NH2	2.31	0.45
1:C:147:LEU:HB3	1:C:270:ILE:HD13	1.98	0.45
1:D:102:ILE:HG21	1:D:901:LEU:HG	1.98	0.45
1:A:598:MET:HA	1:A:638:PHE:HB3	1.99	0.45
1:A:762:LYS:HE3	1:A:771:THR:OG1	2.17	0.45
1:B:615:TRP:HB2	1:B:717:MET:HE3	1.98	0.45



	i a pageini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:79:LYS:O	1:A:82:GLU:HG2	2.17	0.45
1:B:533:ILE:HG12	1:B:562:VAL:HG22	1.99	0.45
1:C:254:LYS:O	1:C:257:PRO:HD2	2.17	0.45
1:C:732:VAL:HG23	1:C:733:VAL:HG23	1.99	0.45
1:D:357:TYR:HD2	1:D:358:TYR:CD2	2.35	0.45
1:B:98:VAL:O	1:B:102:ILE:HG12	2.16	0.45
1:B:106:LEU:HD12	1:B:106:LEU:HA	1.80	0.45
1:B:908:THR:HG23	1:B:951:LEU:HD22	1.99	0.45
1:A:511:ILE:O	1:A:515:ILE:HG13	2.17	0.44
1:A:591:ILE:HB	1:A:594:LYS:O	2.17	0.44
1:B:147:LEU:HD22	1:B:161:VAL:HG11	1.99	0.44
1:D:150:LEU:HD23	1:D:154:VAL:HG21	1.97	0.44
1:D:568:LEU:O	1:D:572:GLN:HG3	2.17	0.44
1:A:597:VAL:CG1	1:A:635:LEU:HD11	2.47	0.44
1:B:888:LYS:O	1:B:892:VAL:HG23	2.17	0.44
1:C:305:ARG:HA	1:C:524:LEU:HD11	1.99	0.44
1:D:657:LEU:HD12	1:D:706:PRO:HG3	1.98	0.44
1:B:336:ASN:HD22	1:B:422:SER:CB	2.30	0.44
1:B:489:TRP:O	1:B:492:SER:OG	2.28	0.44
1:B:598:MET:HA	1:B:638:PHE:HB3	2.00	0.44
1:B:854:LYS:N	1:B:855:PRO:HD2	2.32	0.44
1:A:416:LEU:O	1:A:419:CYS:HB2	2.18	0.44
1:A:615:TRP:CE2	1:A:619:ARG:HD2	2.52	0.44
1:A:533:ILE:HG12	1:A:562:VAL:HG22	1.99	0.44
1:A:734:LYS:HE3	1:A:734:LYS:HB2	1.83	0.44
1:C:334:ARG:NH1	1:D:928:GLU:OE2	2.51	0.44
1:D:454:ASP:OD1	1:D:531:PRO:HD2	2.18	0.44
1:A:601:TYR:HE2	3:A:1004:ACT:H1	1.83	0.44
1:D:828:LEU:O	1:D:832:VAL:HG23	2.18	0.44
1:A:177:HIS:O	1:A:179:THR:N	2.50	0.44
1:B:168:GLN:HG3	1:B:666:GLY:HA2	2.00	0.44
1:B:277:PRO:HG2	1:B:280:VAL:CG2	2.48	0.44
1:C:391:HIS:HB2	1:C:398:SER:HB2	2.00	0.44
1:A:40:LEU:O	1:A:44:ARG:HG3	2.18	0.44
1:A:277:PRO:HG2	1:A:280:VAL:HG23	2.00	0.44
1:A:604:SER:O	1:A:607:ASP:N	2.50	0.44
1:C:536:MET:HE3	1:C:763:ARG:HH22	1.83	0.44
1:A:141:SER:HB2	1:A:145:GLU:OE1	2.18	0.43
1:A:406:PHE:CE1	1:A:412:PHE:HA	2.53	0.43
1:C:41:LEU:HD21	1:C:197:LEU:HD13	2.00	0.43
1:D:147:LEU:O	1:D:151:VAL:HG23	2.18	0.43



	i ageni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:657:LEU:HG	1:D:820:PRO:HB3	2.00	0.43
1:A:647:ARG:NE	1:A:970:GLY:OXT	2.51	0.43
1:A:888:LYS:O	1:A:892:VAL:HG23	2.17	0.43
1:B:469:ILE:HD11	1:B:501:LEU:HD13	1.99	0.43
2:A:1001:GLY:N	1:B:229:GLU:OE1	2.52	0.43
1:B:40:LEU:O	1:B:44:ARG:HG3	2.18	0.43
1:B:406:PHE:CD1	1:B:411:GLU:HG2	2.52	0.43
1:B:737:ARG:HB3	1:B:853:LEU:HD21	2.00	0.43
1:C:113:GLU:O	1:C:117:ILE:HG12	2.17	0.43
1:C:305:ARG:HH22	1:C:396:GLY:HA2	1.83	0.43
1:D:540:PRO:HB3	1:D:581:LEU:HG	1.99	0.43
1:B:42:VAL:HG13	1:B:105:MET:HE2	1.99	0.43
1:B:97:LEU:HD11	1:B:938:LEU:HD13	1.99	0.43
1:C:193:ILE:HG23	1:C:217:LEU:HD11	1.99	0.43
1:A:178:PRO:HB3	1:A:757:GLY:HA3	2.01	0.43
1:A:365:ILE:HG21	1:A:373:VAL:HG22	2.00	0.43
1:B:716:LEU:HD23	1:B:815:MET:CE	2.47	0.43
1:C:885:PRO:O	1:C:887:LEU:N	2.48	0.43
1:D:727:GLU:OE2	1:D:863:LYS:NZ	2.52	0.43
1:D:742:PHE:CZ	1:D:748:GLU:HG3	2.54	0.43
1:A:886:PHE:HA	1:A:889:GLN:HB2	2.00	0.43
1:B:597:VAL:HG12	1:B:635:LEU:HD11	2.00	0.43
1:B:608:ALA:HB1	1:B:612:SER:HB2	2.00	0.43
1:C:931:ASP:OD1	1:C:931:ASP:N	2.50	0.43
1:D:610:ARG:HA	1:D:610:ARG:HD2	1.90	0.43
1:C:70:ASP:O	1:C:74:LYS:HG2	2.17	0.43
1:C:176:ALA:HB2	1:C:289:MET:HG2	2.01	0.43
1:D:766:GLY:O	1:D:771:THR:HG21	2.19	0.43
1:D:776:PRO:O	1:D:780:SER:OG	2.33	0.43
1:A:781:TRP:HA	1:A:784:THR:HG22	2.00	0.43
1:B:249:HIS:HD2	1:B:318:LEU:HD21	1.84	0.43
1:C:886:PHE:HA	1:C:889:GLN:HB2	2.00	0.43
1:D:50:GLN:HG3	1:D:55:PRO:HA	1.99	0.43
1:D:727:GLU:HG2	1:D:793:GLY:HA2	2.00	0.43
1:D:956:ILE:HA	1:D:959:MET:CE	2.49	0.43
1:A:223:ALA:HA	1:B:431:ILE:HD11	2.01	0.43
1:A:899:THR:O	1:A:903:VAL:HG23	2.19	0.43
1:A:922:GLN:HB3	1:A:923:PRO:HD2	2.01	0.43
1:C:98:VAL:O	1:C:102:ILE:HG12	2.19	0.43
1:C:608:ALA:HB1	1:C:612:SER:HB2	2.00	0.43
1:B:753:ARG:NH2	1:B:946:GLU:OE1	2.45	0.43



	hi o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:293:ARG:HG2	1:C:456:ARG:O	2.19	0.43
1:D:391:HIS:HB2	1:D:398:SER:HB2	2.00	0.43
1:A:762:LYS:NZ	1:A:768:GLY:O	2.41	0.42
1:B:845:ASP:HA	1:B:849:VAL:HG23	2.00	0.42
1:D:214:ASP:O	1:D:218:GLN:HG2	2.19	0.42
1:D:580:ARG:HA	1:D:580:ARG:HD3	1.89	0.42
1:B:76:ASP:HB3	1:B:79:LYS:H	1.84	0.42
1:B:264:ASP:CG	1:B:275:ARG:HB3	2.40	0.42
1:C:121:ARG:NH1	1:C:689:GLN:OE1	2.52	0.42
1:C:214:ASP:O	1:C:218:GLN:HG2	2.19	0.42
1:C:716:LEU:HD23	1:C:815:MET:HE1	2.00	0.42
1:D:192:ARG:HD2	1:D:220:GLU:OE2	2.20	0.42
1:A:163:GLU:HA	1:A:166:LYS:HD3	2.00	0.42
1:A:412:PHE:O	1:A:415:PRO:HD2	2.19	0.42
1:B:41:LEU:HD13	1:B:108:LEU:HD22	2.02	0.42
1:C:223:ALA:HA	1:D:332:MET:HE1	2.01	0.42
1:D:732:VAL:HG23	1:D:733:VAL:HG23	2.00	0.42
1:A:366:PRO:HD2	1:A:369:GLU:OE2	2.20	0.42
1:C:334:ARG:NH2	2:C:1001:GLY:O	2.52	0.42
1:D:502:PRO:HG2	1:D:505:LEU:HB2	2.00	0.42
1:D:819:TRP:HD1	1:D:820:PRO:HD2	1.84	0.42
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.75	0.42
1:C:262:ARG:NH2	1:D:212:GLU:OE2	2.53	0.42
1:D:820:PRO:O	1:D:824:VAL:HG23	2.20	0.42
1:B:853:LEU:O	1:B:856:PHE:HB3	2.20	0.42
1:D:371:TYR:CE1	1:D:423:LEU:HG	2.55	0.42
1:A:357:TYR:CD2	1:A:358:TYR:N	2.88	0.42
1:A:878:LYS:HE2	1:A:882:GLU:HG3	2.01	0.42
1:A:664:ILE:HG21	1:A:698:THR:HG23	2.02	0.42
1:B:759:ARG:HG2	1:B:760:PRO:O	2.20	0.42
1:D:845:ASP:CG	1:D:861:ARG:HH12	2.23	0.42
1:C:150:LEU:HD23	1:C:154:VAL:HG21	2.01	0.41
1:D:502:PRO:HA	1:D:503:PRO:HD3	1.81	0.41
1:C:106:LEU:HA	1:C:106:LEU:HD12	1.75	0.41
1:D:336:ASN:ND2	1:D:422:SER:HA	2.32	0.41
1:A:106:LEU:O	1:A:109:ALA:HB3	2.19	0.41
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.79	0.41
1:C:881:LEU:HD23	1:C:881:LEU:HA	1.83	0.41
1:C:431:ILE:HD11	1:D:223:ALA:HA	2.01	0.41
1:A:156:LYS:HE3	1:A:703:MET:HB3	2.02	0.41
1:A:580:ARG:O	1:A:584:VAL:HG23	2.21	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:689:GLN:OE1	1:B:693:ARG:NH1	2.54	0.41
1:B:785:ARG:NH2	1:B:899:THR:OG1	2.52	0.41
1:B:101:SER:O	1:B:105:MET:HG3	2.21	0.41
1:C:762:LYS:HD2	1:C:772:LEU:HA	2.02	0.41
1:D:52:LEU:HD13	1:D:226:ARG:HD2	2.02	0.41
1:D:259:PHE:HE1	1:D:692:GLN:NE2	2.16	0.41
1:D:293:ARG:NH2	1:D:304:THR:OG1	2.52	0.41
1:D:881:LEU:HD11	1:D:887:LEU:HD23	2.02	0.41
1:A:409:ILE:HG22	1:A:413:LEU:HD12	2.02	0.41
1:B:790:VAL:HG11	1:B:832:VAL:HG21	2.03	0.41
1:C:170:VAL:HG11	1:C:694:PHE:HB3	2.01	0.41
1:A:450:LEU:HA	1:A:450:LEU:HD12	1.90	0.41
1:B:308:CYS:O	1:B:312:ARG:HG3	2.21	0.41
1:C:268:LYS:HE2	1:C:268:LYS:HB3	1.80	0.41
1:C:660:PRO:HA	1:C:661:PRO:HD3	1.92	0.41
1:D:315:ALA:HB2	1:D:450:LEU:HB2	2.02	0.41
1:D:854:LYS:N	1:D:855:PRO:HD2	2.36	0.41
1:D:888:LYS:O	1:D:892:VAL:HG23	2.21	0.41
1:B:55:PRO:O	1:B:56:SER:OG	2.23	0.41
1:B:334:ARG:NH2	2:B:1002:GLY:OXT	2.54	0.41
1:C:483:GLU:O	1:C:487:GLN:HG3	2.21	0.41
1:C:828:LEU:O	1:C:832:VAL:HG23	2.21	0.41
1:C:910:LYS:HG2	1:C:917:PHE:CD2	2.56	0.41
1:A:365:ILE:HA	1:A:366:PRO:HD3	1.94	0.41
1:A:938:LEU:HD23	1:A:938:LEU:O	2.21	0.41
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.81	0.41
1:C:102:ILE:O	1:C:106:LEU:HB2	2.21	0.41
1:C:277:PRO:HG2	1:C:280:VAL:HG23	2.03	0.41
1:C:710:LYS:HD2	1:C:713:TRP:CE2	2.56	0.41
1:D:98:VAL:O	1:D:102:ILE:HG12	2.21	0.41
1:D:550:GLN:OE1	1:D:559:LEU:N	2.51	0.41
1:B:277:PRO:HG2	1:B:280:VAL:HG23	2.02	0.40
1:B:661:PRO:O	1:B:663:THR:HG23	2.21	0.40
1:B:762:LYS:HE2	1:B:772:LEU:HD13	2.04	0.40
1:C:144:GLU:OE2	1:C:262:ARG:HD2	2.21	0.40
1:C:899:THR:O	1:C:903:VAL:HG23	2.21	0.40
1:B:192:ARG:HD2	1:B:220:GLU:OE1	2.20	0.40
1:B:638:PHE:CD1	1:B:669:ARG:HB2	2.56	0.40
1:C:932:GLU:H	1:C:932:GLU:HG3	1.52	0.40
1:A:770:THR:HG23	1:A:771:THR:HG23	2.03	0.40
1:C:333:TRP:CD2	1:D:941:LEU:HD11	2.56	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:313:MET:HE3	1:A:313:MET:HB2	1.97	0.40
1:A:325:GLU:O	1:A:329:GLU:HG3	2.21	0.40
1:B:37:TYR:HB3	1:B:112:ALA:HB1	2.04	0.40
1:B:727:GLU:O	1:B:730:SER:OG	2.29	0.40
1:B:847:LEU:HD21	1:B:907:TYR:CZ	2.57	0.40
1:B:930:ALA:N	1:B:931:ASP:HB2	2.37	0.40
1:D:125:LYS:O	1:D:126:LEU:HG	2.22	0.40
1:D:686:LEU:HD23	1:D:686:LEU:HA	1.89	0.40
1:D:853:LEU:O	1:D:856:PHE:HB3	2.21	0.40
1:A:57:LEU:HA	1:A:925:LEU:HD23	2.03	0.40
1:B:482:SER:O	1:B:486:ARG:HG3	2.22	0.40
1:B:660:PRO:HA	1:B:661:PRO:HD3	2.00	0.40
1:C:869:GLN:O	1:C:873:GLN:HG3	2.22	0.40
1:D:511:ILE:O	1:D:515:ILE:HG13	2.21	0.40
1:D:829:LEU:HA	1:D:829:LEU:HD23	1.89	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	entiles
1	А	912/970~(94%)	855 (94%)	53~(6%)	4 (0%)	34	66
1	В	911/970~(94%)	863~(95%)	44 (5%)	4 (0%)	34	66
1	С	912/970~(94%)	867~(95%)	42 (5%)	3~(0%)	41	71
1	D	912/970~(94%)	857 (94%)	54 (6%)	1 (0%)	51	81
All	All	3647/3880~(94%)	3442 (94%)	193 (5%)	12 (0%)	41	71

All (12) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	С	943	PRO
1	В	943	PRO
1	С	330	LEU
1	А	764	ARG
1	А	943	PRO
1	С	651	PRO
1	А	531	PRO
1	В	764	ARG
1	В	768	GLY
1	В	949	PRO
1	D	178	PRO
1	А	178	PRO

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	791/832~(95%)	768~(97%)	23 (3%)	42	69	
1	В	790/832~(95%)	762~(96%)	28~(4%)	36	64	
1	С	791/832~(95%)	761~(96%)	30 (4%)	33	62	
1	D	791/832~(95%)	763~(96%)	28 (4%)	36	64	
All	All	3163/3328~(95%)	3054 (97%)	109 (3%)	37	65	

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	77	THR
1	А	97	LEU
1	А	243	TYR
1	А	283	ILE
1	А	332	MET
1	А	336	ASN
1	А	388	ARG
1	А	393	LEU
1	A	541	SER
1	А	562	VAL



Mol	Chain	Res	Type
1	А	597	VAL
1	А	612	SER
1	А	619	ARG
1	А	683	GLU
1	А	692	GLN
1	А	764	ARG
1	А	809	PHE
1	А	852	GLU
1	А	878	LYS
1	А	882	GLU
1	А	902	ASN
1	А	904	PHE
1	А	932	GLU
1	В	36	GLU
1	В	40	LEU
1	В	58	ARG
1	В	186	LEU
1	В	207	ASP
1	В	243	TYR
1	В	293	ARG
1	В	317	ASN
1	В	328	PHE
1	В	332	MET
1	В	336	ASN
1	В	350	SER
1	В	353	LYS
1	В	388	ARG
1	В	541	SER
1	В	597	VAL
1	В	611	LEU
1	В	612	SER
1	В	619	ARG
1	В	683	GLU
1	В	689	GLN
1	В	692	GLN
1	В	769	ILE
1	В	784	THR
1	В	852	GLU
1	В	893	LEU
1	В	904	PHE
1	В	940	LYS
1	С	40	LEU



Mol	Chain	Res	Type
1	С	58	ARG
1	С	62	GLN
1	С	82	GLU
1	С	88	THR
1	С	97	LEU
1	С	144	GLU
1	С	206	THR
1	С	283	ILE
1	С	332	MET
1	С	336	ASN
1	С	364	GLN
1	С	379	ARG
1	С	388	ARG
1	С	397	VAL
1	С	562	VAL
1	С	610	ARG
1	С	611	LEU
1	С	612	SER
1	С	619	ARG
1	С	687	CYS
1	С	692	GLN
1	С	726	GLU
1	С	727	GLU
1	С	771	THR
1	С	847	LEU
1	С	878	LYS
1	С	891	LEU
1	С	904	PHE
1	C	932	GLU
1	D	58	ARG
1	D	62	GLN
1	D	88	THR
1	D	144	GLU
1	D	206	THR
1	D	243	TYR
1	D	283	ILE
1	D	328	PHE
1	D	332	MET
1	D	350	SER
1	D	361	PHE
1	D	363	LYS
1	D	386	ARG



Mol	Chain	\mathbf{Res}	Type
1	D	388	ARG
1	D	484	ASP
1	D	541	SER
1	D	597	VAL
1	D	611	LEU
1	D	612	SER
1	D	619	ARG
1	D	692	GLN
1	D	825	THR
1	D	852	GLU
1	D	878	LYS
1	D	882	GLU
1	D	893	LEU
1	D	904	PHE
1	D	932	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	211	GLN
1	В	336	ASN
1	С	180	GLN
1	С	211	GLN
1	D	53	HIS
1	D	336	ASN
1	D	659	GLN
1	D	692	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)

18 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	Type	Chain	Dog	Tipk	В	ond leng	gths	Bond angles		gles
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	GLY	С	1001	-	$4,\!4,\!4$	1.02	0	$3,\!4,\!4$	1.53	0
3	ACT	С	1002	-	$3,\!3,\!3$	0.80	0	$3,\!3,\!3$	1.30	0
2	GLY	В	1001	-	$4,\!4,\!4$	1.11	1 (25%)	$3,\!4,\!4$	2.14	2 (66%)
3	ACT	В	1004	-	3,3,3	0.78	0	$3,\!3,\!3$	1.35	0
3	ACT	С	1003	-	3, 3, 3	0.77	0	$3,\!3,\!3$	1.38	0
3	ACT	А	1004	-	$3,\!3,\!3$	0.78	0	$3,\!3,\!3$	1.63	1 (33%)
3	ACT	D	1003	-	3,3,3	0.79	0	$3,\!3,\!3$	1.41	0
3	ACT	В	1005	-	3,3,3	0.73	0	$3,\!3,\!3$	1.60	1 (33%)
3	ACT	D	1002	-	$3,\!3,\!3$	0.79	0	$3,\!3,\!3$	1.62	1 (33%)
3	ACT	С	1005	-	3,3,3	0.82	0	$3,\!3,\!3$	1.36	0
3	ACT	А	1002	-	$3,\!3,\!3$	0.76	0	$3,\!3,\!3$	1.38	0
2	GLY	D	1001	-	$4,\!4,\!4$	0.91	0	$3,\!4,\!4$	1.70	1 (33%)
3	ACT	С	1004	-	$3,\!3,\!3$	0.76	0	$3,\!3,\!3$	1.53	0
2	GLY	А	1001	-	$4,\!4,\!4$	1.13	1 (25%)	$3,\!4,\!4$	1.63	1 (33%)
3	ACT	В	1003	-	3,3,3	0.77	0	$3,\!3,\!3$	1.58	0
3	ACT	D	1004	-	3,3,3	0.76	0	3,3,3	1.17	0
3	ACT	A	1003	-	3,3,3	0.72	0	$\overline{3,3,3}$	1.45	0
2	GLY	В	1002	-	4,4,4	1.06	0	$\overline{3,4,4}$	1.45	0

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	GLY	С	1001	-	-	0/2/2/2	-
2	GLY	В	1001	-	-	2/2/2/2	-
2	GLY	D	1001	-	-	0/2/2/2	-
2	GLY	А	1001	-	-	0/2/2/2	-
2	GLY	В	1002	-	-	2/2/2/2	-



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1001	GLY	OXT-C	-2.11	1.23	1.30
2	А	1001	GLY	OXT-C	-2.06	1.23	1.30

All (2) bond length outliers are listed below:

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1001	GLY	OXT-C-O	-3.01	115.79	123.30
2	А	1001	GLY	OXT-C-O	-2.48	117.11	123.30
2	D	1001	GLY	OXT-C-CA	2.25	122.38	113.45
2	В	1001	GLY	OXT-C-CA	2.17	122.07	113.45
3	А	1004	ACT	OXT-C-O	-2.11	114.28	122.05
3	D	1002	ACT	OXT-C-O	-2.10	114.33	122.05
3	В	1005	ACT	OXT-C-CH3	2.01	123.49	115.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	1001	GLY	O-C-CA-N
2	В	1001	GLY	OXT-C-CA-N
2	В	1002	GLY	OXT-C-CA-N
2	В	1002	GLY	O-C-CA-N

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	1001	GLY	1	0
3	А	1004	ACT	1	0
3	А	1002	ACT	1	0
2	А	1001	GLY	1	0
3	D	1004	ACT	1	0
2	В	1002	GLY	1	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 >	#RSR	RZ>2	$OWAB(Å^2)$	Q<0.9
1	А	918/970~(94%)	-0.10	12 (1%)	77 77	3, 24, 57, 85	0
1	В	917/970~(94%)	-0.23	1 (0%) 9	95 97	0, 17, 50, 88	0
1	С	918/970~(94%)	-0.13	9 (0%) 8	82 82	8, 24, 60, 100	0
1	D	918/970~(94%)	-0.04	12 (1%)	77 77	2, 30, 74, 97	0
All	All	3671/3880~(94%)	-0.12	34 (0%) 8	84 84	0, 23, 63, 100	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	351	GLY	4.5
1	D	352	SER	4.3
1	С	352	SER	3.9
1	D	351	GLY	3.7
1	D	361	PHE	3.5
1	А	353	LYS	3.5
1	С	354	VAL	3.2
1	А	80	LEU	3.0
1	А	351	GLY	3.0
1	D	920	THR	2.9
1	А	352	SER	2.9
1	D	764	ARG	2.8
1	D	355	THR	2.8
1	А	354	VAL	2.7
1	D	362	TRP	2.6
1	D	354	VAL	2.6
1	С	359	ILE	2.6
1	С	362	TRP	2.5
1	А	35	ILE	2.5
1	D	353	LYS	2.4
1	С	353	LYS	2.3



	5	1	1 5	
Mol	Chain	Res	Type	RSRZ
1	D	74	LYS	2.2
1	D	356	LYS	2.2
1	В	38	ASP	2.2
1	А	358	TYR	2.1
1	А	66	GLU	2.1
1	А	476	GLY	2.1
1	С	348	SER	2.1
1	С	358	TYR	2.1
1	А	764	ARG	2.0
1	А	350	SER	2.0
1	D	394	ALA	2.0
1	А	356	LYS	2.0
1	С	931	ASP	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	ACT	С	1003	4/4	0.83	0.22	30,30,30,30	0
3	ACT	С	1005	4/4	0.84	0.27	$37,\!37,\!37,\!37$	0
3	ACT	D	1002	4/4	0.86	0.21	21,21,21,21	0
3	ACT	А	1003	4/4	0.89	0.24	40,40,40,40	0
2	GLY	В	1001	5/5	0.89	0.23	22,22,22,22	0
3	ACT	D	1003	4/4	0.90	0.28	39,39,39,39	0
3	ACT	D	1004	4/4	0.91	0.24	22,22,22,22	0
2	GLY	В	1002	5/5	0.92	0.19	8,8,8,8	0
3	ACT	В	1003	4/4	0.92	0.23	11,11,11,11	0
3	ACT	В	1005	4/4	0.92	0.21	11,11,11,11	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	GLY	С	1001	5/5	0.92	0.22	$18,\!18,\!18,\!18$	0
2	GLY	D	1001	5/5	0.93	0.18	8,8,8,8	0
3	ACT	С	1002	4/4	0.94	0.28	$17,\!17,\!17,\!17$	0
3	ACT	А	1002	4/4	0.94	0.18	16,16,16,16	0
2	GLY	А	1001	5/5	0.94	0.20	9,9,9,9	0
3	ACT	А	1004	4/4	0.95	0.14	20,20,20,20	0
3	ACT	С	1004	4/4	0.95	0.22	$17,\!17,\!17,\!17$	0
3	ACT	В	1004	4/4	0.97	0.16	10,10,10,10	0

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6.5 Other polymers (i)

There are no such residues in this entry.

