

Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 04:42 am BST

PDB ID : 4M0U

Title : crystal structure of human PRS1 Q133P mutant

Authors: Chen, P.; Teng, M.; Li, X.

Deposited on : 2013-08-02

Resolution : 2.74 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 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 : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

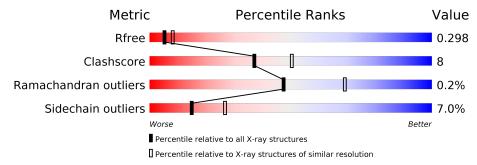
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)

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 on 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%

Mol	Chain	Length	Quality of chain					
1	A	326	75%	16%	• 7%			
1	В	326	75%	17%	• 6%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4701 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.

• Molecule 1 is a protein called Ribose-phosphate pyrophosphokinase 1.

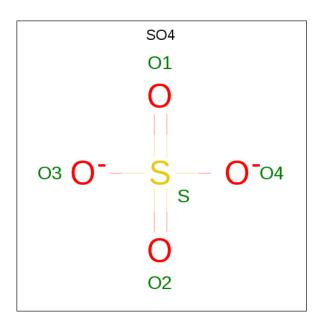
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	303	Total 2310	C 1449	N 406	O 438	S 17	0	0	0
1	В	308	Total 2356	C 1479	N 416	O 444	S 17	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	${f Comment}$	Reference
A	133	PRO	GLN	ENGINEERED MUTATION	UNP P60891
A	319	LEU	=	EXPRESSION TAG	UNP P60891
A	320	GLU	-	EXPRESSION TAG	UNP P60891
A	321	HIS	-	EXPRESSION TAG	UNP P60891
A	322	HIS	-	EXPRESSION TAG	UNP P60891
A	323	HIS	-	EXPRESSION TAG	UNP P60891
A	324	HIS	=	EXPRESSION TAG	UNP P60891
A	325	HIS	-	EXPRESSION TAG	UNP P60891
A	326	HIS	-	EXPRESSION TAG	UNP P60891
В	133	PRO	GLN	ENGINEERED MUTATION	UNP P60891
В	319	LEU	1	EXPRESSION TAG	UNP P60891
В	320	GLU	-	EXPRESSION TAG	UNP P60891
В	321	HIS	1	EXPRESSION TAG	UNP P60891
В	322	HIS	-	EXPRESSION TAG	UNP P60891
В	323	HIS	-	EXPRESSION TAG	UNP P60891
В	324	HIS	-	EXPRESSION TAG	UNP P60891
В	325	HIS	-	EXPRESSION TAG	UNP P60891
В	326	HIS	_	EXPRESSION TAG	UNP P60891

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Δ	1	Total O S	0	0
	7.1	1	5 4 1	0	U
2	Λ.	1	Total O S	0	0
	Λ	1	5 4 1		0
2	В	1	Total O S	0	0
	D	1	5 4 1	0	0
9	D	1	Total O S	0	0
	Б	1	5 4 1		U

• Molecule 3 is water.

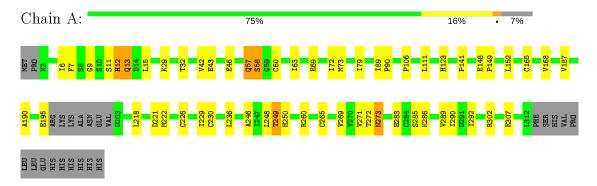
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	В	10	Total O 10 10	0	0



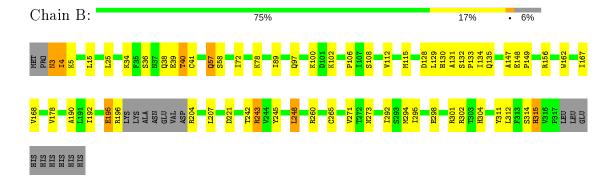
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Ribose-phosphate pyrophosphokinase 1



• Molecule 1: Ribose-phosphate pyrophosphokinase 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	169.88Å 169.88Å 61.76Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.05 - 2.74	Depositor
resolution (A)	34.05 - 2.74	EDS
% Data completeness	92.7 (34.05-2.74)	Depositor
(in resolution range)	92.7 (34.05 - 2.74)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.47 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D D.	0.253 , 0.298	Depositor
R, R_{free}	0.252 , 0.298	DCC
R_{free} test set	823 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.27, 9.6	EDS
L-test for twinning ²	$< L >=0.40, < L^2>=0.23$	Xtriage
Estimated twinning fraction	0.347 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4701	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ 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: SO4

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

Mol	Chain	Boı	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.52	$1/2342 \ (0.0\%)$	0.63	2/3168 (0.1%)	
1	В	0.49	0/2391	0.59	0/3234	
All	All	0.50	$1/4733 \ (0.0\%)$	0.61	2/6402 (0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\mathbf{Ideal}(\mathbf{\mathring{A}})$
1	A	58	SER	C-O	5.87	1.34	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	13	GLN	N-CA-CB	-8.11	96.00	110.60
1	A	60	CYS	N-CA-C	-5.03	97.42	111.00

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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2310	0	2344	36	0
1	В	2356	0	2396	39	0
2	A	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
2	В	10	0	0	0	0
3	A	5	0	0	0	0
3	В	10	0	0	0	0
All	All	4701	0	4740	70	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 8.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom=1 Atom=2 distance (Å) overlap (Å)	Atom-1	Atom-2	Interatomic	Clash
1:B:243:ARG:NH1 1:B:245:TYR:CE1 2.53 0.75 1:A:12:HIS:CG 1:A:12:HIS:O 2.37 0.74 1:A:273:ASN:H 1:A:273:ASN:HD22 1.35 0.72 1:B:243:ARG:NH1 1:B:245:TYR:HE1 1.89 0.69 1:B:243:ARG:NH1 1:B:245:TYR:OH 2.28 0.66 1:A:12:HIS:O 1:A:12:HIS:ND1 2.29 0.65 1:B:57:GLN:HG2 1:B:89:ILE:HG23 1.77 0.65 1:B:192:ILE:HG13 1:B:207:LEU:HD13 1.80 0.64 1:A:72:ILE:CG2 1:B:106:PRO:HG3 2.29 0.61 1:A:32:THR:HG22 1:A:42:VAL:HG22 1.83 0.61 1:B:301:ARG:HH12 1:B:300:PRO:HD2 1.68 0.59 1:A:57:GLN:HE22 1:A:90:PRO:HD2 1.68 0.59 1:B:311:TYR:CE1 1:B:315:HIS:CD2 2.91 0.58 1:A:19:GLY:O 1:A:69:GLU:OE1 2.23 0.57 1:A:14:R:GLU:HB3 1:A:149:PRO:HD3 1.85 0.57 1:B:131:ALA:O 1:B:134:ILE:HD13 2.05 0.57 <	Atom-1	Atom-2	${f distance}({ m \AA})$	$ ho = { m overlap} \; ({ m \AA})$
1:A:12:HIS:CG 1:A:12:HIS:O 2.37 0.74 1:A:273:ASN:H 1:A:273:ASN:HD22 1.35 0.72 1:B:243:ARG:NH1 1:B:245:TYR:HE1 1.89 0.69 1:B:243:ARG:NH1 1:B:245:TYR:OH 2.28 0.66 1:B:57:GLN:HG2 1:B:89:ILE:HG23 1.77 0.65 1:B:57:GLN:HG2 1:B:89:ILE:HG23 1.77 0.65 1:B:192:ILE:HG13 1:B:207:LEU:HD13 1.80 0.64 1:A:72:ILE:CG2 1:B:106:PRO:HG3 2.29 0.61 1:A:32:THR:HG22 1:A:42:VAL:HG22 1.83 0.61 1:B:301:ARG:HH12 1:B:302:ARG:HE 1.51 0.59 1:A:57:GLN:HE22 1:A:90:PRO:HD2 1.68 0.59 1:B:311:TYR:CE1 1:B:315:HIS:CD2 2.91 0.58 1:A:148:GLU:HB3 1:A:149:PRO:HD3 1.85 0.57 1:A:106:PRO:HG3 1:B:72:ILE:HG23 1.85 0.57 1:B:131:ALA:O 1:B:134:ILE:HD13 2.05 0.57 1:B:130:HIS:ND1 1:B:221:ASP:OD2 2.34 0.57 1:B:132:HB:D2 1:A:141:PRO:HB2 1.71 0.56	1:A:72:ILE:HG23	1:B:106:PRO:HG3	1.63	0.79
1:A:273:ASN:H 1:A:273:ASN:HD22 1.35 0.72 1:B:243:ARG:NH1 1:B:245:TYR:HE1 1.89 0.69 1:B:243:ARG:NH1 1:B:245:TYR:OH 2.28 0.66 1:B:12:HIS:O 1:A:12:HIS:ND1 2.29 0.65 1:B:57:GLN:HG2 1:B:89:ILE:HG23 1.77 0.65 1:B:192:ILE:HG13 1:B:207:LEU:HD13 1.80 0.64 1:A:72:ILE:CG2 1:B:106:PRO:HG3 2.29 0.61 1:A:32:THR:HG22 1:A:3 0.61 1:B:301:ARG:HH12 1:B:302:ARG:HE 1.51 0.59 1:A:57:GLN:HE22 1:A:90:PRO:HD2 1.68 0.59 1:B:311:TYR:CE1 1:B:315:HIS:CD2 2.91 0.58 1:A:9:GLY:O 1:A:69:GLU:OE1 2.23 0.57 1:A:148:GLU:HB3 1:A:149:PRO:HD3 1.85 0.57 1:A:106:PRO:HG3 1:B:72:ILE:HG23 1.85 0.57 1:B:131:ALA:O 1:B:134:ILE:HD13 2.05 0.57 1:B:130:HIS:ND1 1:B:221:ASP:OD2 2.34 0.57 1:A:123:HIS:HD2 1:A:147:PRO:HB2 1.71 0.56 1	1:B:243:ARG:NH1	1:B:245:TYR:CE1	2.53	0.75
1:B:243:ARG:NH1 1:B:245:TYR:HE1 1.89 0.69 1:B:243:ARG:NH1 1:B:245:TYR:OH 2.28 0.66 1:A:12:HIS:O 1:A:12:HIS:ND1 2.29 0.65 1:B:57:GLN:HG2 1:B:89:ILE:HG23 1.77 0.65 1:B:192:ILE:HG13 1:B:207:LEU:HD13 1.80 0.64 1:A:72:ILE:CG2 1:B:106:PRO:HG3 2.29 0.61 1:A:32:THR:HG22 1:A:42:VAL:HG22 1.83 0.61 1:B:301:ARG:HH12 1:B:302:ARG:HE 1.51 0.59 1:A:57:GLN:HE22 1:A:90:PRO:HD2 1.68 0.59 1:B:311:TYR:CE1 1:B:315:HIS:CD2 2.91 0.58 1:A:9:GLY:O 1:A:69:GLU:OE1 2.23 0.57 1:A:148:GLU:HB3 1:A:149:PRO:HD3 1.85 0.57 1:A:106:PRO:HG3 1:B:72:ILE:HG23 1.85 0.57 1:B:131:ALA:O 1:B:134:ILE:HD13 2.05 0.57 1:B:130:HIS:ND1 1:B:221:ASP:OD2 2.34 0.57 1:A:123:HIS:HD2 1:A:147:PRO:HB2 1.71 0.56	1:A:12:HIS:CG	1:A:12:HIS:O	2.37	0.74
1:B:243:ARG:NH1 1:B:245:TYR:OH 2.28 0.66 1:A:12:HIS:O 1:A:12:HIS:ND1 2.29 0.65 1:B:57:GLN:HG2 1:B:89:ILE:HG23 1.77 0.65 1:B:192:ILE:HG13 1:B:207:LEU:HD13 1.80 0.64 1:A:72:ILE:CG2 1:B:106:PRO:HG3 2.29 0.61 1:A:32:THR:HG22 1:A:42:VAL:HG22 1.83 0.61 1:B:301:ARG:HH12 1:B:302:ARG:HE 1.51 0.59 1:A:57:GLN:HE22 1:A:90:PRO:HD2 1.68 0.59 1:A:9:GLY:O 1:A:69:PRO:HD2 1.68 0.59 1:B:311:TYR:CE1 1:B:315:HIS:CD2 2.91 0.58 1:A:9:GLY:O 1:A:69:GLY:OE1 2.23 0.57 1:A:148:GLU:HB3 1:A:149:PRO:HD3 1.85 0.57 1:A:106:PRO:HG3 1:B:72:ILE:HG23 1.85 0.57 1:B:131:ALA:O 1:B:134:ILE:HD13 2.05 0.57 1:B:130:HIS:ND1 1:B:221:ASP:OD2 2.34 0.57 1:A:165:CYS:O 1:A:187:VAL:HB 2.06 0.56	1:A:273:ASN:H	1:A:273:ASN:HD22	1.35	0.72
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1:B:131:ALA:O 1:B:134:ILE:HD13 2.05 0.57 1:B:130:HIS:ND1 1:B:221:ASP:OD2 2.34 0.57 1:A:165:CYS:O 1:A:187:VAL:HB 2.06 0.56 1:A:302:ARG:HH11 1:A:307:GLU:HG2 1.71 0.56 1:A:123:HIS:HD2 1:A:141:PRO:HB2 1.71 0.56 1:A:12:HIS:CG 1:A:58:SER:O 2.60 0.55 1:B:129:LEU:HD13 1:B:134:ILE:HB 1.89 0.54 1:B:132:SER:N 1:B:133:PRO:CD 2.69 0.54 1:B:112:VAL:HA 1:B:115:MET:HE3 1.88 0.54 1:A:273:ASN:HD21 1:A:292:ILE:H 1.54 0.54 1:B:243:ARG:NH1 1:B:245:TYR:CZ 2.75 0.53 1:A:168:VAL:HG22 1:A:190:ALA:HB3 1.91 0.53	1:A:148:GLU:HB3	1:A:149:PRO:HD3	1.85	0.57
1:B:130:HIS:ND1 1:B:221:ASP:OD2 2.34 0.57 1:A:165:CYS:O 1:A:187:VAL:HB 2.06 0.56 1:A:302:ARG:HH11 1:A:307:GLU:HG2 1.71 0.56 1:A:123:HIS:HD2 1:A:141:PRO:HB2 1.71 0.56 1:A:12:HIS:CG 1:A:58:SER:O 2.60 0.55 1:B:129:LEU:HD13 1:B:134:ILE:HB 1.89 0.54 1:B:132:SER:N 1:B:133:PRO:CD 2.69 0.54 1:B:112:VAL:HA 1:B:115:MET:HE3 1.88 0.54 1:A:273:ASN:HD21 1:A:292:ILE:H 1.54 0.54 1:B:243:ARG:NH1 1:B:245:TYR:CZ 2.75 0.53 1:A:168:VAL:HG22 1:A:190:ALA:HB3 1.91 0.53	1:A:106:PRO:HG3	1:B:72:ILE:HG23	1.85	0.57
1:A:165:CYS:O 1:A:187:VAL:HB 2.06 0.56 1:A:302:ARG:HH11 1:A:307:GLU:HG2 1.71 0.56 1:A:123:HIS:HD2 1:A:141:PRO:HB2 1.71 0.56 1:A:12:HIS:CG 1:A:58:SER:O 2.60 0.55 1:B:129:LEU:HD13 1:B:134:ILE:HB 1.89 0.54 1:B:132:SER:N 1:B:133:PRO:CD 2.69 0.54 1:B:112:VAL:HA 1:B:115:MET:HE3 1.88 0.54 1:A:273:ASN:HD21 1:A:292:ILE:H 1.54 0.54 1:B:243:ARG:NH1 1:B:245:TYR:CZ 2.75 0.53 1:A:168:VAL:HG22 1:A:190:ALA:HB3 1.91 0.53	1:B:131:ALA:O	1:B:134:ILE:HD13	2.05	0.57
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1:B:129:LEU:HD13 1:B:134:ILE:HB 1.89 0.54 1:B:132:SER:N 1:B:133:PRO:CD 2.69 0.54 1:B:112:VAL:HA 1:B:115:MET:HE3 1.88 0.54 1:A:273:ASN:HD21 1:A:292:ILE:H 1.54 0.54 1:B:243:ARG:NH1 1:B:245:TYR:CZ 2.75 0.53 1:A:168:VAL:HG22 1:A:190:ALA:HB3 1.91 0.53		1:A:141:PRO:HB2	1.71	0.56
1:B:132:SER:N 1:B:133:PRO:CD 2.69 0.54 1:B:112:VAL:HA 1:B:115:MET:HE3 1.88 0.54 1:A:273:ASN:HD21 1:A:292:ILE:H 1.54 0.54 1:B:243:ARG:NH1 1:B:245:TYR:CZ 2.75 0.53 1:A:168:VAL:HG22 1:A:190:ALA:HB3 1.91 0.53	1:A:12:HIS:CG	1:A:58:SER:O	2.60	0.55
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1:A:273:ASN:HD21 1:A:292:ILE:H 1.54 0.54 1:B:243:ARG:NH1 1:B:245:TYR:CZ 2.75 0.53 1:A:168:VAL:HG22 1:A:190:ALA:HB3 1.91 0.53		1:B:133:PRO:CD	2.69	0.54
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1:A:168:VAL:HG22 1:A:190:ALA:HB3 1.91 0.53		1:A:292:ILE:H		
	1:B:243:ARG:NH1	1:B:245:TYR:CZ	2.75	0.53
1:A:42:VAL:HG11				
	1:A:42:VAL:HG11	1:A:73:MET:HG2	1.91	0.53

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Continued from preo		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	$ m overlap~(\AA)$
1:A:226:CYS:N	2:A:1002:SO4:O3	2.43	0.52
1:B:167:ILE:HG22	1:B:178:VAL:HB	1.90	0.52
1:B:4:ILE:HG21	1:B:25:LEU:HD11	1.92	0.51
1:B:298:GLU:HG2	1:B:312:LEU:HD21	1.94	0.50
1:B:148:GLU:HB3	1:B:149:PRO:HD3	1.93	0.50
1:A:63:ILE:HD13	1:B:39:GLU:HG2	1.95	0.48
1:B:4:ILE:CG2	1:B:25:LEU:HD11	2.43	0.48
1:A:57:GLN:NE2	1:A:90:PRO:HD2	2.28	0.48
1:B:273:ASN:OD1	1:B:292:ILE:HG13	2.12	0.48
1:B:132:SER:C	1:B:134:ILE:H	2.18	0.47
1:B:131:ALA:O	1:B:134:ILE:CD1	2.63	0.46
1:B:97:GLN:HB2	1:B:108:SER:HB2	1.98	0.46
1:B:195:GLU:HG2	1:B:204:ARG:O	2.15	0.45
1:A:12:HIS:CB	1:A:58:SER:O	2.64	0.45
1:B:242:THR:HG22	1:B:243:ARG:HG2	1.97	0.45
1:A:271:VAL:HG23	1:A:289:VAL:HG12	1.98	0.44
1:A:272:THR:HG22	1:A:290:ILE:HB	1.99	0.44
1:A:302:ARG:HH11	1:A:307:GLU:CG	2.31	0.44
1:A:221:ASP:O	1:A:249:THR:HG23	2.18	0.43
1:A:230:CYS:SG	1:A:260:ARG:HB3	2.59	0.43
1:A:246:ALA:HB3	1:A:269:VAL:HG22	2.00	0.43
1:B:248:LEU:HB2	1:B:271:VAL:HG12	2.00	0.43
1:B:190:ALA:HB1	1:B:207:LEU:HD11	2.01	0.43
1:B:149:PRO:HG3	1:B:314:SER:HA	2.01	0.43
1:B:34:LYS:HG2	1:B:40:THR:HG23	2.01	0.43
1:A:13:GLN:HE21	1:A:13:GLN:HB3	1.61	0.43
1:A:7:PHE:N	1:A:7:PHE:CD1	2.87	0.42
1:B:168:VAL:HG22	1:B:190:ALA:HB3	2.01	0.42
1:A:218:LEU:HD13	1:A:229:ILE:HG13	2.01	0.42
1:A:273:ASN:N	1:A:273:ASN:HD22	2.11	0.42
1:B:298:GLU:O	1:B:302:ARG:HG2	2.20	0.42
1:B:3:ASN:HB3	1:B:304:HIS:CE1	2.55	0.42
1:B:128:ASP:OD2	1:B:147:ALA:N	2.52	0.41
1:A:222:MET:HB3	1:A:250:HIS:HB2	2.01	0.41
1:A:79:ILE:HD12	1:B:100:LYS:HE3	2.01	0.41
1:B:156:ARG:HA	1:B:162:TRP:CD1	2.56	0.41
1:A:29:LYS:N	1:A:46:GLU:OE2	2.41	0.41
1:A:168:VAL:HG21	1:A:236:LEU:HD21	2.03	0.40
1:B:292:ILE:HG22	1:B:295:ILE:HD12	2.04	0.40
1:A:229:ILE:HD13	1:A:248:LEU:HD11	2.04	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	\mathbf{ntiles}
1	A	299/326~(92%)	276 (92%)	23 (8%)	0	100	100
1	В	304/326~(93%)	287 (94%)	16 (5%)	1 (0%)	41	61
All	All	$603/652 \ (92\%)$	563 (93%)	39 (6%)	1 (0%)	47	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	36	SER

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	$egin{array}{c c} ext{in} & ext{Analysed} & ext{Rotameric} & ext{Outlie} \end{array}$		Outliers	Percentiles
1	A	$254/278 \; (91\%)$	238 (94%)	16 (6%)	18 31
1	В	261/278 (94%)	241 (92%)	20 (8%)	13 23
All	All	515/556 (93%)	479 (93%)	36 (7%)	15 27

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Mol Chain Res		Type
1	A	6	ILE
1	A	11	SER
1	A	12	HIS
1	A	15	LEU
1	A	43	GLU

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Mol	Chain	Res	$egin{array}{c} \textit{Tus page} \\ \mathbf{Type} \end{array}$
1	A	57	GLN
1	1 A		ILE
1			LEU
1	A	152	LEU
1	A	195	GLU
1	A	249	THR
1	A	265	CYS
1	A	273	ASN
1	A	283	HIS
1	A	285	SER
1	A	286	LYS
1	В	3	ASN
1	В	4	ILE
1	В	5	LYS
1	В	15	LEU
1	В	38	GLN
1	В	40	THR
1	В	41	CYS
1	В	57	GLN
1	В	58	SER
1	В	78	LYS
1	В	102	LYS
1	В	135	GLN
1	В	195	GLU
1	В	196	ARG
1	В	243	ARG
1	В	248	LEU
1	В	260	ARG
1	В	265	CYS
1	В	294	MET
1	В	315	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	231	HIS
1	A	273	ASN
1	В	3	ASN
1	В	64	ASN
1	В	186	ASN
1	В	277	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res Link		Dag	Link	B	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
2	SO4	В	402	-	4,4,4	0.17	0	6,6,6	0.10	0		
2	SO4	A	1001	-	4,4,4	0.20	0	6,6,6	0.41	0		
2	SO4	В	401	-	4,4,4	0.15	0	6,6,6	0.26	0		
2	SO4	A	1002	-	4,4,4	0.18	0	6,6,6	0.09	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	SO4	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

