



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:30 PM UTC

PDB ID : 2PPG / pdb\_00002ppg  
Title : Crystal structure of putative isomerase from *Sinorhizobium meliloti*  
Authors : Ramagopal, U.A.; Toro, R.; Dickey, M.; Logan, C.; Groshong, C.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-04-30  
Resolution : 2.49 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

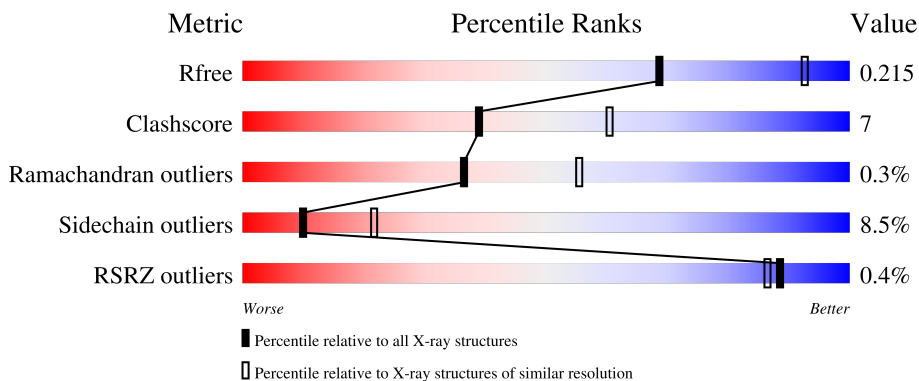
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	399	79% 16% . .
1	B	399	73% 18% 7% %
1	C	399	77% 18% . .
1	D	399	75% 19% . . %

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11799 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 Putative isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	387	2979	1891	533	542	4	9	0	1	0
1	B	370	2845	1807	514	511	4	9	0	0	0
1	C	382	2913	1848	523	529	4	9	0	0	0
1	D	383	2928	1856	527	532	4	9	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP Q92ZS5
A	0	SER	-	cloning artifact	UNP Q92ZS5
A	1	LEU	-	cloning artifact	UNP Q92ZS5
A	79	MSE	MET	modified residue	UNP Q92ZS5
A	109	MSE	MET	modified residue	UNP Q92ZS5
A	199	MSE	MET	modified residue	UNP Q92ZS5
A	216	MSE	MET	modified residue	UNP Q92ZS5
A	232	MSE	MET	modified residue	UNP Q92ZS5
A	275	MSE	MET	modified residue	UNP Q92ZS5
A	291	MSE	MET	modified residue	UNP Q92ZS5
A	300	MSE	MET	modified residue	UNP Q92ZS5
A	359	MSE	MET	modified residue	UNP Q92ZS5
A	390	GLU	-	cloning artifact	UNP Q92ZS5
A	391	GLY	-	cloning artifact	UNP Q92ZS5
A	392	HIS	-	cloning artifact	UNP Q92ZS5
A	393	HIS	-	cloning artifact	UNP Q92ZS5
A	394	HIS	-	cloning artifact	UNP Q92ZS5
A	395	HIS	-	cloning artifact	UNP Q92ZS5
A	396	HIS	-	cloning artifact	UNP Q92ZS5
A	397	HIS	-	cloning artifact	UNP Q92ZS5
B	-1	MSE	-	cloning artifact	UNP Q92ZS5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	cloning artifact	UNP Q92ZS5
B	1	LEU	-	cloning artifact	UNP Q92ZS5
B	79	MSE	MET	modified residue	UNP Q92ZS5
B	109	MSE	MET	modified residue	UNP Q92ZS5
B	199	MSE	MET	modified residue	UNP Q92ZS5
B	216	MSE	MET	modified residue	UNP Q92ZS5
B	232	MSE	MET	modified residue	UNP Q92ZS5
B	275	MSE	MET	modified residue	UNP Q92ZS5
B	291	MSE	MET	modified residue	UNP Q92ZS5
B	300	MSE	MET	modified residue	UNP Q92ZS5
B	359	MSE	MET	modified residue	UNP Q92ZS5
B	390	GLU	-	cloning artifact	UNP Q92ZS5
B	391	GLY	-	cloning artifact	UNP Q92ZS5
B	392	HIS	-	cloning artifact	UNP Q92ZS5
B	393	HIS	-	cloning artifact	UNP Q92ZS5
B	394	HIS	-	cloning artifact	UNP Q92ZS5
B	395	HIS	-	cloning artifact	UNP Q92ZS5
B	396	HIS	-	cloning artifact	UNP Q92ZS5
B	397	HIS	-	cloning artifact	UNP Q92ZS5
C	-1	MSE	-	cloning artifact	UNP Q92ZS5
C	0	SER	-	cloning artifact	UNP Q92ZS5
C	1	LEU	-	cloning artifact	UNP Q92ZS5
C	79	MSE	MET	modified residue	UNP Q92ZS5
C	109	MSE	MET	modified residue	UNP Q92ZS5
C	199	MSE	MET	modified residue	UNP Q92ZS5
C	216	MSE	MET	modified residue	UNP Q92ZS5
C	232	MSE	MET	modified residue	UNP Q92ZS5
C	275	MSE	MET	modified residue	UNP Q92ZS5
C	291	MSE	MET	modified residue	UNP Q92ZS5
C	300	MSE	MET	modified residue	UNP Q92ZS5
C	359	MSE	MET	modified residue	UNP Q92ZS5
C	390	GLU	-	cloning artifact	UNP Q92ZS5
C	391	GLY	-	cloning artifact	UNP Q92ZS5
C	392	HIS	-	cloning artifact	UNP Q92ZS5
C	393	HIS	-	cloning artifact	UNP Q92ZS5
C	394	HIS	-	cloning artifact	UNP Q92ZS5
C	395	HIS	-	cloning artifact	UNP Q92ZS5
C	396	HIS	-	cloning artifact	UNP Q92ZS5
C	397	HIS	-	cloning artifact	UNP Q92ZS5
D	-1	MSE	-	cloning artifact	UNP Q92ZS5
D	0	SER	-	cloning artifact	UNP Q92ZS5
D	1	LEU	-	cloning artifact	UNP Q92ZS5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	79	MSE	MET	modified residue	UNP Q92ZS5
D	109	MSE	MET	modified residue	UNP Q92ZS5
D	199	MSE	MET	modified residue	UNP Q92ZS5
D	216	MSE	MET	modified residue	UNP Q92ZS5
D	232	MSE	MET	modified residue	UNP Q92ZS5
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D	390	GLU	-	cloning artifact	UNP Q92ZS5
D	391	GLY	-	cloning artifact	UNP Q92ZS5
D	392	HIS	-	cloning artifact	UNP Q92ZS5
D	393	HIS	-	cloning artifact	UNP Q92ZS5
D	394	HIS	-	cloning artifact	UNP Q92ZS5
D	395	HIS	-	cloning artifact	UNP Q92ZS5
D	396	HIS	-	cloning artifact	UNP Q92ZS5
D	397	HIS	-	cloning artifact	UNP Q92ZS5

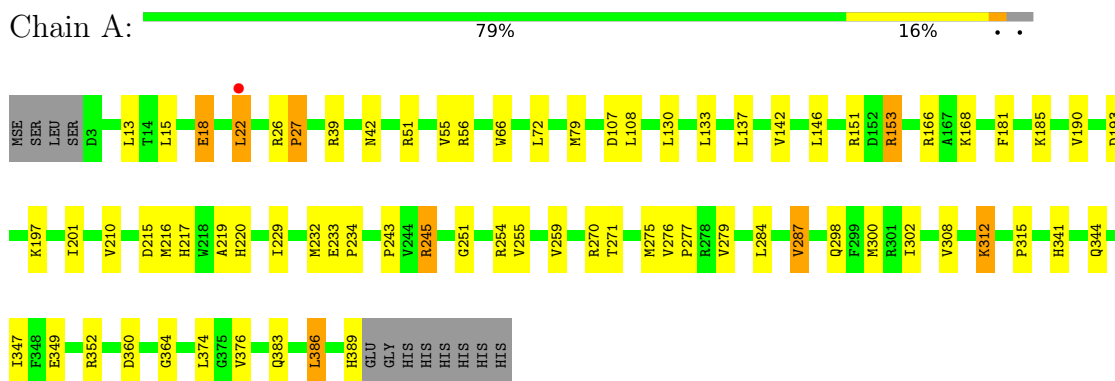
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	46	Total O 46 46	0	0
2	B	22	Total O 22 22	0	0
2	C	28	Total O 28 28	0	0
2	D	38	Total O 38 38	0	0

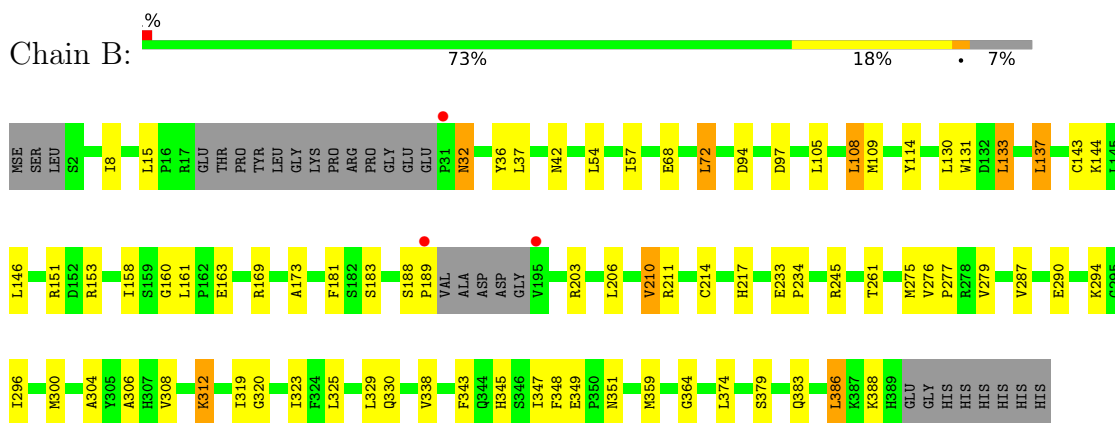
### 3 Residue-property plots [i](#)

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.

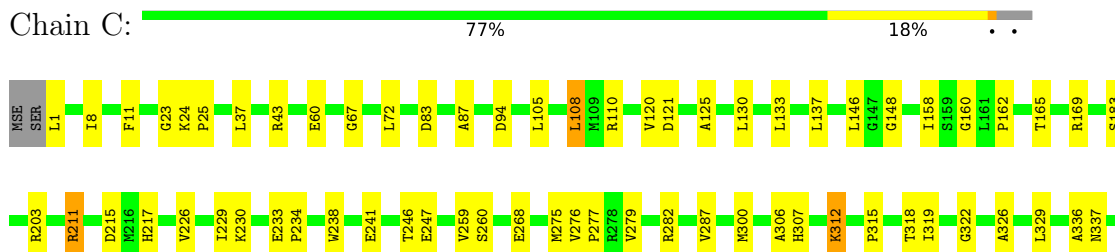
- Molecule 1: Putative isomerase



- Molecule 1: Putative isomerase

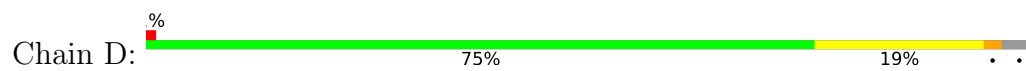


- Molecule 1: Putative isomerase





- Molecule 1: Putative isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.15Å 150.83Å 147.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.00 – 2.49 42.00 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.00-2.49) 99.1 (42.00-2.49)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.48Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.252 (Not available) , 0.215	Depositor DCC
$R_{free}$ test set	2581 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtrriage
Anisotropy	0.795	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.57	0/3038	0.87	1/4109 (0.0%)
1	B	0.55	0/2898	0.85	0/3912
1	C	0.56	0/2968	0.86	0/4013
1	D	0.54	0/2984	0.85	0/4034
All	All	0.56	0/11888	0.86	1/16068 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	CB-CA-C	-5.40	103.37	110.98

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	A	2979	0	2970	37	0
1	B	2845	0	2851	47	0
1	C	2913	0	2904	41	0
1	D	2928	0	2916	39	0
2	A	46	0	0	0	0
2	B	22	0	0	2	0
2	C	28	0	0	1	0
2	D	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11799	0	11641	159	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 (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:MSE:HE2	1:A:232:MSE:HE1	1.29	1.14
1:D:329:LEU:HD12	1:D:359:MSE:HE2	1.33	1.09
1:C:329:LEU:HD12	1:C:359:MSE:HE2	1.12	1.08
1:D:326:ALA:HA	1:D:359:MSE:HE1	1.26	1.08
1:C:326:ALA:HA	1:C:359:MSE:HE1	1.26	1.07
1:B:325:LEU:HG	1:B:359:MSE:HE1	1.33	1.06
1:D:49:PHE:HD2	1:D:49:PHE:H	1.14	0.91
1:B:348:PHE:HE1	1:B:359:MSE:HE2	1.36	0.91
1:C:329:LEU:HD12	1:C:359:MSE:CE	2.00	0.90
1:D:326:ALA:CA	1:D:359:MSE:HE1	2.08	0.82
1:D:326:ALA:HA	1:D:359:MSE:CE	2.11	0.80
1:B:319:ILE:HA	1:B:347:ILE:HG21	1.65	0.79
1:C:329:LEU:CD1	1:C:359:MSE:HE2	2.05	0.76
1:B:348:PHE:CE1	1:B:359:MSE:HE2	2.23	0.74
1:A:383:GLN:HA	1:A:386:LEU:HD22	1.71	0.72
1:B:325:LEU:CG	1:B:359:MSE:HE1	2.16	0.71
1:B:183:SER:OG	1:B:211:ARG:NH1	2.26	0.68
1:B:8:ILE:HG12	1:B:57:ILE:HG12	1.76	0.67
1:A:107:ASP:OD2	1:C:43:ARG:NH2	2.26	0.66
1:C:322:GLY:HA3	1:C:355:LEU:HD11	1.77	0.65
1:D:329:LEU:CD1	1:D:359:MSE:HE2	2.20	0.63
1:A:216:MSE:HE1	1:A:229:ILE:HG12	1.81	0.63
1:C:247:GLU:H	1:C:247:GLU:CD	2.07	0.62
1:D:349:GLU:OE2	1:D:352:ARG:NH1	2.32	0.62
1:C:215:ASP:HA	1:C:241:GLU:HB3	1.83	0.61
1:B:320:GLY:O	1:B:351:ASN:ND2	2.33	0.60
1:B:189:PRO:HG2	1:B:217:HIS:HB2	1.83	0.60
1:D:193:ASP:OD2	1:D:193:ASP:N	2.33	0.60
1:A:26:ARG:HB3	1:A:27:PRO:HD2	1.83	0.59
1:B:383:GLN:HA	1:B:386:LEU:HD22	1.84	0.59
1:A:193:ASP:HB3	1:A:197:LYS:HD2	1.85	0.57
1:C:183:SER:OG	1:C:211:ARG:NH1	2.38	0.57
1:B:133:LEU:O	1:B:137:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LYS:N	1:C:25:PRO:HD3	2.19	0.57
1:D:163:GLU:HB2	1:D:169:ARG:HG2	1.86	0.57
1:D:322:GLY:HA3	1:D:355:LEU:HD11	1.86	0.56
1:D:49:PHE:CD2	1:D:49:PHE:N	2.66	0.56
1:B:144:LYS:NZ	1:C:94:ASP:OD2	2.35	0.56
1:B:290:GLU:H	1:B:294:LYS:NZ	2.04	0.55
1:A:79:MSE:SE	1:A:389:HIS:HB2	2.57	0.54
1:A:216:MSE:HE2	1:A:232:MSE:CE	2.19	0.54
1:D:197:LYS:HA	1:D:200:GLU:HB3	1.90	0.54
1:D:23:GLY:HA2	1:D:24:LYS:CB	2.38	0.54
1:A:276:VAL:HB	1:A:277:PRO:HD3	1.90	0.54
1:C:326:ALA:CA	1:C:359:MSE:HE1	2.18	0.54
1:B:32:ASN:ND2	1:B:36:TYR:H	2.06	0.54
1:A:352:ARG:NH2	1:A:360:ASP:OD1	2.41	0.53
1:B:143:CYS:HB3	1:B:330:GLN:O	2.08	0.53
1:D:344:GLN:HB2	1:D:347:ILE:HG12	1.90	0.53
1:A:271:THR:HA	1:A:298:GLN:HG3	1.90	0.53
1:D:163:GLU:HB2	1:D:169:ARG:CG	2.38	0.53
1:D:68:GLU:HB2	1:D:323:ILE:HB	1.91	0.52
1:A:166:ARG:HG2	1:A:201:ILE:HG21	1.90	0.52
1:B:109:MSE:HE3	1:B:114:TYR:CD2	2.43	0.52
1:D:79:MSE:SE	1:D:389:HIS:HB2	2.60	0.52
1:A:271:THR:HA	1:A:298:GLN:CG	2.39	0.52
1:D:198:GLU:O	1:D:201:ILE:HG22	2.10	0.52
1:D:275:MSE:SE	1:D:287:VAL:HG11	2.60	0.51
1:B:329:LEU:HD11	1:B:359:MSE:HE3	1.93	0.51
1:C:359:MSE:HE3	1:C:369:PRO:HG3	1.92	0.51
1:A:315:PRO:HB2	1:A:341:HIS:CD2	2.47	0.50
1:C:83:ASP:OD2	1:C:389:HIS:ND1	2.19	0.50
1:B:276:VAL:HB	1:B:277:PRO:HD3	1.94	0.49
1:C:146:LEU:HD22	1:C:300:MSE:HG3	1.94	0.49
1:C:23:GLY:CA	1:C:24:LYS:CB	2.89	0.49
1:D:317:ALA:HB1	1:D:347:ILE:HD13	1.94	0.49
1:A:22:LEU:HD22	1:A:39:ARG:HD3	1.95	0.49
1:B:290:GLU:H	1:B:294:LYS:HZ3	1.59	0.49
1:D:252:LEU:HG	1:D:283:ALA:HB1	1.95	0.48
1:B:68:GLU:HB2	1:B:323:ILE:HB	1.95	0.48
1:D:2:SER:OG	1:D:4:ARG:NH2	2.46	0.48
1:B:304:ALA:O	1:B:308:VAL:HG23	2.13	0.48
1:B:173:ALA:HB1	1:B:206:LEU:HD11	1.95	0.48
1:D:278:ARG:HB3	1:D:284:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PHE:CD1	1:A:364:GLY:HA2	2.48	0.48
1:D:249:ILE:H	1:D:249:ILE:HG12	1.50	0.48
1:B:181:PHE:CD1	1:B:364:GLY:HA2	2.48	0.47
1:D:159:SER:HB2	1:D:342:GLU:HG3	1.95	0.47
1:D:146:LEU:HD22	1:D:300:MSE:HG3	1.97	0.47
1:A:233:GLU:N	1:A:234:PRO:HD2	2.29	0.47
1:B:275:MSE:HE1	1:B:306:ALA:HB2	1.96	0.47
1:C:383:GLN:HA	1:C:386:LEU:HD22	1.96	0.47
1:A:18:GLU:H	1:A:18:GLU:CD	2.22	0.47
1:D:116:GLY:HA2	1:D:270:ARG:HG3	1.97	0.47
1:A:216:MSE:CE	1:A:232:MSE:HE1	2.22	0.46
1:A:13:LEU:O	1:A:51:ARG:HA	2.15	0.46
1:B:158:ILE:HD13	1:B:343:PHE:HD2	1.79	0.46
1:C:233:GLU:N	1:C:234:PRO:HD2	2.31	0.45
1:B:105:LEU:HA	1:B:108:LEU:HD22	1.98	0.45
1:B:163:GLU:HB2	1:B:169:ARG:HG2	1.98	0.45
1:A:185:LYS:HE3	1:A:215:ASP:HB2	1.98	0.45
1:C:226:VAL:O	1:C:230:LYS:HG3	2.16	0.45
1:D:199:MSE:HE3	1:D:235:HIS:HB2	1.97	0.45
1:A:275:MSE:SE	1:A:302:ILE:HG23	2.66	0.45
1:B:151:ARG:HH12	1:B:338:VAL:HB	1.82	0.45
1:B:54:LEU:HG	1:B:68:GLU:HG3	1.99	0.45
1:A:146:LEU:HB3	1:A:300:MSE:HE2	1.98	0.45
1:A:245:ARG:HG2	1:C:110:ARG:NH2	2.32	0.45
1:A:308:VAL:HG11	1:D:305:TYR:CE1	2.52	0.45
1:B:203:ARG:NH1	1:B:210:VAL:O	2.39	0.44
1:C:312:LYS:HD2	1:C:312:LYS:HA	1.66	0.44
1:A:151:ARG:HG2	1:A:153:ARG:O	2.17	0.44
1:C:8:ILE:HD12	1:C:87:ALA:HA	1.99	0.44
1:B:188:SER:HB3	1:B:214:CYS:SG	2.57	0.44
1:C:276:VAL:HB	1:C:277:PRO:HD3	2.00	0.44
1:B:379:SER:O	1:B:383:GLN:HG3	2.18	0.43
1:C:120:VAL:O	1:C:121:ASP:C	2.61	0.43
1:D:151:ARG:HD2	1:D:154:ILE:HD13	2.00	0.43
1:A:270:ARG:O	1:A:298:GLN:HG2	2.18	0.43
1:B:188:SER:OG	1:B:189:PRO:HD3	2.17	0.43
1:D:381:GLU:O	1:D:384:GLY:N	2.51	0.43
1:B:97:ASP:HA	1:C:148:GLY:HA3	2.01	0.43
1:D:229:ILE:HA	1:D:232:MSE:HE3	2.01	0.43
1:B:163:GLU:HB2	1:B:169:ARG:CG	2.49	0.43
1:B:319:ILE:HA	1:B:347:ILE:CG2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:GLU:OE2	1:D:261:THR:HG22	2.18	0.43
1:B:32:ASN:HD21	1:B:36:TYR:H	1.66	0.42
1:D:200:GLU:HG3	1:D:201:ILE:N	2.34	0.42
1:A:251:GLY:O	1:A:255:VAL:HG23	2.19	0.42
1:C:160:GLY:C	1:C:162:PRO:HD3	2.44	0.42
1:C:230:LYS:NZ	2:C:421:HOH:O	2.48	0.42
1:C:307:HIS:HD2	1:C:336:ALA:HB3	1.84	0.42
1:B:94:ASP:OD2	1:B:94:ASP:C	2.61	0.42
1:C:337:ASN:OD1	1:C:337:ASN:N	2.52	0.42
1:D:313:VAL:O	1:D:338:VAL:HA	2.19	0.42
1:A:344:GLN:HB3	1:A:347:ILE:HD12	2.02	0.42
1:C:246:THR:OG1	1:C:268:GLU:OE2	2.34	0.42
1:C:307:HIS:CD2	1:C:336:ALA:HB3	2.54	0.42
1:A:56:ARG:HB2	1:A:66:TRP:CZ3	2.55	0.42
1:A:229:ILE:HA	1:A:232:MSE:HE3	2.01	0.42
1:A:255:VAL:O	1:A:259:VAL:HG22	2.19	0.42
1:B:345:HIS:H	1:B:345:HIS:CD2	2.37	0.42
1:A:220:HIS:HB2	1:A:243:PRO:O	2.20	0.41
1:C:203:ARG:HA	1:C:203:ARG:HD3	1.87	0.41
1:A:42:ASN:HD22	1:A:217:HIS:HD2	1.68	0.41
1:A:26:ARG:O	1:A:27:PRO:C	2.64	0.41
1:A:284:LEU:HD23	1:A:284:LEU:N	2.35	0.41
1:A:312:LYS:HD2	1:A:312:LYS:HA	1.81	0.41
1:C:67:GLY:HA3	1:C:125:ALA:O	2.21	0.41
1:C:105:LEU:HA	1:C:108:LEU:HD22	2.02	0.41
1:C:183:SER:HB3	1:C:238:TRP:CZ3	2.56	0.41
1:B:146:LEU:HD13	1:B:300:MSE:SE	2.71	0.41
1:B:233:GLU:N	1:B:234:PRO:CD	2.84	0.41
1:D:39:ARG:HD2	1:D:46:TYR:CE2	2.56	0.41
1:B:72:LEU:HD13	2:B:400:HOH:O	2.20	0.41
1:C:11:PHE:CD1	1:C:386:LEU:HB3	2.56	0.41
1:C:275:MSE:HE1	1:C:306:ALA:HB2	2.02	0.41
1:D:105:LEU:HD23	1:D:105:LEU:HA	1.85	0.41
1:D:116:GLY:CA	1:D:270:ARG:HG3	2.51	0.41
1:D:278:ARG:HB3	1:D:284:LEU:HD22	2.02	0.41
1:C:24:LYS:H	1:C:25:PRO:HD3	1.85	0.41
1:B:131:TRP:CD1	1:B:296:ILE:HB	2.56	0.41
1:C:229:ILE:HG21	1:C:259:VAL:HG21	2.02	0.40
1:C:315:PRO:HD2	1:C:340:CYS:O	2.20	0.40
1:C:165:THR:O	1:C:169:ARG:HG3	2.21	0.40
1:B:151:ARG:NH1	1:B:338:VAL:HB	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ARG:NH1	2:B:398:HOH:O	2.37	0.40
1:B:312:LYS:HD2	1:B:312:LYS:HA	1.83	0.40
1:B:181:PHE:CE1	1:B:364:GLY:HA2	2.57	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	Percentiles	
1	A	386/399 (97%)	366 (95%)	18 (5%)	2 (0%)	24	43
1	B	364/399 (91%)	343 (94%)	20 (6%)	1 (0%)	36	55
1	C	378/399 (95%)	361 (96%)	17 (4%)	0	100	100
1	D	379/399 (95%)	365 (96%)	13 (3%)	1 (0%)	36	55
All	All	1507/1596 (94%)	1435 (95%)	68 (4%)	4 (0%)	36	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ALA
1	D	16	PRO
1	A	27	PRO
1	B	160	GLY

### 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	A	300/301 (100%)	277 (92%)	23 (8%)	12	25
1	B	287/301 (95%)	267 (93%)	20 (7%)	14	29
1	C	291/301 (97%)	268 (92%)	23 (8%)	11	24
1	D	294/301 (98%)	261 (89%)	33 (11%)	6	12
All	All	1172/1204 (97%)	1073 (92%)	99 (8%)	10	22

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	18	GLU
1	A	22	LEU
1	A	55	VAL
1	A	72	LEU
1	A	108	LEU
1	A	130	LEU
1	A	133	LEU
1	A	137	LEU
1	A	142	VAL
1	A	153	ARG
1	A	168	LYS
1	A	190	VAL
1	A	210	VAL
1	A	245	ARG
1	A	254	ARG
1	A	279	VAL
1	A	287	VAL
1	A	312	LYS
1	A	349	GLU
1	A	374	LEU
1	A	376	VAL
1	A	386	LEU
1	B	15	LEU
1	B	32	ASN
1	B	37	LEU
1	B	42	ASN
1	B	72	LEU
1	B	108	LEU
1	B	130	LEU
1	B	133	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	137	LEU
1	B	153	ARG
1	B	161	LEU
1	B	210	VAL
1	B	261	THR
1	B	279	VAL
1	B	287	VAL
1	B	312	LYS
1	B	349	GLU
1	B	374	LEU
1	B	386	LEU
1	B	388	LYS
1	C	1	LEU
1	C	37	LEU
1	C	60	GLU
1	C	72	LEU
1	C	108	LEU
1	C	130	LEU
1	C	133	LEU
1	C	137	LEU
1	C	158	ILE
1	C	211	ARG
1	C	217	HIS
1	C	260	SER
1	C	279	VAL
1	C	282	ARG
1	C	287	VAL
1	C	312	LYS
1	C	318	THR
1	C	319	ILE
1	C	355	LEU
1	C	362	LEU
1	C	374	LEU
1	C	386	LEU
1	C	388	LYS
1	D	10	SER
1	D	15	LEU
1	D	17	ARG
1	D	37	LEU
1	D	49	PHE
1	D	72	LEU
1	D	108	LEU

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Mol	Chain	Res	Type
1	D	111	VAL
1	D	130	LEU
1	D	133	LEU
1	D	137	LEU
1	D	145	LEU
1	D	153	ARG
1	D	154	ILE
1	D	168	LYS
1	D	193	ASP
1	D	195	VAL
1	D	200	GLU
1	D	217	HIS
1	D	249	ILE
1	D	250	ASP
1	D	261	THR
1	D	279	VAL
1	D	302	ILE
1	D	318	THR
1	D	319	ILE
1	D	347	ILE
1	D	351	ASN
1	D	362	LEU
1	D	374	LEU
1	D	385	LEU
1	D	386	LEU
1	D	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	A	220	HIS
1	A	235	HIS
1	B	32	ASN
1	B	42	ASN
1	B	61	ASN
1	B	273	HIS
1	B	310	HIS
1	C	220	HIS
1	C	273	HIS
1	C	307	HIS
1	D	220	HIS

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	378/399 (94%)	-0.54	1 (0%) 90 87	19, 34, 61, 89	1 (0%)
1	B	361/399 (90%)	-0.27	3 (0%) 82 80	22, 40, 75, 86	0
1	C	373/399 (93%)	-0.41	0 100 100	25, 38, 64, 81	0
1	D	374/399 (93%)	-0.31	2 (0%) 87 85	25, 39, 77, 98	0
All	All	1486/1596 (93%)	-0.38	6 (0%) 88 86	19, 38, 73, 98	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	VAL	3.8
1	B	31	PRO	3.5
1	D	350	PRO	3.3
1	A	22	LEU	3.1
1	D	49	PHE	2.9
1	B	189	PRO	2.2

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.