



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:16 AM EDT

PDB ID : 2PCE / pdb\_00002pce  
Title : Crystal structure of putative mandelate racemase/muconate lactonizing enzyme from *Roseovarius nubinhibens* ISM  
Authors : Bonanno, J.B.; Rutter, M.; Bain, K.T.; Lau, C.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-03-29  
Resolution : 2.00 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

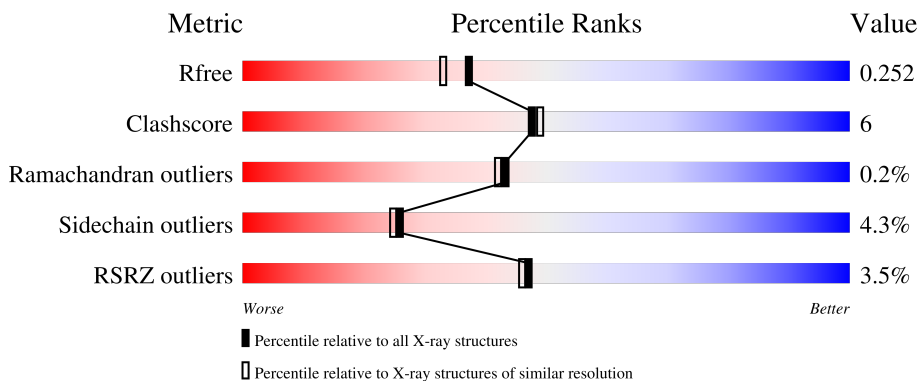
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

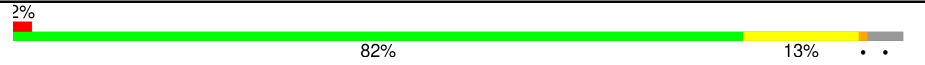



The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	386	 2% 82% 13% . .
1	B	386	 6% 82% 12% . .
1	C	386	 3% 81% 15% . .
1	D	386	 2% 81% 14% . .

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Mol	Chain	Length	Quality of chain
1	E	386	<p>2% 85% 11% .</p>
1	F	386	<p>6% 78% 16% . .</p>
1	G	386	<p>3% 79% 16% . .</p>
1	H	386	<p>4% 83% 12% . .</p>

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	D	401	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23281 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 mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	372	Total 2796	C 1741	N 514	O 525	S 16	0	4	0
1	B	371	Total 2770	C 1724	N 507	O 523	S 16	0	2	0
1	C	372	Total 2777	C 1727	N 511	O 523	S 16	0	1	0
1	D	372	Total 2777	C 1727	N 511	O 523	S 16	0	1	0
1	E	372	Total 2777	C 1727	N 511	O 523	S 16	0	1	0
1	F	370	Total 2771	C 1725	N 510	O 520	S 16	0	2	0
1	G	372	Total 2788	C 1735	N 513	O 524	S 16	0	3	0
1	H	372	Total 2784	C 1732	N 513	O 523	S 16	0	2	0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	111	Total	O	0	0
			111	111		
3	C	102	Total	O	0	0
			102	102		
3	D	128	Total	O	0	0
			128	128		

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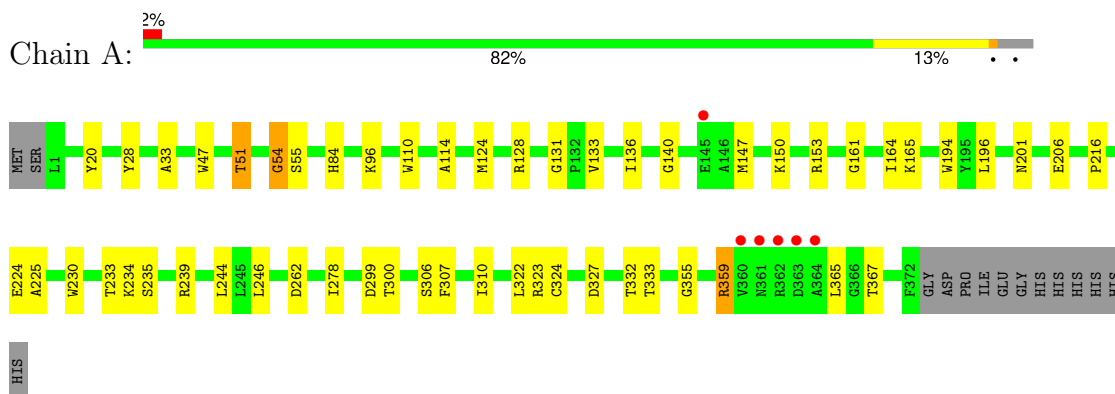
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	143	Total 143	O 143	0	0
3	F	129	Total 129	O 129	0	0
3	G	114	Total 114	O 114	0	0
3	H	110	Total 110	O 110	0	0

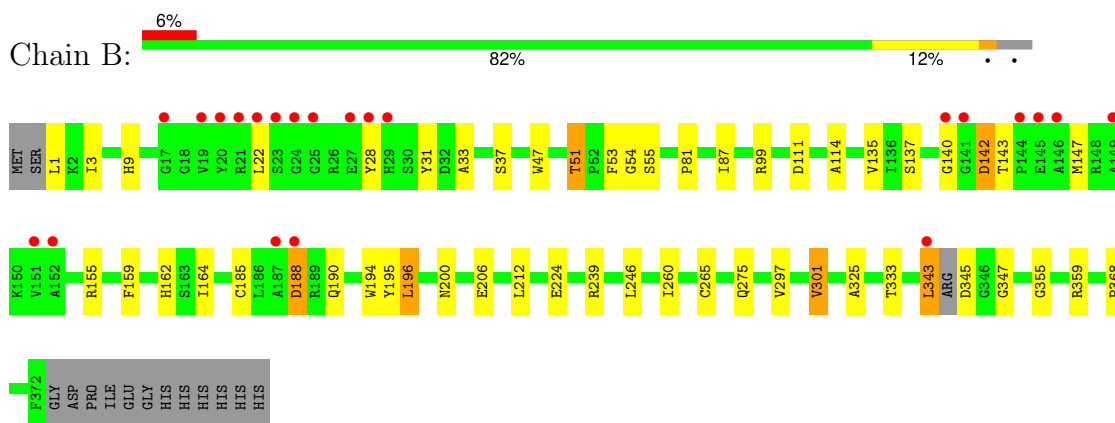
### 3 Residue-property plots [i](#)

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.

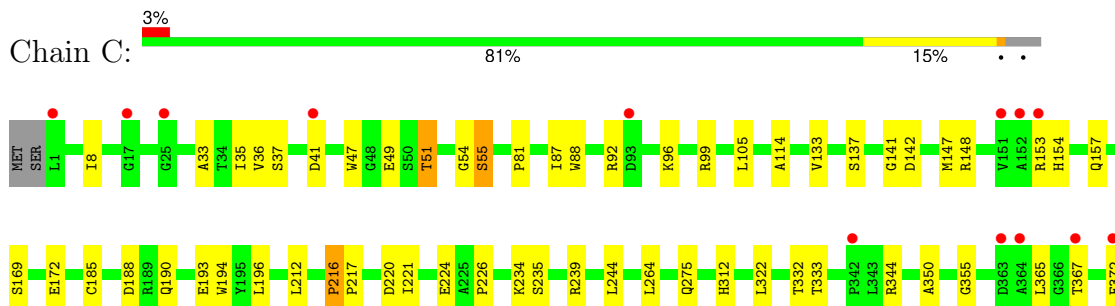
- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme



- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme




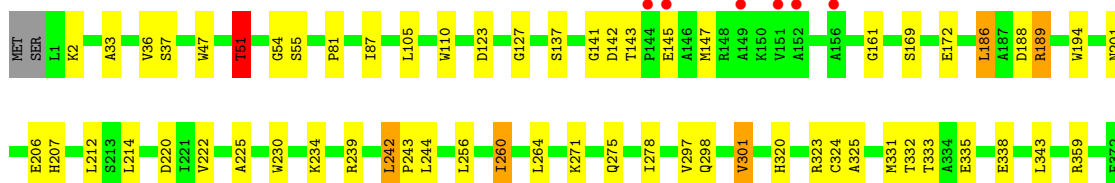
- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme



GLY  
ASP  
PRO  
ILE  
GLU  
GLY  
HIS  
HIS  
HIS  
HIS  
HIS


- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme

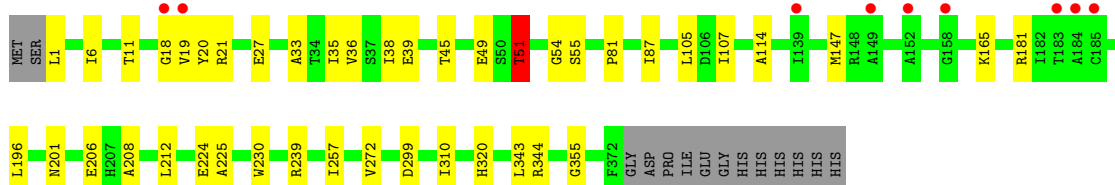
Chain D: 




GLY  
ASP  
PRO  
ILE  
GLU  
GLY  
HIS  
HIS  
HIS  
HIS  
HIS

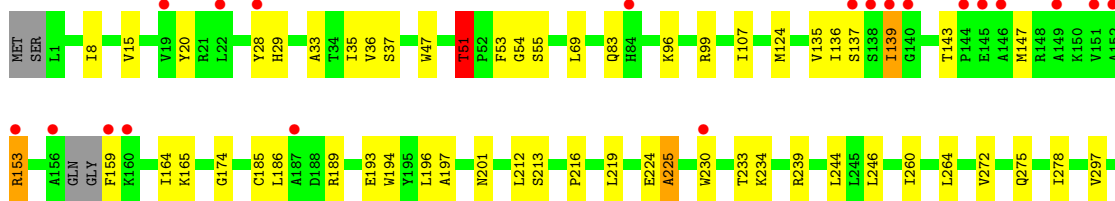
- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme

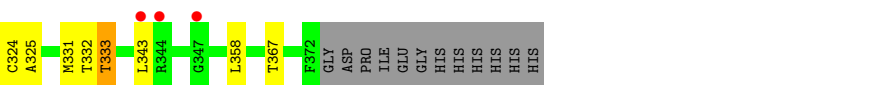
Chain E: 




- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme

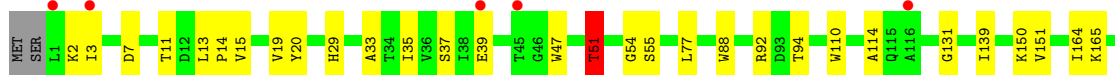
Chain F: 

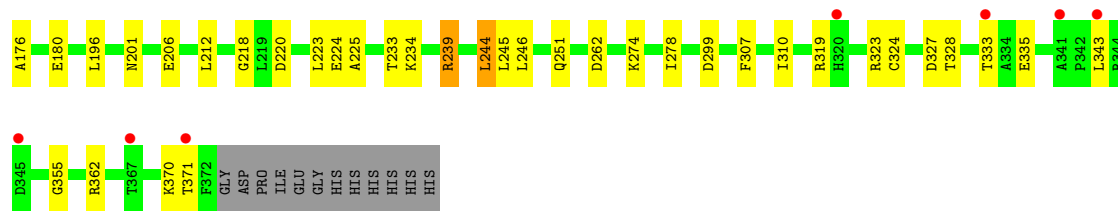


Chain G: 

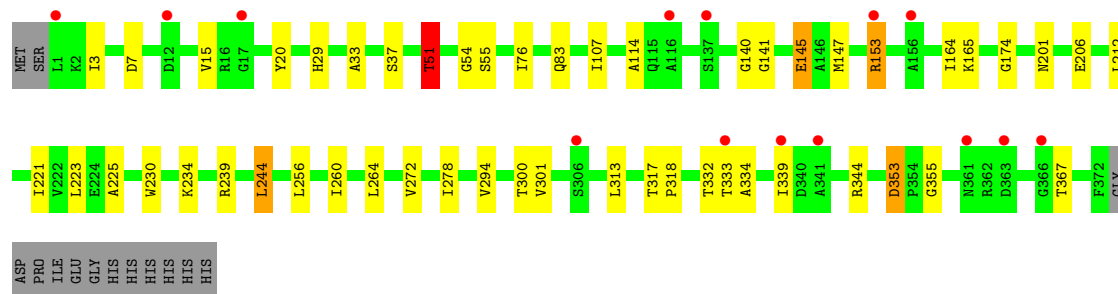
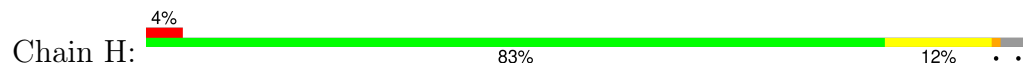
- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme

Chain G: 





- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.69Å 174.41Å 108.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.00) 96.9 (20.00-2.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.00Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.202 , 0.250 0.205 , 0.252	Depositor DCC
$R_{free}$ test set	10475 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtrriage
Anisotropy	0.323	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.010 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.16 % 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 9.2445e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.02	0/2853	1.05	5/3877 (0.1%)
1	B	0.94	0/2822	1.04	2/3834 (0.1%)
1	C	0.88	0/2827	1.04	5/3841 (0.1%)
1	D	0.97	2/2827 (0.1%)	1.05	4/3841 (0.1%)
1	E	0.96	1/2827 (0.0%)	1.04	3/3841 (0.1%)
1	F	0.99	4/2824 (0.1%)	1.03	6/3836 (0.2%)
1	G	0.91	1/2845 (0.0%)	1.03	5/3866 (0.1%)
1	H	0.94	1/2838 (0.0%)	1.07	6/3856 (0.2%)
All	All	0.95	9/22663 (0.0%)	1.04	36/30792 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	8

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	THR	CA-CB	6.75	1.61	1.53
1	F	51	THR	CA-CB	6.41	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	51	THR	CA-CB	6.13	1.59	1.53
1	D	51	THR	C-O	-5.46	1.20	1.25
1	F	225	ALA	C-O	-5.34	1.21	1.23
1	G	51	THR	CA-CB	5.28	1.60	1.52
1	F	197	ALA	CA-CB	-5.24	1.46	1.53
1	F	35	ILE	CA-CB	5.10	1.60	1.54
1	H	51	THR	CA-CB	5.08	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	55	SER	N-CA-C	13.28	128.95	113.15
1	C	55	SER	N-CA-C	-12.71	93.81	113.89
1	D	55	SER	N-CA-C	-10.73	96.94	113.89
1	B	55	SER	N-CA-C	-10.62	98.99	114.39
1	G	55	SER	N-CA-C	-10.31	97.59	113.89
1	A	55	SER	N-CA-C	-9.89	98.78	113.61
1	H	55	SER	N-CA-C	-9.01	100.09	113.61
1	F	55	SER	N-CA-C	-8.66	100.66	114.09
1	D	242	LEU	CA-C-N	-7.28	112.50	119.85
1	D	242	LEU	C-N-CA	-7.28	112.50	119.85
1	A	131	GLY	CA-C-N	6.71	126.62	119.85
1	A	131	GLY	C-N-CA	6.71	126.62	119.85
1	E	55	SER	N-CA-CB	-5.86	101.44	110.46
1	H	334	ALA	N-CA-C	5.75	118.12	110.53
1	G	51	THR	CB-CA-C	5.65	119.35	110.71
1	H	174	GLY	CA-C-N	5.52	125.35	119.28
1	H	174	GLY	C-N-CA	5.52	125.35	119.28
1	C	216	PRO	CA-C-N	5.38	125.68	119.92
1	C	216	PRO	C-N-CA	5.38	125.68	119.92
1	E	51	THR	CB-CA-C	5.38	118.43	111.01
1	F	51	THR	CB-CA-C	5.37	118.92	110.71
1	F	333	THR	N-CA-CB	-5.35	102.66	110.53
1	B	111	ASP	N-CA-C	-5.34	105.35	111.07
1	C	216	PRO	O-C-N	5.31	123.64	121.15
1	D	55	SER	N-CA-CB	5.28	118.55	110.95
1	H	300	THR	N-CA-C	-5.27	105.23	110.97
1	C	235	SER	N-CA-CB	5.25	117.93	110.16
1	G	131	GLY	CA-C-N	-5.21	114.88	120.03
1	G	131	GLY	C-N-CA	-5.21	114.88	120.03
1	F	174	GLY	CA-C-N	5.16	125.20	119.32
1	F	174	GLY	C-N-CA	5.16	125.20	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	PRO	O-C-N	5.14	123.68	121.31
1	H	294	VAL	N-CA-C	-5.13	104.45	110.05
1	F	216	PRO	O-C-N	5.11	123.66	121.31
1	A	300	THR	N-CA-C	-5.07	105.64	111.07
1	G	239	ARG	CG-CD-NE	-5.04	100.90	112.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	GLY	Peptide
1	B	54	GLY	Peptide
1	C	54	GLY	Peptide
1	D	54	GLY	Peptide
1	E	54	GLY	Peptide
1	F	54	GLY	Peptide
1	G	54	GLY	Peptide
1	H	54	GLY	Peptide

## 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	2796	0	2821	27	0
1	B	2770	0	2790	30	0
1	C	2777	0	2797	33	0
1	D	2777	0	2797	33	0
1	E	2777	0	2797	29	0
1	F	2771	0	2792	41	0
1	G	2788	0	2811	33	0
1	H	2784	0	2804	29	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	164	0	0	4	0
3	B	111	0	0	3	0
3	C	102	0	0	2	0
3	D	128	0	0	3	0
3	E	143	0	0	5	0
3	F	129	0	0	1	0
3	G	114	0	0	0	0
3	H	110	0	0	0	0
All	All	23281	0	22409	251	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 6.

All (251) 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:D:142:ASP:H	1:D:147:MET:HE3	1.06	1.11
1:C:142:ASP:H	1:C:147:MET:HE3	1.07	1.08
1:E:147:MET:HE1	1:E:181:ARG:HB3	1.37	1.01
3:E:428:HOH:O	1:F:83:GLN:HG2	1.60	1.00
1:H:234:LYS:HG2	1:H:264:LEU:HD11	1.47	0.97
1:C:142:ASP:N	1:C:147:MET:HE3	1.79	0.97
1:H:153:ARG:HG3	1:H:153:ARG:HH11	1.27	0.95
1:D:141:GLY:HA2	1:D:147:MET:CE	1.98	0.94
1:G:139:ILE:HD13	1:G:151:VAL:HG22	1.52	0.90
1:E:147:MET:HE1	1:E:181:ARG:CB	2.02	0.89
1:C:141:GLY:HA2	1:C:147:MET:CE	2.03	0.88
1:D:142:ASP:N	1:D:147:MET:HE3	1.88	0.88
1:A:359:ARG:HG3	1:A:359:ARG:HH11	1.40	0.84
1:F:143:THR:O	1:F:147:MET:HG3	1.79	0.83
1:E:208:ALA:O	1:E:212:LEU:HD13	1.80	0.82
1:H:153:ARG:HH11	1:H:153:ARG:CG	1.93	0.80
1:C:196:LEU:HD22	1:C:224:GLU:HB2	1.63	0.80
1:B:155:ARG:NH1	1:B:188:ASP:O	2.14	0.79
1:G:139:ILE:CD1	1:G:151:VAL:HG22	2.13	0.78
1:G:139:ILE:HD13	1:G:151:VAL:CG2	2.14	0.78
1:B:142:ASP:H	1:B:147:MET:HE3	1.49	0.77
1:G:176:ALA:O	1:G:180:GLU:HG3	1.85	0.76
1:G:33:ALA:HA	1:G:51:THR:HB	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ALA:HA	1:D:51:THR:HB	1.70	0.74
1:C:114:ALA:HB3	1:C:355:GLY:HA2	1.70	0.73
1:F:33:ALA:HA	1:F:51:THR:HB	1.69	0.73
1:D:141:GLY:HA2	1:D:147:MET:HE2	1.71	0.73
1:B:143:THR:HB	3:B:411:HOH:O	1.86	0.73
1:H:33:ALA:HA	1:H:51:THR:HB	1.71	0.73
1:F:153:ARG:HG3	1:F:153:ARG:HH11	1.55	0.72
1:E:196:LEU:HD22	1:E:224:GLU:HB2	1.75	0.69
1:E:196:LEU:HD13	1:E:224:GLU:OE1	1.93	0.69
1:C:234:LYS:HG2	1:C:264:LEU:HD13	1.75	0.68
1:H:234:LYS:HG2	1:H:264:LEU:CD1	2.22	0.68
1:G:299:ASP:HB2	1:G:310:ILE:HD11	1.76	0.67
3:C:437:HOH:O	1:H:83:GLN:HG2	1.95	0.66
1:E:320:HIS:HD2	3:E:465:HOH:O	1.76	0.66
1:B:33:ALA:HA	1:B:51:THR:HB	1.77	0.66
1:H:153:ARG:HG3	1:H:153:ARG:NH1	2.04	0.66
1:D:301:VAL:HG23	1:D:331:MET:HE2	1.78	0.65
1:A:299:ASP:HB2	1:A:310:ILE:HD11	1.79	0.64
1:A:359:ARG:HG3	1:A:359:ARG:NH1	2.05	0.64
1:B:114:ALA:HB3	1:B:355:GLY:HA2	1.80	0.63
1:F:196:LEU:HD22	1:F:224:GLU:HB2	1.80	0.63
1:G:196:LEU:HD13	1:G:224:GLU:OE1	1.99	0.63
1:C:226:PRO:HG3	1:C:244:LEU:HD11	1.82	0.62
1:E:33:ALA:HA	1:E:51:THR:HB	1.81	0.62
1:D:147:MET:HA	3:D:432:HOH:O	2.00	0.61
1:H:256:LEU:O	1:H:260:ILE:HD13	2.00	0.61
1:E:114:ALA:HB3	1:E:355:GLY:HA2	1.83	0.61
1:F:343:LEU:HD12	1:F:343:LEU:N	2.16	0.60
1:C:81:PRO:HA	1:C:87:ILE:HD11	1.82	0.60
1:B:155:ARG:HH11	1:B:190:GLN:HG2	1.66	0.59
1:B:28:TYR:CE2	1:B:53:PHE:HE2	2.20	0.59
1:D:142:ASP:H	1:D:147:MET:CE	1.98	0.59
1:H:145:GLU:H	1:H:145:GLU:CD	2.09	0.58
1:B:143:THR:CB	3:B:411:HOH:O	2.46	0.58
1:C:99:ARG:HD3	1:C:275:GLN:O	2.03	0.58
1:F:20:TYR:OH	1:F:165:LYS:HE3	2.03	0.58
1:G:114:ALA:HB3	1:G:355:GLY:HA2	1.84	0.58
1:C:8:ILE:CD1	1:C:372:PHE:HE2	2.16	0.58
1:B:28:TYR:CE2	1:B:53:PHE:CE2	2.91	0.58
1:C:33:ALA:HA	1:C:51:THR:HB	1.85	0.57
1:F:189:ARG:NH2	1:F:193:GLU:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:MET:HB3	1:C:185:CYS:SG	2.44	0.57
1:A:33:ALA:HA	1:A:51:THR:HB	1.87	0.57
1:C:141:GLY:HA2	1:C:147:MET:HE3	1.86	0.57
1:G:307:PHE:HB2	1:G:328:THR:OG1	2.05	0.57
1:D:320:HIS:HD2	3:D:444:HOH:O	1.87	0.56
1:F:301:VAL:HG23	1:F:331:MET:HE2	1.87	0.56
1:H:147:MET:HE1	1:H:165:LYS:O	2.05	0.56
1:H:223:LEU:HB3	1:H:244:LEU:HD12	1.88	0.56
1:C:190:GLN:O	1:C:193:GLU:HG3	2.06	0.56
1:G:11:THR:HG22	1:G:35:ILE:CD1	2.35	0.56
1:H:141:GLY:HA2	1:H:147:MET:HE3	1.87	0.55
1:H:140:GLY:O	1:H:147:MET:HE3	2.05	0.55
1:A:47:TRP:CZ3	1:A:365:LEU:CD1	2.90	0.55
1:F:186:LEU:HD12	1:F:219:LEU:HD22	1.89	0.55
1:F:164:ILE:O	1:F:164:ILE:HG13	2.07	0.54
1:H:7:ASP:HB2	1:H:37:SER:OG	2.08	0.53
1:H:230[A]:TRP:CD1	1:H:234:LYS:HE2	2.43	0.53
1:G:20:TYR:OH	1:G:165:LYS:HE2	2.09	0.53
1:E:11:THR:HG22	1:E:35:ILE:CD1	2.39	0.53
1:D:201:ASN:HD22	1:D:225:ALA:HB1	1.73	0.53
1:C:55:SER:OG	1:G:94:THR:O	2.26	0.53
1:E:147:MET:HE1	1:E:181:ARG:CG	2.38	0.53
1:F:136:ILE:HG23	1:F:137:SER:O	2.09	0.53
1:A:196[B]:LEU:HD11	1:A:224:GLU:HB2	1.91	0.53
1:B:142:ASP:N	1:B:147:MET:HE3	2.20	0.53
1:B:1:LEU:N	3:B:418:HOH:O	2.37	0.53
1:F:8:ILE:HD13	1:F:36:VAL:HG22	1.91	0.52
1:C:114:ALA:CB	1:C:355:GLY:HA2	2.38	0.52
1:B:196:LEU:HD22	1:B:224:GLU:HB2	1.90	0.52
1:F:194:TRP:CH2	1:F:196:LEU:HG	2.45	0.51
1:E:320:HIS:CD2	3:E:465:HOH:O	2.59	0.51
1:H:114:ALA:HB3	1:H:355:GLY:HA2	1.92	0.51
1:G:234:LYS:HE2	1:G:262:ASP:CG	2.35	0.51
1:F:201:ASN:HD22	1:F:225:ALA:HB1	1.75	0.51
1:C:141:GLY:HA2	1:C:147:MET:HE1	1.90	0.51
1:C:37:SER:HB3	1:C:47:TRP:CZ3	2.46	0.51
1:A:233:THR:HG21	1:A:246:LEU:HD21	1.93	0.50
1:F:147:MET:HB3	1:F:185:CYS:SG	2.51	0.50
1:F:297:VAL:O	1:F:325:ALA:HA	2.12	0.50
1:A:194:TRP:CZ3	1:A:196[A]:LEU:HG	2.47	0.50
1:E:230[A]:TRP:CD1	3:E:492:HOH:O	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:SER:HB3	1:D:47:TRP:CZ3	2.46	0.50
1:A:201:ASN:HD22	1:A:225:ALA:HB1	1.77	0.49
1:E:299:ASP:HB2	1:E:310:ILE:HD11	1.93	0.49
1:B:155:ARG:NH1	1:B:190:GLN:HG2	2.26	0.49
1:B:359:ARG:HG3	1:B:359:ARG:HH11	1.76	0.49
1:D:297:VAL:O	1:D:325:ALA:HA	2.13	0.49
1:G:3:ILE:HG22	1:G:77:LEU:HD23	1.95	0.49
1:A:230[B]:TRP:HD1	3:A:470:HOH:O	1.95	0.49
1:F:196:LEU:HD13	1:F:224:GLU:OE1	2.13	0.49
1:F:278:ILE:HG23	1:F:313:LEU:HD21	1.94	0.49
1:A:323:ARG:O	1:A:324:CYS:HB2	2.13	0.49
1:D:110:TRP:CD1	1:D:278:ILE:HB	2.48	0.49
1:F:323:ARG:O	1:F:324:CYS:HB2	2.13	0.49
1:A:20:TYR:OH	1:A:165:LYS:HE2	2.13	0.49
1:A:133:VAL:HG13	1:A:322:LEU:HD21	1.95	0.49
1:F:107:ILE:HD11	1:F:272:VAL:CG1	2.43	0.49
1:D:256:LEU:O	1:D:260:ILE:HD12	2.13	0.48
1:G:196:LEU:HD21	1:G:245:LEU:HD13	1.95	0.48
1:B:246:LEU:HG	1:B:265:CYS:HB3	1.95	0.48
1:F:8:ILE:HD12	1:F:69:LEU:HD13	1.95	0.48
1:B:343:LEU:HA	1:B:347:GLY:O	2.14	0.48
1:G:370:LYS:HD2	1:G:371:THR:H	1.78	0.48
1:B:135:VAL:HG23	1:B:159:PHE:CE1	2.49	0.48
1:E:20:TYR:OH	1:E:165:LYS:HE2	2.13	0.48
1:F:37:SER:HB3	1:F:47:TRP:CZ3	2.48	0.48
1:F:153:ARG:HH11	1:F:153:ARG:CG	2.27	0.47
1:C:312:HIS:CE1	1:C:350:ALA:HB1	2.49	0.47
1:E:201:ASN:HD22	1:E:225:ALA:HB1	1.78	0.47
1:E:343:LEU:N	1:E:343:LEU:HD12	2.29	0.47
1:G:327:ASP:OD1	1:G:343:LEU:HD11	2.14	0.47
1:A:84[B]:HIS:HD2	3:A:461:HOH:O	1.97	0.47
1:B:196:LEU:CD2	1:B:224:GLU:HB2	2.43	0.47
1:G:110:TRP:CD1	1:G:278:ILE:HB	2.50	0.47
1:E:257:ILE:HD12	1:F:260:ILE:HD13	1.97	0.47
1:D:222:VAL:HG22	1:D:243:PRO:HG2	1.97	0.46
1:A:128:ARG:HD3	3:A:545:HOH:O	2.16	0.46
1:C:8:ILE:HD12	1:C:372:PHE:HE2	1.79	0.46
1:F:107:ILE:HD11	1:F:272:VAL:HG11	1.97	0.46
1:G:196:LEU:HD22	1:G:224:GLU:HB2	1.96	0.46
1:D:234:LYS:HG2	1:D:264:LEU:HD13	1.96	0.46
1:B:140:GLY:O	1:B:147:MET:HE2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ASP:HA	1:D:127:GLY:HA2	1.97	0.45
1:E:49:GLU:OE2	1:E:51:THR:CG2	2.64	0.45
1:B:37:SER:HB3	1:B:47:TRP:CZ3	2.52	0.45
1:B:99:ARG:HD3	1:B:275:GLN:O	2.15	0.45
1:B:162:HIS:CD2	1:B:195:TYR:CE2	3.04	0.45
1:C:196:LEU:HD13	1:C:224:GLU:OE1	2.16	0.45
1:F:135:VAL:HG23	1:F:159:PHE:CD1	2.51	0.45
1:D:338:GLU:HB2	1:D:359:ARG:HB2	1.97	0.45
1:D:169:SER:OG	1:D:172:GLU:HG3	2.16	0.45
1:G:13:LEU:HA	1:G:14:PRO:HD3	1.86	0.45
1:D:230[B]:TRP:HD1	3:D:441:HOH:O	1.99	0.45
1:H:20:TYR:OH	1:H:165:LYS:HE2	2.17	0.45
1:C:8:ILE:HD11	1:C:372:PHE:HE2	1.81	0.45
1:H:353:ASP:OD2	1:H:353:ASP:N	2.50	0.44
1:A:114:ALA:HB3	1:A:355:GLY:HA2	1.99	0.44
1:G:19:VAL:HG22	1:G:29:HIS:CE1	2.52	0.44
1:C:153:ARG:O	1:C:157:GLN:HG3	2.17	0.44
1:E:21:ARG:HG2	1:E:27:GLU:HG2	1.99	0.44
1:G:37:SER:HB3	1:G:47:TRP:CZ3	2.52	0.44
1:A:47:TRP:CZ3	1:A:365:LEU:HD11	2.53	0.44
1:F:15:VAL:HG23	1:F:29:HIS:C	2.42	0.44
1:A:124:MET:HE3	1:A:124:MET:HB3	1.82	0.44
1:E:11:THR:HG22	1:E:35:ILE:HD11	2.00	0.44
1:C:216:PRO:HA	1:C:217:PRO:HD3	1.82	0.44
1:A:307:PHE:CE1	1:A:327:ASP:HA	2.53	0.43
1:C:133:VAL:HG13	1:C:322:LEU:HD21	2.00	0.43
1:F:124:MET:HB3	1:F:124:MET:HE3	1.83	0.43
1:H:201:ASN:HD22	1:H:225:ALA:HB1	1.83	0.43
1:D:271:LYS:HA	1:D:298:GLN:O	2.18	0.43
1:F:213:SER:O	1:G:218:GLY:HA2	2.18	0.43
1:F:99:ARG:HD3	1:F:275:GLN:O	2.18	0.43
1:F:234:LYS:HG2	1:F:264:LEU:HD13	1.99	0.43
1:G:220:ASP:OD2	1:G:220:ASP:C	2.62	0.43
1:H:153:ARG:CG	1:H:153:ARG:NH1	2.64	0.43
1:A:140:GLY:O	1:A:147:MET:HE3	2.18	0.43
1:D:141:GLY:HA2	1:D:147:MET:HE3	1.96	0.43
1:C:137:SER:HB2	1:C:154:HIS:CD2	2.54	0.43
1:D:169:SER:HG	1:D:172:GLU:HG3	1.83	0.43
1:G:15:VAL:HG23	1:G:29:HIS:C	2.43	0.43
1:H:230[B]:TRP:O	1:H:234:LYS:HG3	2.19	0.43
1:D:359:ARG:HG3	1:D:359:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ILE:HG12	1:E:38:ILE:HG12	1.99	0.43
1:H:230[A]:TRP:CE2	1:H:264:LEU:HD22	2.53	0.43
1:C:36:VAL:HG11	1:C:105:LEU:HD23	2.00	0.43
1:C:148:ARG:NH2	1:C:188:ASP:OD1	2.48	0.43
1:F:308:ALA:HB2	1:F:358:LEU:HD21	2.01	0.43
1:A:359:ARG:HH11	1:A:359:ARG:CG	2.18	0.43
1:B:297:VAL:O	1:B:325:ALA:HA	2.19	0.43
1:H:107:ILE:HD11	1:H:272:VAL:CG1	2.49	0.43
1:B:3:ILE:HG13	1:B:81:PRO:HD3	2.00	0.42
1:C:49:GLU:OE2	1:C:51:THR:CG2	2.67	0.42
1:E:18:GLY:O	1:E:19:VAL:C	2.62	0.42
1:G:223:LEU:HB3	1:G:244:LEU:HD12	2.01	0.42
1:C:220:ASP:HB2	1:D:214:LEU:HD21	2.00	0.42
1:E:344:ARG:HE	1:E:344:ARG:HB3	1.51	0.42
1:G:233:THR:HG21	1:G:246:LEU:HD21	2.00	0.42
1:A:153:ARG:NH2	3:A:460:HOH:O	2.52	0.42
1:E:49:GLU:OE2	1:E:51:THR:HG21	2.19	0.42
1:F:230[B]:TRP:HD1	3:F:420:HOH:O	2.02	0.42
1:B:359:ARG:HG3	1:B:359:ARG:NH1	2.35	0.42
1:D:36:VAL:HG11	1:D:105:LEU:HD23	2.00	0.42
1:H:278:ILE:HG23	1:H:313:LEU:HD21	2.00	0.42
1:C:194:TRP:CH2	1:C:196:LEU:HG	2.54	0.42
3:C:437:HOH:O	1:H:83:GLN:CG	2.61	0.42
1:E:107:ILE:HD11	1:E:272:VAL:CG1	2.49	0.42
1:H:3:ILE:HD13	1:H:76:ILE:HD12	2.00	0.42
1:B:22:LEU:HD22	1:B:200:ASN:OD1	2.20	0.42
1:B:147:MET:HB3	1:B:185:CYS:SG	2.60	0.42
1:F:28:TYR:CE2	1:F:53:PHE:HE2	2.38	0.42
1:H:15:VAL:HG23	1:H:29:HIS:C	2.44	0.42
1:G:11:THR:HG22	1:G:35:ILE:HD11	2.01	0.42
1:G:251:GLN:HG2	1:G:274:LYS:HG3	2.01	0.42
1:F:201:ASN:ND2	1:F:225:ALA:HB1	2.35	0.41
1:D:323:ARG:O	1:D:324:CYS:HB2	2.20	0.41
1:D:207:HIS:CD2	1:D:207:HIS:C	2.98	0.41
1:G:88:TRP:CD1	1:G:92:ARG:HD2	2.55	0.41
1:C:88:TRP:O	1:C:92:ARG:HG3	2.20	0.41
1:D:161:GLY:HA2	1:D:194:TRP:O	2.21	0.41
1:E:36:VAL:HG11	1:E:105:LEU:HD23	2.02	0.41
1:G:201:ASN:HD22	1:G:225:ALA:HB1	1.86	0.41
1:D:220:ASP:OD2	1:D:220:ASP:C	2.63	0.41
1:G:7:ASP:HB2	1:G:37:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:THR:HA	1:H:318:PRO:HD2	1.90	0.41
1:A:110:TRP:CD1	1:A:278:ILE:HB	2.56	0.41
1:F:139:ILE:O	1:F:165:LYS:HG2	2.20	0.41
1:G:323:ARG:O	1:G:324:CYS:HB2	2.21	0.41
1:B:31:TYR:CE1	1:B:301:VAL:HG21	2.55	0.41
1:C:169:SER:OG	1:C:172:GLU:HG3	2.21	0.41
1:F:233:THR:HG21	1:F:246:LEU:HD21	2.02	0.41
1:A:20:TYR:HB3	1:A:28:TYR:HB2	2.02	0.41
1:A:136:ILE:HG13	1:A:161:GLY:C	2.46	0.41
1:A:234:LYS:HE2	1:A:262:ASP:OD1	2.21	0.41
1:B:9:HIS:CE1	1:B:368:PRO:HG3	2.56	0.41
1:F:343:LEU:N	1:F:343:LEU:CD1	2.83	0.41
1:F:8:ILE:CD1	1:F:36:VAL:HG22	2.50	0.41
1:A:299:ASP:CB	1:A:310:ILE:HD11	2.47	0.40
1:D:81:PRO:HA	1:D:87:ILE:HD11	2.03	0.40
1:E:1:LEU:N	3:E:520:HOH:O	2.54	0.40
1:F:196:LEU:HD22	1:F:224:GLU:CB	2.47	0.40
1:D:143:THR:O	1:D:147:MET:HG3	2.21	0.40
1:E:81:PRO:HA	1:E:87:ILE:HD11	2.03	0.40
1:B:194:TRP:CH2	1:B:196:LEU:HG	2.56	0.40
1:D:186:LEU:HD13	1:D:189:ARG:NH1	2.37	0.40
1:E:39:GLU:HG2	1:E:45:THR:OG1	2.21	0.40
1:H:230[A]:TRP:HD1	1:H:234:LYS:CE	2.34	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	374/386 (97%)	363 (97%)	10 (3%)	1 (0%)	36 35
1	B	369/386 (96%)	355 (96%)	13 (4%)	1 (0%)	36 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	371/386 (96%)	359 (97%)	11 (3%)	1 (0%)	36	35
1	D	371/386 (96%)	358 (96%)	12 (3%)	1 (0%)	36	35
1	E	371/386 (96%)	360 (97%)	11 (3%)	0	100	100
1	F	368/386 (95%)	351 (95%)	16 (4%)	1 (0%)	36	35
1	G	373/386 (97%)	362 (97%)	11 (3%)	0	100	100
1	H	372/386 (96%)	361 (97%)	10 (3%)	1 (0%)	36	35
All	All	2969/3088 (96%)	2869 (97%)	94 (3%)	6 (0%)	43	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	ASP
1	A	54	GLY
1	B	301	VAL
1	H	301	VAL
1	F	301	VAL
1	D	301	VAL

### 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	286/294 (97%)	273 (96%)	13 (4%)	24	23
1	B	283/294 (96%)	269 (95%)	14 (5%)	22	20
1	C	283/294 (96%)	272 (96%)	11 (4%)	28	28
1	D	283/294 (96%)	265 (94%)	18 (6%)	16	12
1	E	283/294 (96%)	280 (99%)	3 (1%)	65	73
1	F	283/294 (96%)	273 (96%)	10 (4%)	32	32
1	G	285/294 (97%)	272 (95%)	13 (5%)	24	22
1	H	284/294 (97%)	269 (95%)	15 (5%)	20	18
All	All	2270/2352 (96%)	2173 (96%)	97 (4%)	26	25

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	96	LYS
1	A	150	LYS
1	A	164	ILE
1	A	206	GLU
1	A	235	SER
1	A	239	ARG
1	A	244	LEU
1	A	306	SER
1	A	332	THR
1	A	333	THR
1	A	359	ARG
1	A	367	THR
1	B	51	THR
1	B	87	ILE
1	B	137	SER
1	B	142	ASP
1	B	164	ILE
1	B	188	ASP
1	B	196	LEU
1	B	206	GLU
1	B	212	LEU
1	B	239	ARG
1	B	260	ILE
1	B	333	THR
1	B	343	LEU
1	B	345	ASP
1	C	35	ILE
1	C	51	THR
1	C	96	LYS
1	C	212	LEU
1	C	221	ILE
1	C	239	ARG
1	C	332	THR
1	C	333	THR
1	C	344	ARG
1	C	365	LEU
1	C	367	THR
1	D	2	LYS
1	D	51	THR
1	D	137	SER
1	D	145	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	186	LEU
1	D	188	ASP
1	D	189	ARG
1	D	206	GLU
1	D	212	LEU
1	D	239	ARG
1	D	242	LEU
1	D	244	LEU
1	D	260	ILE
1	D	275	GLN
1	D	332	THR
1	D	333	THR
1	D	335	GLU
1	D	343	LEU
1	E	51	THR
1	E	206	GLU
1	E	239	ARG
1	F	51	THR
1	F	96	LYS
1	F	139	ILE
1	F	153	ARG
1	F	212	LEU
1	F	239	ARG
1	F	244	LEU
1	F	332	THR
1	F	333	THR
1	F	367	THR
1	G	2	LYS
1	G	39	GLU
1	G	51	THR
1	G	150	LYS
1	G	164	ILE
1	G	206	GLU
1	G	212	LEU
1	G	239	ARG
1	G	244	LEU
1	G	319	ARG
1	G	333	THR
1	G	335	GLU
1	G	362	ARG
1	H	51	THR
1	H	145	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	153	ARG
1	H	164	ILE
1	H	206	GLU
1	H	212	LEU
1	H	221	ILE
1	H	239	ARG
1	H	244	LEU
1	H	332	THR
1	H	333	THR
1	H	339	ILE
1	H	344	ARG
1	H	353	ASP
1	H	367	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	9	HIS
1	A	190	GLN
1	A	201	ASN
1	B	9	HIS
1	B	29	HIS
1	B	201	ASN
1	C	201	ASN
1	D	83	GLN
1	D	84	HIS
1	D	157	GLN
1	D	201	ASN
1	E	157	GLN
1	E	201	ASN
1	E	320	HIS
1	F	29	HIS
1	F	154	HIS
1	F	201	ASN
1	F	320	HIS
1	G	29	HIS
1	G	201	ASN
1	G	320	HIS
1	H	201	ASN
1	H	320	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](#)

8 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	F	401	-	4,4,4	0.73	0	6,6,6	1.24	0
2	PO4	D	401	-	4,4,4	1.40	1 (25%)	6,6,6	1.92	3 (50%)
2	PO4	B	401	-	4,4,4	0.82	0	6,6,6	0.87	0
2	PO4	E	401	-	4,4,4	1.16	0	6,6,6	1.84	2 (33%)
2	PO4	H	401	-	4,4,4	1.08	0	6,6,6	1.12	1 (16%)
2	PO4	A	401	-	4,4,4	0.97	0	6,6,6	1.39	1 (16%)
2	PO4	C	401	-	4,4,4	0.64	0	6,6,6	1.29	1 (16%)
2	PO4	G	401	-	4,4,4	0.97	0	6,6,6	0.89	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	PO4	P-O3	-2.08	1.48	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	PO4	O4-P-O3	3.30	118.19	107.91
2	D	401	PO4	O3-P-O2	2.71	116.36	107.91
2	C	401	PO4	O4-P-O1	-2.64	101.63	110.95
2	E	401	PO4	O4-P-O2	-2.35	100.61	107.91
2	D	401	PO4	O4-P-O1	2.34	119.24	110.95
2	A	401	PO4	O2-P-O1	-2.28	102.89	110.95
2	D	401	PO4	O4-P-O3	-2.26	100.89	107.91
2	H	401	PO4	O4-P-O1	-2.22	103.08	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

### 6.1 Protein, DNA and RNA chains

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	372/386 (96%)	-0.07	6 (1%) 70 70	13, 30, 42, 61	4 (1%)
1	B	371/386 (96%)	0.37	22 (5%) 28 27	14, 35, 56, 73	2 (0%)
1	C	372/386 (96%)	0.46	13 (3%) 47 46	14, 39, 53, 65	1 (0%)
1	D	372/386 (96%)	0.10	6 (1%) 70 70	14, 31, 50, 57	1 (0%)
1	E	372/386 (96%)	0.16	9 (2%) 59 59	12, 32, 45, 53	1 (0%)
1	F	370/386 (95%)	0.35	23 (6%) 26 25	15, 34, 51, 60	2 (0%)
1	G	372/386 (96%)	0.39	12 (3%) 50 49	14, 35, 53, 59	3 (0%)
1	H	372/386 (96%)	0.32	14 (3%) 44 43	15, 34, 52, 61	2 (0%)
All	All	2973/3088 (96%)	0.26	105 (3%) 47 46	12, 34, 51, 73	16 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	151	VAL	4.7
1	F	139	ILE	4.7
1	F	156	ALA	4.5
1	D	156	ALA	4.2
1	B	152	ALA	4.1
1	B	19	VAL	4.1
1	F	149	ALA	3.9
1	F	137	SER	3.9
1	B	28	TYR	3.8
1	C	364	ALA	3.7
1	H	153	ARG	3.7
1	B	27	GLU	3.5
1	B	22	LEU	3.5
1	B	23	SER	3.5
1	B	145	GLU	3.4
1	H	361	ASN	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	149	ALA	3.4
1	C	41	ASP	3.4
1	F	138	SER	3.4
1	F	146	ALA	3.4
1	F	159	PHE	3.4
1	E	184	ALA	3.3
1	C	363	ASP	3.3
1	D	152	ALA	3.1
1	H	17	GLY	3.1
1	A	361	ASN	3.1
1	B	144	PRO	3.1
1	F	152	ALA	3.0
1	G	3	ILE	3.0
1	D	145	GLU	2.9
1	F	347	GLY	2.9
1	C	367	THR	2.9
1	H	116	ALA	2.9
1	H	1	LEU	2.8
1	E	158	GLY	2.8
1	B	20	TYR	2.8
1	C	1	LEU	2.8
1	F	19	VAL	2.8
1	G	1	LEU	2.8
1	B	151	VAL	2.8
1	A	363	ASP	2.7
1	C	93	ASP	2.7
1	B	17	GLY	2.7
1	G	343	LEU	2.7
1	H	12	ASP	2.7
1	A	364	ALA	2.6
1	E	19	VAL	2.6
1	H	363	ASP	2.6
1	F	343	LEU	2.6
1	B	24	GLY	2.6
1	F	28	TYR	2.5
1	A	145	GLU	2.5
1	G	39	GLU	2.5
1	G	341	ALA	2.5
1	H	366	GLY	2.5
1	C	153	ARG	2.5
1	B	187	ALA	2.5
1	C	342	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	156	ALA	2.5
1	E	139	ILE	2.5
1	B	149	ALA	2.4
1	D	149	ALA	2.4
1	B	21	ARG	2.4
1	F	187	ALA	2.4
1	B	141	GLY	2.4
1	G	345	ASP	2.4
1	G	333	THR	2.4
1	H	333	THR	2.4
1	G	116	ALA	2.4
1	F	145	GLU	2.3
1	E	18	GLY	2.3
1	H	306	SER	2.3
1	G	367	THR	2.3
1	C	17	GLY	2.3
1	A	362	ARG	2.3
1	F	160	LYS	2.3
1	B	146	ALA	2.3
1	B	29	HIS	2.3
1	D	144	PRO	2.3
1	C	152	ALA	2.3
1	B	140	GLY	2.3
1	F	84[A]	HIS	2.2
1	F	344	ARG	2.2
1	B	25	GLY	2.2
1	E	185	CYS	2.2
1	B	343	LEU	2.2
1	G	45	THR	2.2
1	F	140	GLY	2.2
1	C	372	PHE	2.1
1	E	183	THR	2.1
1	A	360	VAL	2.1
1	C	151	VAL	2.1
1	F	22	LEU	2.1
1	F	144	PRO	2.1
1	G	371	THR	2.1
1	H	339	ILE	2.1
1	F	230[A]	TRP	2.1
1	D	151	VAL	2.1
1	E	152	ALA	2.1
1	H	341	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	137	SER	2.1
1	B	188	ASP	2.1
1	F	153	ARG	2.0
1	G	320	HIS	2.0
1	C	25	GLY	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 oligosaccharides 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	PO4	F	401	5/5	0.90	0.11	34,36,36,42	0
2	PO4	B	401	5/5	0.91	0.10	38,42,45,48	0
2	PO4	D	401	5/5	0.93	0.08	31,34,39,43	0
2	PO4	E	401	5/5	0.93	0.09	41,43,44,46	0
2	PO4	C	401	5/5	0.93	0.09	40,41,46,47	0
2	PO4	G	401	5/5	0.93	0.09	44,44,45,48	0
2	PO4	A	401	5/5	0.94	0.10	35,36,40,44	0
2	PO4	H	401	5/5	0.95	0.08	38,39,39,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.