Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:57 PM GMT

PDB ID	:	3X43
Title	:	Crystal structure of O-ureido-L-serine synthase
Authors	:	Matoba, Y.; Uda, N.; Oda, K.; Sugiyama, M.
Deposited on	:	2015-03-13
Resolution	:	2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

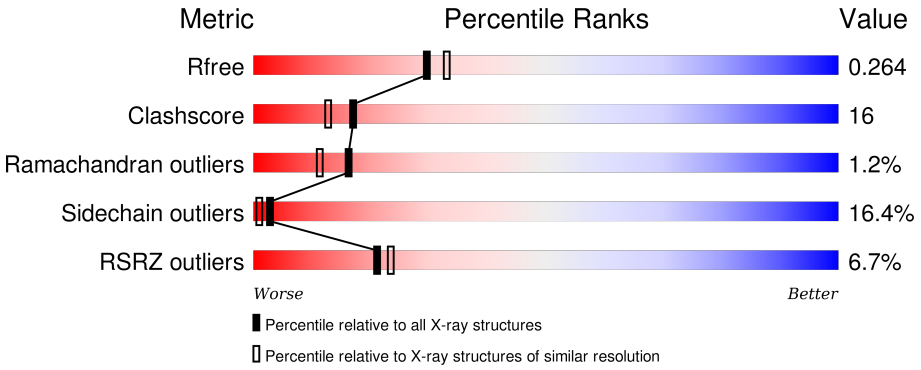
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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. 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	A	332	4% 62% 27% 6% 5%
1	B	332	6% 60% 27% 8% .
1	C	332	6% 62% 26% 7% 5%
1	D	332	6% 64% 25% 5% 5%
1	E	332	12% 58% 30% 8% 5%

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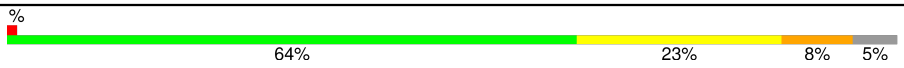
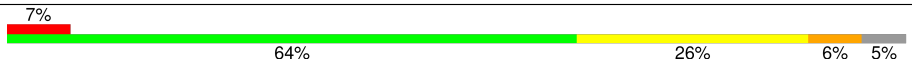
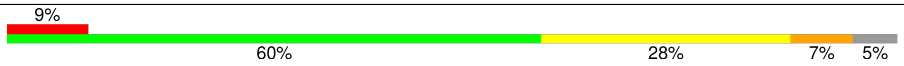
Mol	Chain	Length	Quality of chain
1	F	332	
1	G	332	
1	H	332	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20024 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 O-ureido-L-serine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2381	1502	419	452	8			
1	B	319	Total	C	N	O	S	0	0	0
			2404	1516	422	458	8			
1	C	317	Total	C	N	O	S	0	0	0
			2389	1508	420	453	8			
1	D	316	Total	C	N	O	S	0	0	0
			2381	1502	419	452	8			
1	E	317	Total	C	N	O	S	0	0	0
			2389	1508	420	453	8			
1	F	316	Total	C	N	O	S	0	0	0
			2381	1502	419	452	8			
1	G	317	Total	C	N	O	S	0	0	0
			2389	1508	420	453	8			
1	H	316	Total	C	N	O	S	0	0	0
			2381	1502	419	452	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	LEU	-	EXPRESSION TAG	UNP D2Z027
A	326	GLU	-	EXPRESSION TAG	UNP D2Z027
A	327	HIS	-	EXPRESSION TAG	UNP D2Z027
A	328	HIS	-	EXPRESSION TAG	UNP D2Z027
A	329	HIS	-	EXPRESSION TAG	UNP D2Z027
A	330	HIS	-	EXPRESSION TAG	UNP D2Z027
A	331	HIS	-	EXPRESSION TAG	UNP D2Z027
A	332	HIS	-	EXPRESSION TAG	UNP D2Z027
B	325	LEU	-	EXPRESSION TAG	UNP D2Z027
B	326	GLU	-	EXPRESSION TAG	UNP D2Z027
B	327	HIS	-	EXPRESSION TAG	UNP D2Z027
B	328	HIS	-	EXPRESSION TAG	UNP D2Z027
B	329	HIS	-	EXPRESSION TAG	UNP D2Z027

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Chain	Residue	Modelled	Actual	Comment	Reference
B	330	HIS	-	EXPRESSION TAG	UNP D2Z027
B	331	HIS	-	EXPRESSION TAG	UNP D2Z027
B	332	HIS	-	EXPRESSION TAG	UNP D2Z027
C	325	LEU	-	EXPRESSION TAG	UNP D2Z027
C	326	GLU	-	EXPRESSION TAG	UNP D2Z027
C	327	HIS	-	EXPRESSION TAG	UNP D2Z027
C	328	HIS	-	EXPRESSION TAG	UNP D2Z027
C	329	HIS	-	EXPRESSION TAG	UNP D2Z027
C	330	HIS	-	EXPRESSION TAG	UNP D2Z027
C	331	HIS	-	EXPRESSION TAG	UNP D2Z027
C	332	HIS	-	EXPRESSION TAG	UNP D2Z027
D	325	LEU	-	EXPRESSION TAG	UNP D2Z027
D	326	GLU	-	EXPRESSION TAG	UNP D2Z027
D	327	HIS	-	EXPRESSION TAG	UNP D2Z027
D	328	HIS	-	EXPRESSION TAG	UNP D2Z027
D	329	HIS	-	EXPRESSION TAG	UNP D2Z027
D	330	HIS	-	EXPRESSION TAG	UNP D2Z027
D	331	HIS	-	EXPRESSION TAG	UNP D2Z027
D	332	HIS	-	EXPRESSION TAG	UNP D2Z027
E	325	LEU	-	EXPRESSION TAG	UNP D2Z027
E	326	GLU	-	EXPRESSION TAG	UNP D2Z027
E	327	HIS	-	EXPRESSION TAG	UNP D2Z027
E	328	HIS	-	EXPRESSION TAG	UNP D2Z027
E	329	HIS	-	EXPRESSION TAG	UNP D2Z027
E	330	HIS	-	EXPRESSION TAG	UNP D2Z027
E	331	HIS	-	EXPRESSION TAG	UNP D2Z027
E	332	HIS	-	EXPRESSION TAG	UNP D2Z027
F	325	LEU	-	EXPRESSION TAG	UNP D2Z027
F	326	GLU	-	EXPRESSION TAG	UNP D2Z027
F	327	HIS	-	EXPRESSION TAG	UNP D2Z027
F	328	HIS	-	EXPRESSION TAG	UNP D2Z027
F	329	HIS	-	EXPRESSION TAG	UNP D2Z027
F	330	HIS	-	EXPRESSION TAG	UNP D2Z027
F	331	HIS	-	EXPRESSION TAG	UNP D2Z027
F	332	HIS	-	EXPRESSION TAG	UNP D2Z027
G	325	LEU	-	EXPRESSION TAG	UNP D2Z027
G	326	GLU	-	EXPRESSION TAG	UNP D2Z027
G	327	HIS	-	EXPRESSION TAG	UNP D2Z027
G	328	HIS	-	EXPRESSION TAG	UNP D2Z027
G	329	HIS	-	EXPRESSION TAG	UNP D2Z027
G	330	HIS	-	EXPRESSION TAG	UNP D2Z027
G	331	HIS	-	EXPRESSION TAG	UNP D2Z027

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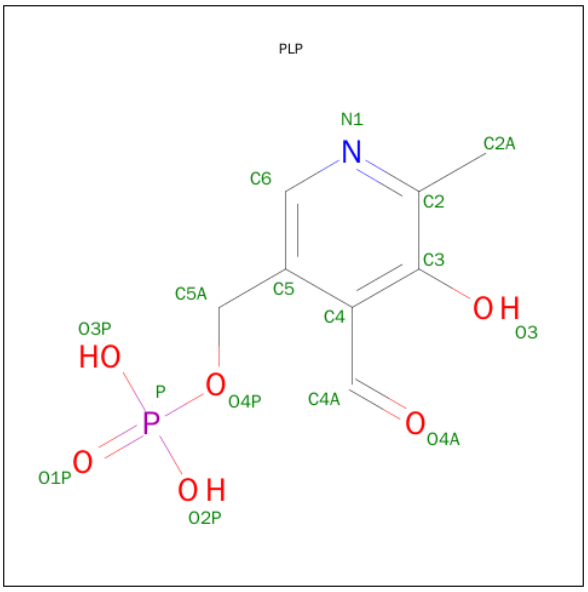
Chain	Residue	Modelled	Actual	Comment	Reference
G	332	HIS	-	EXPRESSION TAG	UNP D2Z027
H	325	LEU	-	EXPRESSION TAG	UNP D2Z027
H	326	GLU	-	EXPRESSION TAG	UNP D2Z027
H	327	HIS	-	EXPRESSION TAG	UNP D2Z027
H	328	HIS	-	EXPRESSION TAG	UNP D2Z027
H	329	HIS	-	EXPRESSION TAG	UNP D2Z027
H	330	HIS	-	EXPRESSION TAG	UNP D2Z027
H	331	HIS	-	EXPRESSION TAG	UNP D2Z027
H	332	HIS	-	EXPRESSION TAG	UNP D2Z027

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

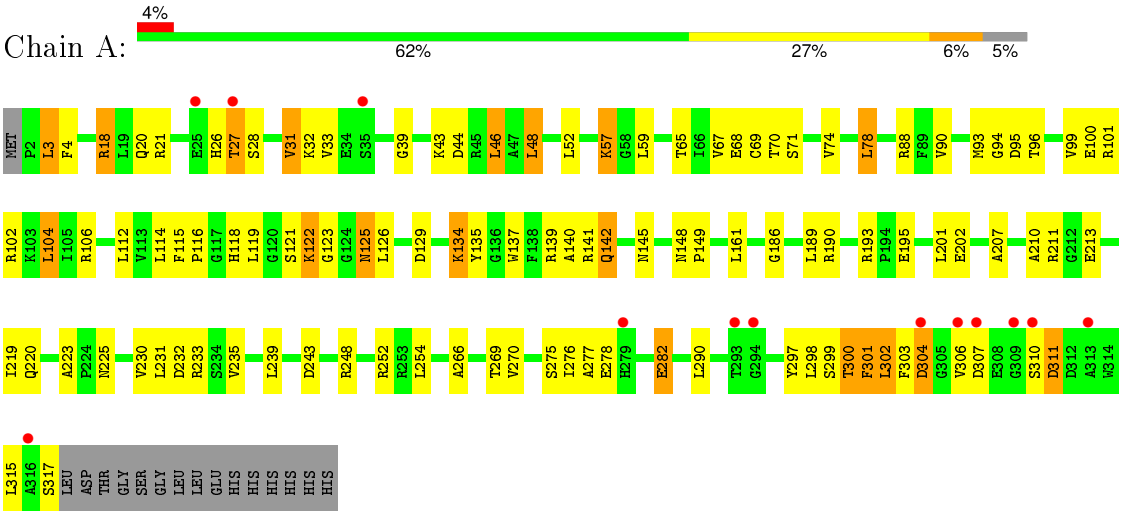
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	B	102	Total	O	0	0
			102	102		
3	C	96	Total	O	0	0
			96	96		
3	D	114	Total	O	0	0
			114	114		
3	E	106	Total	O	0	0
			106	106		
3	F	98	Total	O	0	0
			98	98		
3	G	97	Total	O	0	0
			97	97		
3	H	85	Total	O	0	0
			85	85		

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 errors 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.

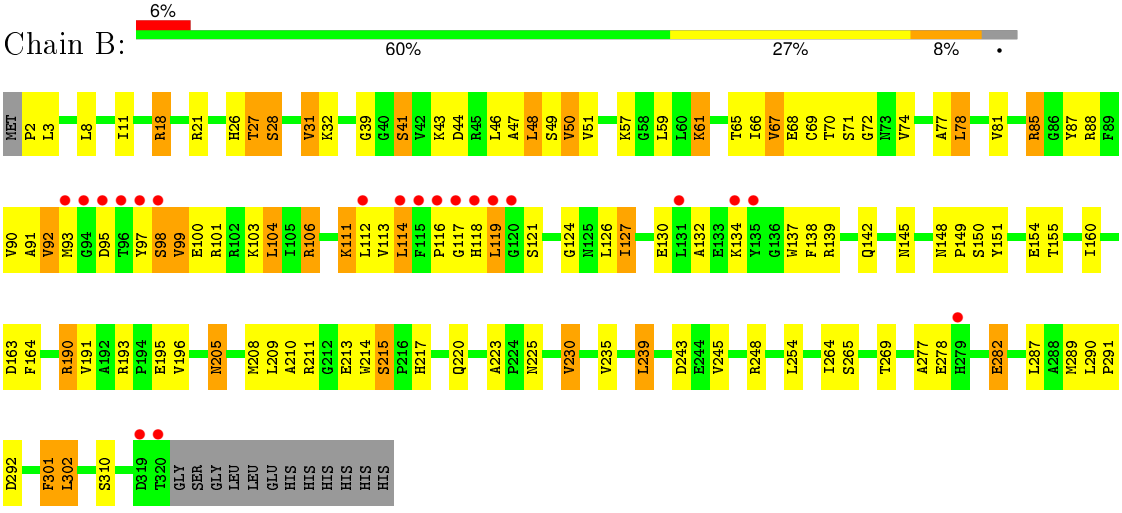
- Molecule 1: O-ureido-L-serine synthase

Chain A:



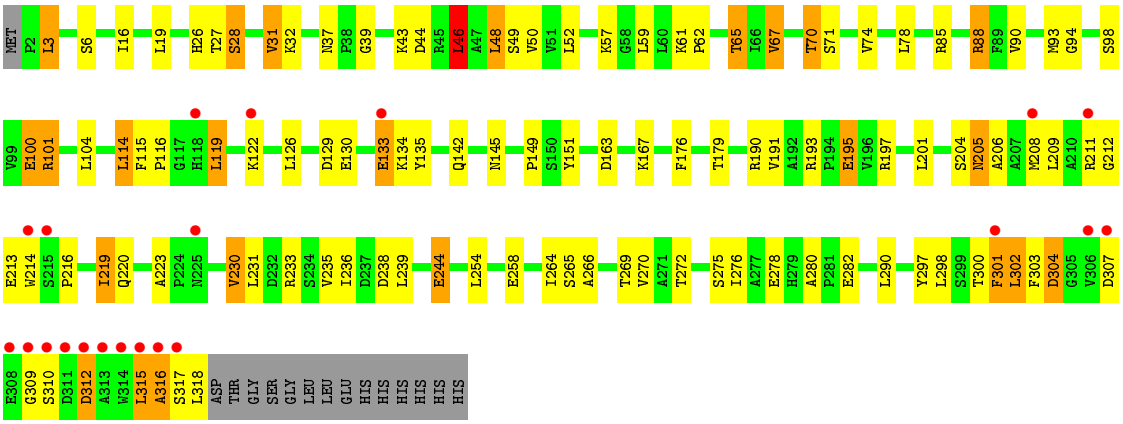
- Molecule 1: O-ureido-L-serine synthase

Chain B:



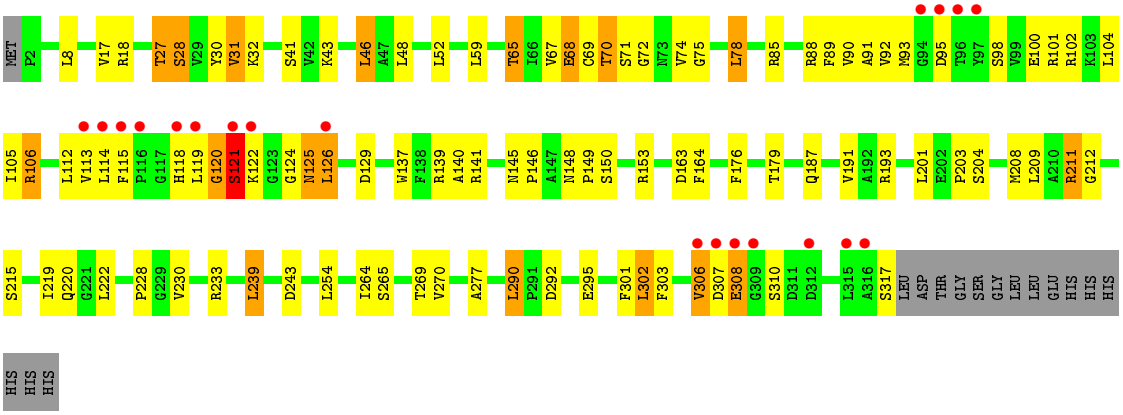
- Molecule 1: O-ureido-L-serine synthase

Chain C:



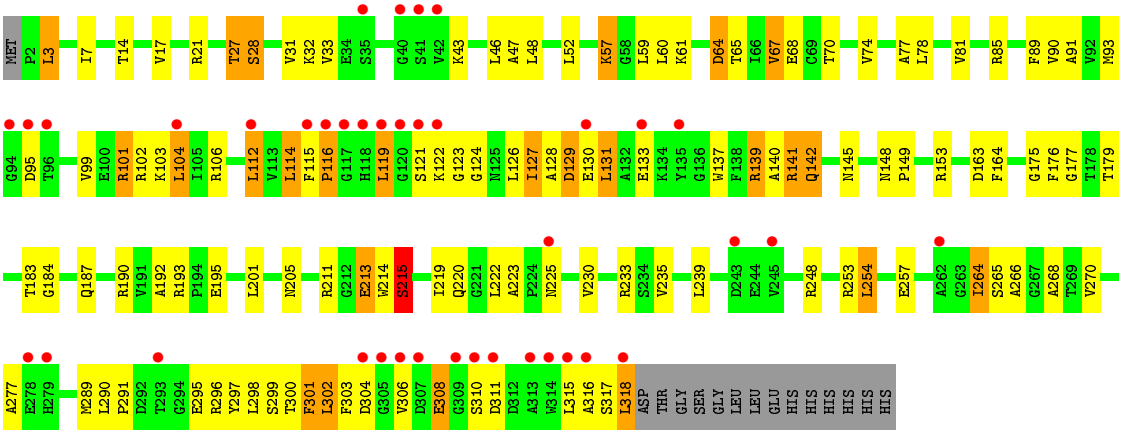
• Molecule 1: O-ureido-L-serine synthase

Chain D:



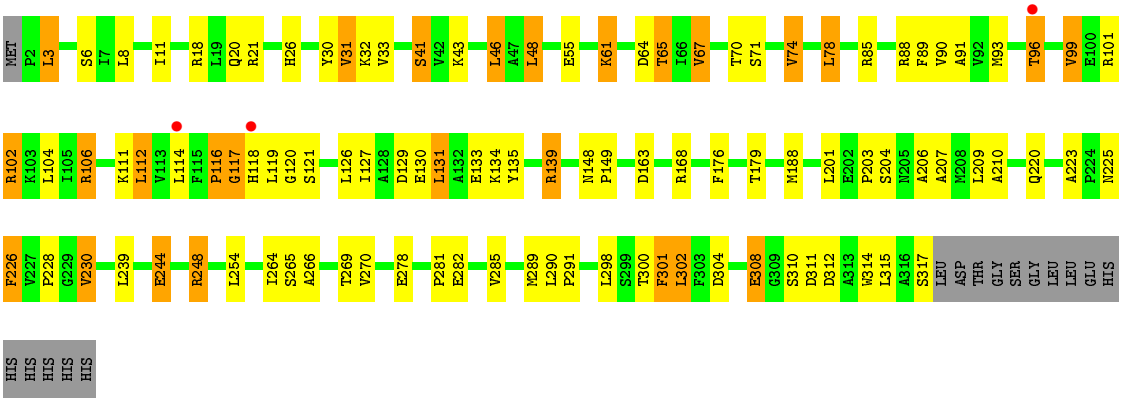
• Molecule 1: O-ureido-L-serine synthase

Chain E:



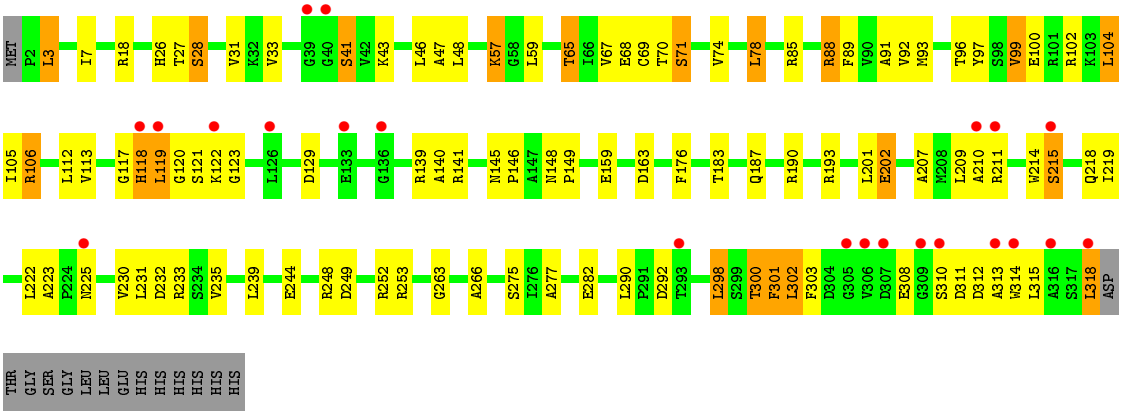
• Molecule 1: O-ureido-L-serine synthase

Chain F:



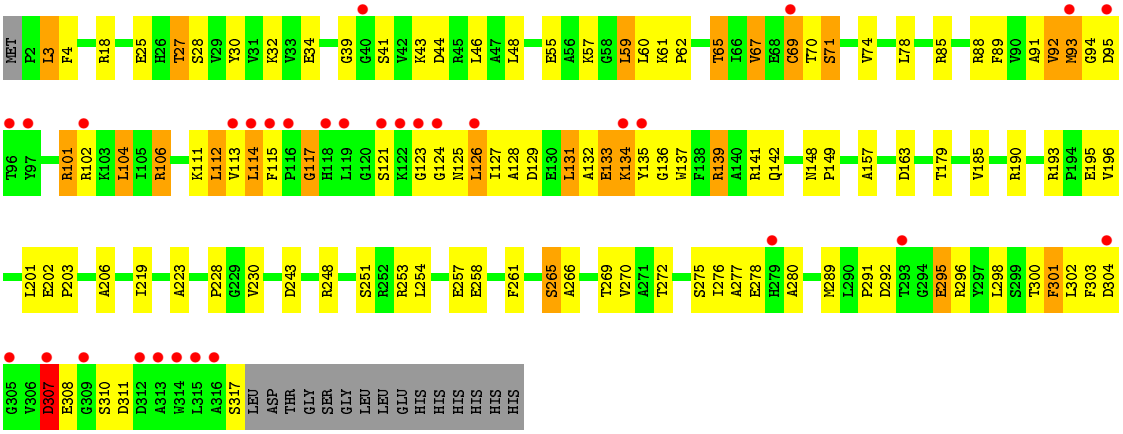
• Molecule 1: O-ureido-L-serine synthase

Chain G:



• Molecule 1: O-ureido-L-serine synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.48Å 154.13Å 118.52Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	29.83 – 2.25 36.64 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.83-2.25) 99.9 (36.64-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 2.24Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.264 0.209 , 0.264	Depositor DCC
R_{free} test set	6179 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.7	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 122927 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20024	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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 30.39 % 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 1.3181e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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	0.34	0/2427	0.60	0/3295
1	B	0.33	0/2450	0.59	0/3327
1	C	0.34	0/2435	0.61	1/3306 (0.0%)
1	D	0.37	0/2427	0.61	1/3295 (0.0%)
1	E	0.33	0/2435	0.58	2/3306 (0.1%)
1	F	0.37	0/2427	0.62	0/3295
1	G	0.33	0/2435	0.59	0/3306
1	H	0.33	0/2427	0.59	0/3295
All	All	0.34	0/19463	0.60	4/26425 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	46	LEU	CA-CB-CG	5.46	127.85	115.30
1	E	175	GLY	N-CA-C	-5.32	99.81	113.10
1	D	46	LEU	CA-CB-CG	5.26	127.41	115.30
1	E	177	GLY	N-CA-C	-5.01	100.56	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2381	0	2374	75	0
1	B	2404	0	2396	95	0
1	C	2389	0	2385	85	0
1	D	2381	0	2374	87	0
1	E	2389	0	2385	97	0
1	F	2381	0	2374	70	0
1	G	2389	0	2385	81	0
1	H	2381	0	2374	81	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
2	E	15	0	6	0	0
2	F	15	0	6	0	0
2	G	15	0	6	0	0
2	H	15	0	6	0	0
3	A	111	0	0	2	0
3	B	102	0	0	1	0
3	C	96	0	0	6	0
3	D	114	0	0	2	0
3	E	106	0	0	0	0
3	F	98	0	0	1	0
3	G	97	0	0	1	0
3	H	85	0	0	1	0
All	All	20024	0	19095	626	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 16.

All (626) 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:57:LYS:HB3	1:A:59:LEU:HD13	1.30	1.07
1:B:114:LEU:H	1:C:310:SER:HB2	1.21	1.06
1:D:68:GLU:HA	1:D:139:ARG:HH21	1.17	1.04
1:B:67:VAL:HG12	1:B:90:VAL:HB	1.44	0.95
1:F:26:HIS:HB2	1:F:282:GLU:HG2	1.48	0.94
1:A:300:THR:HG22	1:A:302:LEU:H	1.32	0.92
1:E:214:TRP:O	1:E:215:SER:HB3	1.69	0.91
1:D:67:VAL:HG12	1:D:90:VAL:HB	1.53	0.90
1:B:31:VAL:HG22	1:B:290:LEU:HD13	1.53	0.90
1:E:67:VAL:HG13	1:E:90:VAL:HB	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:HG12	1:A:90:VAL:HB	1.51	0.89
1:C:116:PRO:HB2	1:C:119:LEU:HD23	1.56	0.88
1:H:69:CYS:HB2	1:H:125:ASN:HD21	1.39	0.86
1:B:57:LYS:HB3	1:B:59:LEU:HD13	1.58	0.86
1:E:116:PRO:HB2	1:E:119:LEU:HD23	1.58	0.85
1:C:129:ASP:O	1:C:133:GLU:HG2	1.76	0.85
1:A:27:THR:HG21	1:A:277:ALA:HB1	1.58	0.85
1:H:300:THR:HG22	1:H:301:PHE:H	1.41	0.84
1:B:210:ALA:HB2	1:B:239:LEU:HD13	1.60	0.83
1:G:248:ARG:HG2	1:G:302:LEU:HD23	1.57	0.83
1:D:70:THR:HG21	1:D:75:GLY:H	1.42	0.82
1:G:300:THR:HG22	1:G:302:LEU:H	1.46	0.81
1:H:65:THR:HB	1:H:88:ARG:HB3	1.62	0.80
1:C:31:VAL:HG13	1:C:290:LEU:HD22	1.64	0.78
1:B:124:GLY:HA2	1:B:127:ILE:HG22	1.66	0.77
1:D:95:ASP:HA	1:D:114:LEU:HD22	1.64	0.77
1:F:3:LEU:HD13	1:G:163:ASP:HB3	1.67	0.76
1:A:70:THR:O	1:A:93:MET:HG3	1.87	0.74
1:G:57:LYS:HB3	1:G:59:LEU:HD13	1.68	0.74
1:H:70:THR:OG1	1:H:93:MET:HB3	1.86	0.74
1:E:300:THR:HG22	1:E:301:PHE:H	1.52	0.74
1:A:3:LEU:HD13	1:D:163:ASP:HB3	1.67	0.74
1:A:67:VAL:HG11	1:A:137:TRP:CE3	2.22	0.74
1:H:43:LYS:HE2	1:H:74:VAL:HG23	1.70	0.74
1:B:3:LEU:HD13	1:C:163:ASP:HB3	1.68	0.73
1:G:119:LEU:HD23	1:G:123:GLY:HA3	1.70	0.73
1:C:190:ARG:HD2	3:C:506:HOH:O	1.87	0.73
1:C:65:THR:HB	1:C:88:ARG:HB3	1.68	0.73
1:B:116:PRO:HG2	1:B:119:LEU:HD12	1.70	0.73
1:G:31:VAL:HG13	1:G:290:LEU:HD22	1.70	0.73
1:B:114:LEU:N	1:C:310:SER:HB2	2.01	0.73
1:E:31:VAL:HG13	1:E:290:LEU:HD22	1.71	0.72
1:E:163:ASP:HB3	1:H:3:LEU:HD13	1.71	0.72
1:C:74:VAL:HG21	1:C:142:GLN:OE1	1.89	0.72
1:F:207:ALA:HB1	1:F:210:ALA:HB3	1.72	0.72
1:D:68:GLU:HA	1:D:139:ARG:NH2	2.00	0.72
1:G:300:THR:CG2	1:G:302:LEU:H	2.02	0.72
1:E:31:VAL:CG1	1:E:290:LEU:HD22	2.20	0.72
1:H:70:THR:HG21	1:H:91:ALA:HB1	1.72	0.71
1:F:31:VAL:HG13	1:F:290:LEU:HD22	1.72	0.71
1:D:69:CYS:HB3	1:D:125:ASN:HD22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:VAL:HG22	1:D:290:LEU:HD13	1.73	0.71
1:F:65:THR:HB	1:F:88:ARG:HD2	1.71	0.70
1:C:254:LEU:HD11	1:C:270:VAL:HG21	1.73	0.70
1:C:116:PRO:O	1:C:119:LEU:HB2	1.91	0.70
1:A:67:VAL:HG11	1:A:137:TRP:HE3	1.57	0.70
1:F:135:TYR:OH	1:G:318:LEU:HG	1.92	0.70
1:G:231:LEU:HD12	1:G:232:ASP:N	2.07	0.70
1:E:68:GLU:OE2	1:E:140:ALA:HB3	1.92	0.70
1:A:68:GLU:OE2	1:A:140:ALA:HB3	1.90	0.70
1:B:99:VAL:O	1:B:103:LYS:HG3	1.91	0.70
1:A:26:HIS:HB2	1:A:282:GLU:HG2	1.71	0.70
1:G:231:LEU:HD12	1:G:232:ASP:H	1.56	0.69
1:A:31:VAL:HG22	1:A:290:LEU:HD13	1.74	0.69
1:H:300:THR:HG22	1:H:301:PHE:N	2.07	0.69
1:F:70:THR:O	1:F:93:MET:HG2	1.92	0.69
1:A:31:VAL:HG13	1:A:290:LEU:HD22	1.76	0.68
1:C:31:VAL:CG1	1:C:290:LEU:HD22	2.24	0.68
1:E:298:LEU:HA	1:E:303:PHE:CD1	2.28	0.67
1:A:149:PRO:HG3	1:A:230:VAL:HG13	1.75	0.67
1:B:67:VAL:CG1	1:B:90:VAL:HB	2.24	0.67
1:F:129:ASP:O	1:F:133:GLU:HG2	1.93	0.67
1:D:70:THR:HG21	1:D:75:GLY:N	2.09	0.67
1:C:43:LYS:HE2	1:C:74:VAL:CG2	2.25	0.67
1:D:93:MET:HE1	1:D:102:ARG:HA	1.76	0.66
1:E:77:ALA:O	1:E:81:VAL:HG23	1.95	0.66
1:B:26:HIS:HB2	1:B:282:GLU:HG2	1.77	0.66
1:C:31:VAL:HG22	1:C:290:LEU:HD13	1.77	0.66
1:B:106:ARG:NH2	1:B:112:LEU:H	1.94	0.66
1:C:43:LYS:HE2	1:C:74:VAL:HG23	1.78	0.66
1:G:300:THR:HG23	1:G:301:PHE:N	2.09	0.66
1:A:122:LYS:HB2	1:A:225:ASN:HD21	1.58	0.66
1:D:254:LEU:HD11	1:D:270:VAL:HG21	1.75	0.66
1:H:92:VAL:HG21	1:H:128:ALA:HB2	1.75	0.66
1:E:310:SER:HB2	1:H:114:LEU:HG	1.77	0.66
1:G:311:ASP:O	1:G:313:ALA:N	2.28	0.65
1:B:43:LYS:HE2	1:B:74:VAL:CG2	2.25	0.65
1:D:65:THR:HB	1:D:88:ARG:HB3	1.78	0.65
1:G:31:VAL:CG1	1:G:290:LEU:HD22	2.26	0.65
1:E:43:LYS:HE2	1:E:74:VAL:HG22	1.78	0.65
1:H:123:GLY:O	1:H:126:LEU:HB2	1.96	0.65
1:D:113:VAL:O	1:D:113:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:GLN:HG3	1:G:244:GLU:OE1	1.98	0.64
1:B:114:LEU:HG	1:C:310:SER:CB	2.27	0.64
1:H:70:THR:CG2	1:H:91:ALA:HB1	2.27	0.64
1:H:149:PRO:HG3	1:H:230:VAL:HG13	1.79	0.64
1:A:311:ASP:CG	1:D:106:ARG:HH22	2.01	0.64
1:B:31:VAL:HG22	1:B:290:LEU:CD1	2.24	0.64
1:D:67:VAL:HG11	1:D:137:TRP:CE3	2.32	0.64
1:H:106:ARG:NH1	1:H:112:LEU:HD11	2.13	0.64
1:B:43:LYS:HE2	1:B:74:VAL:HG22	1.80	0.64
1:F:301:PHE:HA	1:F:304:ASP:HB2	1.78	0.64
1:A:201:LEU:HD21	1:A:269:THR:HG22	1.80	0.64
1:A:57:LYS:HB3	1:A:59:LEU:CD1	2.19	0.64
1:C:67:VAL:HG13	1:C:90:VAL:HB	1.79	0.63
1:A:231:LEU:HD12	1:A:232:ASP:H	1.63	0.63
1:F:134:LYS:HE3	1:G:318:LEU:HD21	1.78	0.63
1:B:248:ARG:HG2	1:B:302:LEU:HD23	1.80	0.63
1:E:43:LYS:HE2	1:E:74:VAL:CG2	2.28	0.63
1:D:69:CYS:HB3	1:D:125:ASN:ND2	2.12	0.63
1:H:69:CYS:HB2	1:H:125:ASN:ND2	2.11	0.63
1:E:163:ASP:HB3	1:H:3:LEU:CD1	2.29	0.63
1:A:207:ALA:HB1	1:A:210:ALA:HB3	1.81	0.62
1:B:264:ILE:HD11	1:B:302:LEU:HB2	1.81	0.62
1:B:98:SER:HB2	1:B:100:GLU:HG2	1.82	0.62
1:A:65:THR:OG1	1:A:88:ARG:HD2	1.99	0.62
1:E:306:VAL:HG13	1:H:106:ARG:HG2	1.80	0.62
1:G:183:THR:O	1:G:187:GLN:HG3	2.00	0.62
1:F:265:SER:O	1:F:269:THR:HG23	1.99	0.62
1:H:27:THR:HG21	1:H:277:ALA:HB1	1.82	0.62
1:H:67:VAL:HG22	1:H:137:TRP:HB3	1.82	0.62
1:A:67:VAL:HG23	1:A:139:ARG:HD2	1.81	0.61
1:D:264:ILE:HD11	1:D:302:LEU:HB2	1.82	0.61
1:H:148:ASN:HB3	1:H:149:PRO:CD	2.29	0.61
1:D:233:ARG:HG3	3:D:517:HOH:O	2.00	0.61
1:B:39:GLY:N	1:B:44:ASP:OD1	2.32	0.61
1:G:43:LYS:HE2	1:G:74:VAL:HG22	1.80	0.61
1:C:276:ILE:O	1:C:280:ALA:HB2	1.99	0.61
1:G:219:ILE:HG21	1:G:222:LEU:HD12	1.81	0.61
1:H:298:LEU:HD12	1:H:303:PHE:HE2	1.66	0.61
1:H:65:THR:HG21	1:H:88:ARG:HH11	1.66	0.61
1:D:31:VAL:CG2	1:D:290:LEU:HD13	2.30	0.61
1:B:114:LEU:HG	1:C:310:SER:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ALA:HB1	1:C:290:LEU:HG	1.82	0.61
1:D:302:LEU:HD22	1:D:302:LEU:O	1.99	0.61
1:C:298:LEU:HA	1:C:303:PHE:CD1	2.35	0.61
1:B:70:THR:CG2	1:B:91:ALA:HB1	2.31	0.61
1:E:266:ALA:O	1:E:270:VAL:HG23	2.01	0.60
1:F:61:LYS:HD2	1:F:64:ASP:OD1	2.00	0.60
1:F:31:VAL:HG22	1:F:290:LEU:HD13	1.82	0.60
1:C:300:THR:HG22	1:C:301:PHE:N	2.17	0.60
1:G:141:ARG:HH11	1:G:141:ARG:HG3	1.67	0.60
1:H:57:LYS:O	1:H:59:LEU:HD13	2.02	0.59
1:E:93:MET:O	1:E:114:LEU:HD12	2.01	0.59
1:F:41:SER:HB3	3:F:539:HOH:O	2.02	0.59
1:G:190:ARG:HD2	3:G:517:HOH:O	2.02	0.59
1:H:298:LEU:HD12	1:H:303:PHE:CE2	2.37	0.59
1:H:289:MET:O	1:H:291:PRO:HD3	2.01	0.59
1:G:214:TRP:CD1	1:G:225:ASN:HA	2.36	0.59
1:E:219:ILE:HG21	1:E:222:LEU:HD12	1.82	0.59
1:D:148:ASN:HB3	1:D:149:PRO:CD	2.32	0.59
1:G:99:VAL:HA	1:G:102:ARG:HD3	1.83	0.59
1:C:134:LYS:HE2	1:C:135:TYR:CZ	2.38	0.58
1:F:99:VAL:HA	1:F:102:ARG:CG	2.33	0.58
1:G:46:LEU:HD12	1:G:47:ALA:N	2.19	0.58
1:F:18:ARG:NH1	1:F:20:GLN:HE22	2.01	0.58
1:E:148:ASN:HB3	1:E:149:PRO:CD	2.34	0.58
1:E:164:PHE:O	1:E:193:ARG:NH2	2.36	0.58
1:A:116:PRO:HB2	1:A:119:LEU:HD13	1.84	0.58
1:E:119:LEU:O	1:E:123:GLY:HA3	2.04	0.58
1:B:69:CYS:HA	1:B:92:VAL:HG23	1.84	0.58
1:F:43:LYS:HE2	1:F:74:VAL:HG23	1.86	0.58
1:F:74:VAL:HG13	1:F:78:LEU:HD22	1.85	0.58
1:C:278:GLU:HG2	3:C:595:HOH:O	2.03	0.58
1:A:31:VAL:HG22	1:A:290:LEU:CD1	2.34	0.57
1:B:114:LEU:HD21	1:C:309:GLY:HA2	1.86	0.57
1:B:66:ILE:HG23	1:B:138:PHE:HD2	1.68	0.57
1:H:148:ASN:HB3	1:H:149:PRO:HD3	1.86	0.57
1:F:18:ARG:HH12	1:F:20:GLN:HE22	1.52	0.57
1:D:67:VAL:HG11	1:D:137:TRP:HE3	1.69	0.57
1:A:116:PRO:HB2	1:A:119:LEU:CD1	2.33	0.57
1:B:50:VAL:HG22	1:B:145:ASN:ND2	2.20	0.57
1:D:27:THR:CG2	1:D:28:SER:N	2.68	0.57
1:H:128:ALA:HA	1:H:131:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ALA:HA	1:B:137:TRP:HB2	1.86	0.57
1:B:46:LEU:HD12	1:B:47:ALA:N	2.19	0.57
1:C:57:LYS:HB3	1:C:59:LEU:HD13	1.86	0.57
1:H:102:ARG:HG3	1:H:102:ARG:HH21	1.68	0.57
1:D:126:LEU:HD22	1:D:129:ASP:OD2	2.05	0.56
1:H:43:LYS:HE2	1:H:74:VAL:CG2	2.35	0.56
1:H:113:VAL:O	1:H:113:VAL:HG23	2.05	0.56
1:B:148:ASN:HB3	1:B:149:PRO:CD	2.35	0.56
1:B:67:VAL:HA	1:B:90:VAL:O	2.06	0.56
1:D:70:THR:HG22	1:D:72:GLY:H	1.70	0.56
1:H:266:ALA:O	1:H:270:VAL:HG23	2.05	0.56
1:E:57:LYS:HB3	1:E:59:LEU:HD13	1.87	0.56
1:E:302:LEU:HD22	1:E:302:LEU:O	2.06	0.56
1:D:65:THR:HB	1:D:88:ARG:HD2	1.88	0.56
1:B:31:VAL:HG13	1:B:290:LEU:HD22	1.88	0.56
1:G:41:SER:HB2	1:G:292:ASP:HB3	1.86	0.56
1:H:101:ARG:HA	1:H:104:LEU:HD23	1.87	0.56
1:C:231:LEU:HD21	1:C:233:ARG:HG2	1.87	0.56
1:B:70:THR:HG22	1:B:91:ALA:HB1	1.88	0.55
1:D:8:LEU:HD12	1:D:85:ARG:HD3	1.87	0.55
1:E:303:PHE:HD2	1:E:306:VAL:HG21	1.71	0.55
1:G:65:THR:HB	1:G:88:ARG:HB3	1.88	0.55
1:A:211:ARG:HB2	1:A:213:GLU:HG2	1.87	0.55
1:C:48:LEU:HD22	1:C:52:LEU:HG	1.88	0.55
1:C:61:LYS:HB3	1:C:62:PRO:HD2	1.89	0.55
1:D:101:ARG:O	1:D:105:ILE:HD12	2.06	0.55
1:A:122:LYS:HB2	1:A:225:ASN:ND2	2.21	0.55
1:D:126:LEU:HA	1:D:129:ASP:HB2	1.88	0.55
1:H:93:MET:O	1:H:114:LEU:HA	2.07	0.55
1:G:129:ASP:CG	1:G:139:ARG:HH11	2.10	0.55
1:E:31:VAL:HG22	1:E:290:LEU:HD13	1.89	0.55
1:G:27:THR:CG2	1:G:28:SER:N	2.70	0.55
1:C:26:HIS:HB2	1:C:282:GLU:OE2	2.06	0.55
1:E:124:GLY:HA2	1:E:127:ILE:HG13	1.89	0.54
1:G:148:ASN:HB3	1:G:149:PRO:CD	2.36	0.54
1:B:93:MET:SD	1:B:112:LEU:HD11	2.47	0.54
1:C:46:LEU:O	1:C:50:VAL:HG23	2.07	0.54
1:F:31:VAL:HG22	1:F:290:LEU:CD1	2.37	0.54
1:G:300:THR:CG2	1:G:301:PHE:N	2.71	0.54
1:B:248:ARG:HB2	1:B:301:PHE:CZ	2.43	0.54
1:E:265:SER:O	1:E:268:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HD11	1:D:295:GLU:HG3	1.89	0.54
1:E:141:ARG:O	1:E:145:ASN:HB2	2.08	0.54
1:A:148:ASN:HB3	1:A:149:PRO:CD	2.38	0.54
1:A:65:THR:HB	1:A:137:TRP:CD1	2.42	0.54
1:E:211:ARG:O	1:E:213:GLU:HG2	2.08	0.54
1:D:306:VAL:O	1:D:307:ASP:HB2	2.07	0.54
1:H:253:ARG:O	1:H:257:GLU:HB2	2.08	0.54
1:A:297:TYR:O	1:A:300:THR:HB	2.07	0.54
1:D:102:ARG:HB3	1:D:112:LEU:HD21	1.90	0.54
1:A:302:LEU:HD13	1:A:303:PHE:CE1	2.43	0.53
1:G:263:GLY:O	1:G:266:ALA:HB3	2.08	0.53
1:G:43:LYS:HE2	1:G:74:VAL:CG2	2.38	0.53
1:E:27:THR:HG23	1:E:28:SER:N	2.23	0.53
1:E:32:LYS:O	1:E:290:LEU:HB2	2.08	0.53
1:C:37:ASN:HB3	1:C:44:ASP:OD1	2.09	0.53
1:B:68:GLU:HG3	1:B:69:CYS:N	2.23	0.53
1:A:310:SER:HB2	1:D:114:LEU:H	1.72	0.53
1:G:31:VAL:HG22	1:G:290:LEU:CD1	2.38	0.53
1:C:297:TYR:CB	1:C:302:LEU:HD12	2.38	0.53
1:E:148:ASN:HB3	1:E:149:PRO:HD3	1.91	0.53
1:F:116:PRO:HB2	1:F:118:HIS:CD2	2.44	0.53
1:A:43:LYS:HE2	1:A:74:VAL:CG2	2.39	0.53
1:B:114:LEU:H	1:C:310:SER:CB	2.09	0.53
1:B:46:LEU:HD12	1:B:46:LEU:C	2.29	0.53
1:F:46:LEU:C	1:F:46:LEU:HD12	2.28	0.53
1:F:31:VAL:CG1	1:F:290:LEU:HD22	2.38	0.53
1:B:39:GLY:HA3	1:B:44:ASP:OD2	2.09	0.53
1:G:96:THR:OG1	1:G:117:GLY:HA3	2.09	0.53
1:F:67:VAL:HG23	1:F:139:ARG:HG2	1.90	0.53
1:H:70:THR:OG1	1:H:71:SER:N	2.42	0.53
1:H:134:LYS:HE2	1:H:135:TYR:CZ	2.43	0.53
1:F:93:MET:O	1:F:114:LEU:HA	2.09	0.53
1:C:264:ILE:HD12	1:C:297:TYR:CD1	2.44	0.53
1:C:208:MET:O	1:C:212:GLY:HA2	2.08	0.53
1:E:70:THR:O	1:E:93:MET:HG2	2.09	0.53
1:C:315:LEU:O	1:C:316:ALA:HB2	2.09	0.53
1:F:264:ILE:HD13	1:F:301:PHE:HE2	1.74	0.52
1:H:276:ILE:O	1:H:280:ALA:HB2	2.09	0.52
1:H:89:PHE:CE2	1:H:91:ALA:HB2	2.44	0.52
1:E:59:LEU:HD12	1:E:59:LEU:N	2.24	0.52
1:D:126:LEU:HA	1:D:129:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD22	1:C:258:GLU:HG3	1.90	0.52
1:F:163:ASP:HB3	1:G:3:LEU:HD13	1.90	0.52
1:D:92:VAL:HG22	1:D:113:VAL:CG2	2.40	0.52
1:B:193:ARG:HB3	1:B:196:VAL:HG23	1.92	0.52
1:A:119:LEU:HB3	1:A:123:GLY:HA3	1.92	0.52
1:E:99:VAL:HG22	1:E:103:LYS:HD2	1.92	0.52
1:E:129:ASP:O	1:E:133:GLU:HG3	2.10	0.52
1:C:201:LEU:HD12	1:C:201:LEU:O	2.09	0.52
1:E:192:ALA:HB2	1:F:188:MET:HE2	1.92	0.52
1:H:94:GLY:HA2	1:H:115:PHE:O	2.09	0.52
1:C:297:TYR:HB2	1:C:302:LEU:HD12	1.93	0.51
1:G:31:VAL:HG22	1:G:290:LEU:HD13	1.92	0.51
1:A:297:TYR:HB2	1:A:302:LEU:HD12	1.91	0.51
1:F:96:THR:OG1	1:F:117:GLY:HA3	2.10	0.51
1:B:70:THR:O	1:B:70:THR:HG23	2.10	0.51
1:F:289:MET:O	1:F:291:PRO:HD3	2.10	0.51
1:H:254:LEU:O	1:H:258:GLU:HB2	2.11	0.51
1:D:153:ARG:HD3	1:D:187:GLN:OE1	2.11	0.51
1:F:127:ILE:HG22	1:F:131:LEU:HD11	1.91	0.51
1:B:163:ASP:HB3	1:C:3:LEU:HD13	1.91	0.51
1:D:106:ARG:NH1	1:D:112:LEU:HB2	2.25	0.51
1:F:114:LEU:HD12	1:G:310:SER:H	1.76	0.51
1:F:203:PRO:HB2	1:F:206:ALA:HB3	1.93	0.50
1:C:98:SER:OG	1:C:100:GLU:HG3	2.11	0.50
1:A:298:LEU:HA	1:A:303:PHE:CD1	2.46	0.50
1:D:102:ARG:HD2	1:D:112:LEU:HD21	1.94	0.50
1:F:176:PHE:CZ	1:F:209:LEU:HG	2.45	0.50
1:B:74:VAL:HG12	1:B:78:LEU:HD22	1.93	0.50
1:E:295:GLU:HG2	1:H:295:GLU:HG2	1.93	0.50
1:F:179:THR:HG23	1:F:228:PRO:HG2	1.93	0.50
1:H:179:THR:HG23	1:H:228:PRO:HG2	1.93	0.50
1:E:116:PRO:O	1:E:119:LEU:HB2	2.10	0.50
1:C:16:ILE:HG12	1:C:32:LYS:HG3	1.93	0.50
1:A:266:ALA:O	1:A:270:VAL:HG23	2.12	0.50
1:H:265:SER:O	1:H:269:THR:HG23	2.12	0.50
1:B:113:VAL:O	1:B:113:VAL:HG23	2.11	0.50
1:A:300:THR:CG2	1:A:301:PHE:N	2.74	0.50
1:A:306:VAL:HG12	1:D:106:ARG:HG2	1.93	0.50
1:D:95:ASP:HB3	1:D:114:LEU:HB3	1.92	0.50
1:G:266:ALA:HB1	1:G:290:LEU:HG	1.94	0.50
1:E:27:THR:HG21	1:E:277:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HG23	3:A:529:HOH:O	2.10	0.50
1:C:191:VAL:HG21	1:D:191:VAL:HG21	1.94	0.50
1:B:211:ARG:HB3	1:B:213:GLU:HG2	1.94	0.50
1:H:65:THR:HG21	1:H:88:ARG:NH1	2.27	0.50
1:G:201:LEU:HD12	1:G:201:LEU:C	2.32	0.50
1:H:61:LYS:HB3	1:H:62:PRO:HD2	1.93	0.50
1:G:159:GLU:HG2	3:H:508:HOH:O	2.11	0.50
1:F:18:ARG:NH1	1:F:20:GLN:NE2	2.59	0.50
1:E:128:ALA:HB3	1:E:139:ARG:NH2	2.26	0.50
1:A:254:LEU:HD11	1:A:270:VAL:HG21	1.94	0.50
1:D:201:LEU:HD21	1:D:269:THR:HA	1.92	0.50
1:F:65:THR:HB	1:F:88:ARG:HB3	1.94	0.49
1:E:31:VAL:HG11	1:E:290:LEU:HD22	1.94	0.49
1:C:201:LEU:HD12	1:C:201:LEU:C	2.33	0.49
1:A:231:LEU:HD12	1:A:232:ASP:N	2.27	0.49
1:B:243:ASP:OD1	1:B:245:VAL:HB	2.12	0.49
1:H:300:THR:CG2	1:H:301:PHE:H	2.19	0.49
1:E:300:THR:HG22	1:E:301:PHE:N	2.24	0.49
1:F:114:LEU:HD12	1:G:310:SER:N	2.27	0.49
1:G:106:ARG:NH1	1:G:112:LEU:HD12	2.27	0.49
1:B:85:ARG:NH1	1:B:85:ARG:HG2	2.28	0.49
1:E:214:TRP:CG	1:E:215:SER:N	2.81	0.49
1:E:115:PHE:CE1	1:E:119:LEU:HB3	2.47	0.49
1:C:300:THR:C	1:C:302:LEU:H	2.16	0.49
1:D:93:MET:CE	1:D:112:LEU:HD11	2.43	0.49
1:B:77:ALA:O	1:B:81:VAL:HG23	2.13	0.49
1:A:39:GLY:N	1:A:44:ASP:OD1	2.35	0.49
1:A:102:ARG:HG2	1:A:112:LEU:HD21	1.93	0.49
1:E:115:PHE:HE1	1:E:119:LEU:HB3	1.77	0.49
1:B:85:ARG:CG	1:B:85:ARG:HH11	2.26	0.48
1:B:97:TYR:O	1:B:98:SER:C	2.51	0.48
1:E:127:ILE:O	1:E:131:LEU:HD12	2.12	0.48
1:G:68:GLU:OE2	1:G:140:ALA:HB3	2.12	0.48
1:B:164:PHE:O	1:B:193:ARG:NH2	2.46	0.48
1:D:176:PHE:CD1	1:D:179:THR:HG22	2.48	0.48
1:H:39:GLY:N	1:H:44:ASP:OD1	2.35	0.48
1:A:94:GLY:HA2	1:A:115:PHE:O	2.13	0.48
1:E:17:VAL:HG12	1:H:4:PHE:HB2	1.95	0.48
1:B:302:LEU:HD22	1:B:302:LEU:O	2.13	0.48
1:G:59:LEU:N	1:G:59:LEU:HD12	2.29	0.48
1:C:94:GLY:HA2	1:C:115:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:SER:O	1:C:318:LEU:HB2	2.13	0.48
1:C:31:VAL:HG22	1:C:290:LEU:CD1	2.41	0.48
1:C:272:THR:O	1:C:276:ILE:HG13	2.14	0.48
1:G:148:ASN:HB3	1:G:149:PRO:HD3	1.94	0.48
1:B:8:LEU:HD13	1:B:48:LEU:HD23	1.94	0.48
1:D:100:GLU:HG2	1:D:101:ARG:N	2.29	0.48
1:H:203:PRO:HB3	1:H:219:ILE:HD12	1.95	0.48
1:C:70:THR:O	1:C:93:MET:HB3	2.14	0.48
1:B:2:PRO:HG2	3:C:510:HOH:O	2.12	0.48
1:C:101:ARG:HD3	1:C:101:ARG:HA	1.49	0.48
1:E:201:LEU:C	1:E:201:LEU:HD12	2.35	0.48
1:E:68:GLU:CD	1:E:140:ALA:HB3	2.34	0.48
1:H:127:ILE:HG22	1:H:131:LEU:HD11	1.95	0.48
1:B:148:ASN:HB3	1:B:149:PRO:HD3	1.96	0.48
1:E:67:VAL:HA	1:E:90:VAL:O	2.14	0.47
1:H:128:ALA:HB3	1:H:139:ARG:NH2	2.29	0.47
1:F:248:ARG:HB3	1:F:301:PHE:CZ	2.49	0.47
1:D:27:THR:HG23	1:D:28:SER:N	2.30	0.47
1:C:57:LYS:CB	1:C:59:LEU:HD13	2.44	0.47
1:H:18:ARG:HB2	1:H:30:TYR:CE2	2.49	0.47
1:E:214:TRP:O	1:E:215:SER:CB	2.52	0.47
1:E:248:ARG:HG2	1:E:302:LEU:HD23	1.95	0.47
1:E:126:LEU:O	1:E:130:GLU:HG3	2.15	0.47
1:G:207:ALA:HB1	1:G:210:ALA:HB3	1.96	0.47
1:D:92:VAL:HG22	1:D:113:VAL:HG21	1.95	0.47
1:F:18:ARG:HB2	1:F:30:TYR:CE2	2.49	0.47
1:B:149:PRO:HG3	1:B:230:VAL:HG22	1.96	0.47
1:H:115:PHE:CD2	1:H:117:GLY:HA3	2.49	0.47
1:E:289:MET:O	1:E:291:PRO:HD3	2.14	0.47
1:C:193:ARG:NH1	3:C:547:HOH:O	2.46	0.47
1:B:27:THR:HG21	1:B:277:ALA:HB1	1.96	0.47
1:H:201:LEU:HD22	1:H:272:THR:OG1	2.14	0.47
1:E:124:GLY:HA2	1:E:127:ILE:CG1	2.44	0.47
1:D:208:MET:HE3	1:D:212:GLY:HA2	1.94	0.47
1:E:106:ARG:NH1	1:H:307:ASP:HB3	2.29	0.47
1:A:248:ARG:CZ	1:A:252:ARG:NH1	2.77	0.47
1:A:300:THR:HG22	1:A:302:LEU:N	2.14	0.47
1:D:211:ARG:HH11	1:D:211:ARG:HG2	1.80	0.47
1:B:31:VAL:CG2	1:B:290:LEU:CD1	2.92	0.47
1:A:93:MET:O	1:A:114:LEU:HA	2.15	0.47
1:H:254:LEU:HD11	1:H:270:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HB2	1:A:213:GLU:CG	2.45	0.47
1:C:197:ARG:NH2	1:C:238:ASP:OD1	2.48	0.47
1:F:308:GLU:CD	1:F:308:GLU:H	2.18	0.47
1:E:310:SER:OG	1:H:113:VAL:HA	2.15	0.47
1:B:106:ARG:NH1	1:B:112:LEU:HB3	2.29	0.47
1:C:201:LEU:HD21	1:C:269:THR:HA	1.96	0.47
1:H:115:PHE:CE2	1:H:124:GLY:HA3	2.49	0.47
1:D:93:MET:HE2	1:D:112:LEU:HD11	1.97	0.47
1:B:116:PRO:HG2	1:B:119:LEU:CD1	2.41	0.47
1:D:18:ARG:HB2	1:D:30:TYR:CE2	2.50	0.47
1:F:225:ASN:O	1:F:226:PHE:HB3	2.15	0.47
1:C:67:VAL:CG1	1:C:90:VAL:HB	2.45	0.47
1:F:149:PRO:HG3	1:F:230:VAL:HG22	1.96	0.47
1:D:43:LYS:HE2	1:D:74:VAL:CG2	2.45	0.47
1:E:99:VAL:HG13	1:E:103:LYS:HD2	1.97	0.46
1:B:18:ARG:NH2	3:B:588:HOH:O	2.47	0.46
1:C:317:SER:N	3:C:550:HOH:O	2.47	0.46
1:F:65:THR:HG21	1:F:88:ARG:HH11	1.79	0.46
1:G:176:PHE:HZ	1:G:202:GLU:OE1	1.99	0.46
1:C:149:PRO:HG3	1:C:230:VAL:HG22	1.96	0.46
1:B:265:SER:O	1:B:269:THR:HG23	2.15	0.46
1:D:219:ILE:HG21	1:D:222:LEU:HD12	1.97	0.46
1:A:300:THR:HG23	1:A:301:PHE:N	2.31	0.46
1:D:70:THR:O	1:D:93:MET:HB3	2.15	0.46
1:H:93:MET:HE2	1:H:112:LEU:HB3	1.97	0.46
1:A:18:ARG:NH1	1:A:20:GLN:OE1	2.49	0.46
1:B:68:GLU:HG3	1:B:69:CYS:H	1.81	0.46
1:F:315:LEU:HD11	1:G:113:VAL:HG22	1.97	0.46
1:E:192:ALA:HB2	1:F:188:MET:CE	2.46	0.46
1:F:8:LEU:HD12	1:F:85:ARG:HD3	1.98	0.46
1:E:27:THR:CG2	1:E:28:SER:N	2.78	0.46
1:H:115:PHE:O	1:H:115:PHE:CG	2.68	0.46
1:E:102:ARG:HD2	1:H:308:GLU:O	2.16	0.46
1:E:139:ARG:HD2	1:E:141:ARG:NH2	2.31	0.46
1:B:208:MET:SD	1:B:214:TRP:HB2	2.56	0.46
1:A:74:VAL:HG21	1:A:142:GLN:OE1	2.16	0.46
1:E:46:LEU:C	1:E:46:LEU:HD12	2.35	0.46
1:F:168:ARG:O	1:F:285:VAL:HG11	2.16	0.46
1:G:27:THR:HG21	1:G:277:ALA:HB1	1.97	0.45
1:F:163:ASP:O	1:G:3:LEU:HD22	2.15	0.45
1:H:203:PRO:HG2	1:H:206:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:C	1:A:46:LEU:HD12	2.37	0.45
1:G:7:ILE:HG13	1:G:7:ILE:O	2.15	0.45
1:H:129:ASP:O	1:H:132:ALA:HB3	2.17	0.45
1:B:67:VAL:HG11	1:B:137:TRP:CE3	2.51	0.45
1:D:101:ARG:HA	1:D:101:ARG:HD3	1.72	0.45
1:H:300:THR:CG2	1:H:301:PHE:N	2.77	0.45
1:E:254:LEU:HD11	1:E:270:VAL:HG21	1.99	0.45
1:F:298:LEU:HD21	1:G:104:LEU:HD13	1.97	0.45
1:F:3:LEU:CD1	1:G:163:ASP:HB3	2.42	0.45
1:D:65:THR:HG21	1:D:88:ARG:HH11	1.81	0.45
1:B:32:LYS:O	1:B:290:LEU:HB2	2.16	0.45
1:F:244:GLU:HG2	1:F:244:GLU:H	1.50	0.45
1:E:7:ILE:HG13	1:E:7:ILE:O	2.16	0.45
1:C:209:LEU:HD22	1:C:233:ARG:CZ	2.46	0.45
1:B:49:SER:HB2	1:B:151:TYR:CD1	2.51	0.45
1:C:205:ASN:OD1	1:C:205:ASN:N	2.38	0.45
1:H:248:ARG:HG3	1:H:301:PHE:CE1	2.52	0.45
1:B:92:VAL:HG11	1:B:127:ILE:HG23	1.97	0.45
1:C:219:ILE:CD1	1:C:244:GLU:HB3	2.46	0.45
1:C:219:ILE:HG23	1:C:264:ILE:HG22	1.98	0.45
1:A:43:LYS:HE2	1:A:74:VAL:HG23	1.99	0.45
1:D:203:PRO:HB3	1:D:219:ILE:HD12	1.98	0.45
1:B:90:VAL:HG13	1:B:111:LYS:O	2.16	0.45
1:A:129:ASP:OD1	1:A:139:ARG:NH1	2.50	0.45
1:G:70:THR:O	1:G:93:MET:HB3	2.16	0.45
1:G:69:CYS:HA	1:G:92:VAL:O	2.16	0.45
1:D:31:VAL:CG2	1:D:290:LEU:CD1	2.94	0.45
1:F:102:ARG:CB	1:F:112:LEU:HD21	2.47	0.45
1:G:46:LEU:C	1:G:46:LEU:HD12	2.36	0.45
1:F:281:PRO:O	1:F:282:GLU:C	2.55	0.45
1:E:301:PHE:HA	1:E:304:ASP:CG	2.37	0.45
1:A:148:ASN:HB3	1:A:149:PRO:HD3	1.99	0.44
1:D:303:PHE:O	1:D:306:VAL:HG22	2.18	0.44
1:D:145:ASN:HA	1:D:146:PRO:HD2	1.87	0.44
1:F:302:LEU:O	1:F:302:LEU:HD22	2.18	0.44
1:E:298:LEU:HD23	1:E:303:PHE:CE1	2.53	0.44
1:C:300:THR:CG2	1:C:301:PHE:N	2.80	0.44
1:G:71:SER:HB3	1:G:97:TYR:CZ	2.52	0.44
1:A:95:ASP:HA	1:A:102:ARG:HH11	1.82	0.44
1:E:65:THR:HB	1:E:137:TRP:CD1	2.52	0.44
1:B:217:HIS:H	1:B:217:HIS:CD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:PHE:HA	1:F:304:ASP:CB	2.46	0.44
1:G:219:ILE:CG2	1:G:222:LEU:HD12	2.46	0.44
1:F:55:GLU:OE1	1:F:85:ARG:NH2	2.45	0.44
1:D:41:SER:HB2	1:D:292:ASP:HB3	1.98	0.44
1:B:113:VAL:HA	1:C:310:SER:HB2	2.00	0.44
1:B:151:TYR:CE2	1:B:155:THR:HG21	2.53	0.44
1:E:3:LEU:HD22	1:H:163:ASP:O	2.18	0.44
1:B:205:ASN:N	1:B:205:ASN:OD1	2.33	0.44
1:G:89:PHE:CE2	1:G:91:ALA:HB2	2.52	0.44
1:E:153:ARG:HG2	1:E:184:GLY:O	2.17	0.44
1:C:65:THR:HA	1:C:88:ARG:O	2.18	0.44
1:G:298:LEU:HD22	1:G:303:PHE:CZ	2.52	0.44
1:H:261:PHE:HZ	1:H:303:PHE:HZ	1.66	0.44
1:F:102:ARG:H	1:F:102:ARG:HG2	1.58	0.44
1:C:46:LEU:C	1:C:46:LEU:HD12	2.38	0.44
1:D:120:GLY:O	1:D:121:SER:O	2.35	0.44
1:C:176:PHE:CD1	1:C:179:THR:HG22	2.53	0.44
1:B:230:VAL:HG13	1:B:230:VAL:O	2.18	0.43
1:E:264:ILE:HG12	1:E:297:TYR:CE1	2.54	0.43
1:B:92:VAL:HG11	1:B:127:ILE:CG2	2.49	0.43
1:E:114:LEU:HD12	1:E:114:LEU:HA	1.88	0.43
1:D:140:ALA:O	1:D:141:ARG:HB2	2.18	0.43
1:F:266:ALA:O	1:F:270:VAL:HG23	2.17	0.43
1:G:214:TRP:CD2	1:G:215:SER:N	2.86	0.43
1:D:78:LEU:HB3	1:D:89:PHE:CE1	2.53	0.43
1:D:164:PHE:O	1:D:193:ARG:NH2	2.51	0.43
1:F:201:LEU:HD21	1:F:269:THR:HA	2.01	0.43
1:G:141:ARG:HH11	1:G:141:ARG:CG	2.31	0.43
1:C:211:ARG:HH21	1:C:213:GLU:CD	2.21	0.43
1:E:104:LEU:HD13	1:E:104:LEU:HA	1.87	0.43
1:G:233:ARG:C	1:G:235:VAL:H	2.21	0.43
1:H:65:THR:HB	1:H:88:ARG:HD2	2.01	0.43
1:E:303:PHE:CD2	1:E:306:VAL:HG21	2.52	0.43
1:F:55:GLU:CD	1:F:85:ARG:HH21	2.20	0.43
1:H:32:LYS:HE3	1:H:34:GLU:OE1	2.19	0.43
1:C:27:THR:HG22	1:C:28:SER:N	2.34	0.43
1:F:89:PHE:CE2	1:F:91:ALA:HB2	2.54	0.43
1:F:32:LYS:O	1:F:290:LEU:HB2	2.19	0.43
1:D:91:ALA:O	1:D:113:VAL:HG22	2.19	0.43
1:E:48:LEU:HD11	1:E:52:LEU:HD11	2.01	0.43
1:A:193:ARG:HD2	3:A:523:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:CG1	1:A:137:TRP:CE3	2.97	0.43
1:G:118:HIS:C	1:G:120:GLY:H	2.22	0.43
1:D:32:LYS:O	1:D:290:LEU:HB2	2.19	0.43
1:G:225:ASN:OD1	1:G:225:ASN:C	2.56	0.43
1:D:27:THR:HG21	1:D:277:ALA:HB1	2.00	0.43
1:C:312:ASP:HA	1:C:315:LEU:HB2	2.01	0.43
1:E:253:ARG:O	1:E:257:GLU:HB2	2.19	0.43
1:D:85:ARG:HA	1:D:85:ARG:HD2	1.92	0.43
1:A:48:LEU:HD22	1:A:52:LEU:HG	2.01	0.43
1:D:308:GLU:H	1:D:308:GLU:HG2	1.44	0.43
1:C:70:THR:OG1	1:C:71:SER:N	2.51	0.43
1:D:118:HIS:C	1:D:120:GLY:H	2.21	0.43
1:B:190:ARG:HG3	1:B:191:VAL:N	2.31	0.43
1:G:78:LEU:HD12	1:G:78:LEU:HA	1.89	0.42
1:C:100:GLU:HG3	1:C:100:GLU:H	1.59	0.42
1:B:27:THR:HG23	1:B:28:SER:N	2.33	0.42
1:A:186:GLY:HA3	1:A:235:VAL:HG11	2.01	0.42
1:H:127:ILE:O	1:H:131:LEU:HD12	2.19	0.42
1:B:8:LEU:HD22	1:B:11:ILE:HD11	2.01	0.42
1:E:183:THR:O	1:E:187:GLN:HG3	2.19	0.42
1:G:249:ASP:O	1:G:253:ARG:HG3	2.19	0.42
1:H:102:ARG:NH2	1:H:102:ARG:HG3	2.34	0.42
1:E:106:ARG:NH2	1:H:311:ASP:OD2	2.52	0.42
1:C:195:GLU:HG3	3:C:543:HOH:O	2.18	0.42
1:G:74:VAL:HG12	1:G:78:LEU:HD22	2.01	0.42
1:A:118:HIS:CD2	1:A:119:LEU:HD12	2.54	0.42
1:C:93:MET:O	1:C:114:LEU:HA	2.17	0.42
1:F:148:ASN:HB3	1:F:149:PRO:CD	2.49	0.42
1:C:49:SER:OG	1:C:151:TYR:HB2	2.19	0.42
1:E:68:GLU:OE1	1:E:142:GLN:NE2	2.47	0.42
1:H:39:GLY:HA3	1:H:44:ASP:OD2	2.19	0.42
1:A:4:PHE:HB2	1:D:17:VAL:HG12	2.01	0.42
1:G:209:LEU:HB2	1:G:239:LEU:HD11	2.01	0.42
1:H:93:MET:CE	1:H:112:LEU:HB3	2.49	0.42
1:D:115:PHE:CZ	1:D:124:GLY:HA3	2.54	0.42
1:B:95:ASP:HB3	1:B:117:GLY:H	1.85	0.42
1:B:65:THR:HB	1:B:137:TRP:CD1	2.55	0.42
1:E:57:LYS:CB	1:E:59:LEU:HD13	2.49	0.42
1:E:59:LEU:CD1	1:E:59:LEU:N	2.82	0.42
1:G:27:THR:HG23	1:G:28:SER:N	2.35	0.42
1:B:310:SER:N	1:C:114:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LEU:HA	1:C:303:PHE:CE1	2.55	0.42
1:D:8:LEU:CD1	1:D:85:ARG:HD3	2.50	0.42
1:B:289:MET:O	1:B:291:PRO:HD3	2.20	0.42
1:E:112:LEU:HA	1:E:112:LEU:HD13	1.90	0.42
1:C:167:LYS:O	1:C:193:ARG:NH2	2.53	0.42
1:E:253:ARG:HG2	1:E:257:GLU:OE2	2.19	0.42
1:D:209:LEU:CB	1:D:239:LEU:HD11	2.49	0.42
1:A:69:CYS:HB3	1:A:125:ASN:HD22	1.84	0.42
1:H:133:GLU:HG2	1:H:133:GLU:H	1.37	0.42
1:B:85:ARG:HH11	1:B:85:ARG:HG2	1.85	0.42
1:D:179:THR:HG23	1:D:228:PRO:HG2	2.01	0.42
1:G:233:ARG:O	1:G:235:VAL:N	2.52	0.42
1:A:141:ARG:O	1:A:145:ASN:HB2	2.20	0.42
1:E:153:ARG:NH1	1:E:187:GLN:OE1	2.53	0.41
1:G:300:THR:HG22	1:G:302:LEU:HB2	2.02	0.41
1:E:176:PHE:CD1	1:E:179:THR:HG22	2.55	0.41
1:E:46:LEU:HD12	1:E:47:ALA:N	2.35	0.41
1:E:89:PHE:CE2	1:E:91:ALA:HB2	2.54	0.41
1:B:41:SER:HB2	1:B:292:ASP:HB3	2.01	0.41
1:F:11:ILE:HD12	1:F:48:LEU:HG	2.02	0.41
1:C:297:TYR:HB3	1:C:302:LEU:HD12	2.02	0.41
1:B:27:THR:CG2	1:B:28:SER:N	2.83	0.41
1:G:113:VAL:O	1:G:113:VAL:HG12	2.20	0.41
1:H:132:ALA:O	1:H:136:GLY:N	2.52	0.41
1:E:176:PHE:HB2	1:E:179:THR:HA	2.03	0.41
1:C:206:ALA:HA	1:C:214:TRP:HA	2.02	0.41
1:H:55:GLU:OE1	1:H:85:ARG:NH2	2.54	0.41
1:A:78:LEU:HA	1:A:78:LEU:HD12	1.93	0.41
1:A:297:TYR:CB	1:A:302:LEU:HD12	2.51	0.41
1:D:65:THR:HG23	1:D:137:TRP:CD1	2.56	0.41
1:F:106:ARG:NH2	1:G:311:ASP:OD2	2.53	0.41
1:D:113:VAL:O	1:D:113:VAL:CG2	2.68	0.41
1:F:67:VAL:HG13	1:F:90:VAL:HB	2.03	0.41
1:B:104:LEU:HA	1:B:104:LEU:HD13	1.90	0.41
1:D:48:LEU:HD11	1:D:52:LEU:HD11	2.02	0.41
1:G:248:ARG:HD2	1:G:248:ARG:C	2.40	0.41
1:A:306:VAL:CG1	1:D:106:ARG:HG2	2.50	0.41
1:G:218:GLN:HG3	1:G:244:GLU:CD	2.41	0.41
1:B:8:LEU:HD11	1:B:81:VAL:HG13	2.02	0.41
1:D:204:SER:HB2	3:D:556:HOH:O	2.20	0.41
1:B:3:LEU:HA	1:B:3:LEU:HD12	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ALA:HB1	1:E:290:LEU:HG	2.02	0.41
1:C:219:ILE:HG22	1:C:265:SER:HA	2.02	0.41
1:E:93:MET:O	1:E:114:LEU:HA	2.21	0.41
1:D:265:SER:O	1:D:269:THR:HG23	2.19	0.41
1:B:49:SER:HB2	1:B:151:TYR:CG	2.56	0.41
1:E:316:ALA:C	1:E:318:LEU:H	2.24	0.41
1:B:61:LYS:O	1:B:87:TYR:HE1	2.04	0.41
1:F:102:ARG:HB3	1:F:112:LEU:HD21	2.03	0.41
1:E:101:ARG:HG2	1:E:101:ARG:H	1.61	0.41
1:G:145:ASN:HA	1:G:146:PRO:HD2	1.96	0.41
1:A:298:LEU:CD1	1:D:100:GLU:HB2	2.51	0.41
1:G:118:HIS:CE1	1:G:119:LEU:HD12	2.56	0.41
1:D:69:CYS:CB	1:D:125:ASN:HD22	2.29	0.41
1:A:32:LYS:O	1:A:290:LEU:HB2	2.21	0.41
1:D:148:ASN:HB3	1:D:149:PRO:HD3	2.00	0.41
1:C:50:VAL:HG13	1:C:145:ASN:ND2	2.35	0.41
1:C:39:GLY:HA3	1:C:44:ASP:OD2	2.21	0.41
1:A:248:ARG:NE	1:A:252:ARG:NH1	2.68	0.41
1:B:160:ILE:HG12	1:B:287:LEU:HD21	2.02	0.41
1:H:60:LEU:HA	1:H:60:LEU:HD23	1.96	0.41
1:A:134:LYS:HG2	1:A:135:TYR:CE2	2.55	0.41
1:C:219:ILE:N	1:C:219:ILE:HD13	2.35	0.41
1:G:100:GLU:O	1:G:104:LEU:HD22	2.20	0.41
1:D:120:GLY:O	1:D:121:SER:C	2.59	0.41
1:H:41:SER:HB2	1:H:292:ASP:HB3	2.03	0.41
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.93	0.41
1:E:102:ARG:HE	1:E:102:ARG:HB2	1.76	0.40
1:B:50:VAL:HG12	1:B:51:VAL:N	2.36	0.40
1:B:205:ASN:HB2	1:B:215:SER:OG	2.21	0.40
1:G:233:ARG:C	1:G:235:VAL:N	2.74	0.40
1:A:69:CYS:HB3	1:A:125:ASN:ND2	2.37	0.40
1:H:157:ALA:HB2	1:H:185:VAL:HA	2.03	0.40
1:B:248:ARG:CG	1:B:302:LEU:HA	2.51	0.40
1:D:302:LEU:HD13	1:D:303:PHE:CE1	2.56	0.40
1:F:311:ASP:HB3	1:F:314:TRP:HB3	2.03	0.40
1:E:14:THR:HB	1:E:33:VAL:O	2.21	0.40
1:E:298:LEU:HA	1:E:303:PHE:CE1	2.56	0.40
1:A:161:LEU:HD22	1:B:154:GLU:HG2	2.02	0.40
1:G:26:HIS:HB2	1:G:282:GLU:HG2	2.03	0.40
1:H:193:ARG:HB3	1:H:196:VAL:HG23	2.03	0.40
1:F:111:LYS:HE3	1:G:314:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:GLU:H	1:E:308:GLU:HG2	1.67	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	314/332 (95%)	294 (94%)	17 (5%)	3 (1%)	19	16
1	B	317/332 (96%)	293 (92%)	19 (6%)	5 (2%)	12	7
1	C	315/332 (95%)	285 (90%)	26 (8%)	4 (1%)	15	10
1	D	314/332 (95%)	292 (93%)	20 (6%)	2 (1%)	30	30
1	E	315/332 (95%)	288 (91%)	23 (7%)	4 (1%)	15	10
1	F	314/332 (95%)	294 (94%)	15 (5%)	5 (2%)	12	7
1	G	315/332 (95%)	288 (91%)	24 (8%)	3 (1%)	19	16
1	H	314/332 (95%)	286 (91%)	24 (8%)	4 (1%)	15	10
All	All	2518/2656 (95%)	2320 (92%)	168 (7%)	30 (1%)	16	11

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	ALA
1	D	121	SER
1	E	215	SER
1	G	312	ASP
1	H	117	GLY
1	H	121	SER
1	D	120	GLY
1	E	64	ASP
1	F	120	GLY

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Mol	Chain	Res	Type
1	A	304	ASP
1	B	98	SER
1	B	225	ASN
1	B	118	HIS
1	C	223	ALA
1	C	304	ASP
1	E	116	PRO
1	H	223	ALA
1	H	307	ASP
1	A	307	ASP
1	B	223	ALA
1	C	216	PRO
1	A	223	ALA
1	E	223	ALA
1	F	223	ALA
1	F	226	PHE
1	G	118	HIS
1	F	116	PRO
1	F	117	GLY
1	G	223	ALA
1	B	72	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	247/261 (95%)	203 (82%)	44 (18%)	2	1
1	B	250/261 (96%)	206 (82%)	44 (18%)	2	1
1	C	248/261 (95%)	210 (85%)	38 (15%)	3	2
1	D	247/261 (95%)	215 (87%)	32 (13%)	5	3
1	E	248/261 (95%)	201 (81%)	47 (19%)	2	0
1	F	247/261 (95%)	205 (83%)	42 (17%)	2	1
1	G	248/261 (95%)	214 (86%)	34 (14%)	4	2
1	H	247/261 (95%)	203 (82%)	44 (18%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1982/2088 (95%)	1657 (84%)	325 (16%)	3 1

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	18	ARG
1	A	21	ARG
1	A	27	THR
1	A	28	SER
1	A	31	VAL
1	A	33	VAL
1	A	46	LEU
1	A	48	LEU
1	A	57	LYS
1	A	71	SER
1	A	78	LEU
1	A	96	THR
1	A	99	VAL
1	A	100	GLU
1	A	101	ARG
1	A	104	LEU
1	A	106	ARG
1	A	121	SER
1	A	122	LYS
1	A	125	ASN
1	A	126	LEU
1	A	134	LYS
1	A	142	GLN
1	A	190	ARG
1	A	195	GLU
1	A	202	GLU
1	A	219	ILE
1	A	220	GLN
1	A	233	ARG
1	A	239	LEU
1	A	243	ASP
1	A	275	SER
1	A	276	ILE
1	A	278	GLU
1	A	282	GLU
1	A	299	SER

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Mol	Chain	Res	Type
1	A	300	THR
1	A	301	PHE
1	A	302	LEU
1	A	304	ASP
1	A	311	ASP
1	A	315	LEU
1	A	317	SER
1	B	18	ARG
1	B	21	ARG
1	B	27	THR
1	B	28	SER
1	B	31	VAL
1	B	41	SER
1	B	48	LEU
1	B	50	VAL
1	B	61	LYS
1	B	67	VAL
1	B	71	SER
1	B	78	LEU
1	B	85	ARG
1	B	88	ARG
1	B	92	VAL
1	B	99	VAL
1	B	101	ARG
1	B	104	LEU
1	B	106	ARG
1	B	111	LYS
1	B	114	LEU
1	B	119	LEU
1	B	121	SER
1	B	126	LEU
1	B	127	ILE
1	B	130	GLU
1	B	134	LYS
1	B	139	ARG
1	B	142	GLN
1	B	150	SER
1	B	190	ARG
1	B	195	GLU
1	B	205	ASN
1	B	209	LEU
1	B	215	SER

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Mol	Chain	Res	Type
1	B	220	GLN
1	B	230	VAL
1	B	235	VAL
1	B	239	LEU
1	B	254	LEU
1	B	278	GLU
1	B	282	GLU
1	B	301	PHE
1	B	302	LEU
1	C	3	LEU
1	C	6	SER
1	C	28	SER
1	C	31	VAL
1	C	46	LEU
1	C	48	LEU
1	C	65	THR
1	C	67	VAL
1	C	70	THR
1	C	78	LEU
1	C	85	ARG
1	C	88	ARG
1	C	100	GLU
1	C	101	ARG
1	C	104	LEU
1	C	114	LEU
1	C	119	LEU
1	C	122	LYS
1	C	126	LEU
1	C	130	GLU
1	C	133	GLU
1	C	195	GLU
1	C	204	SER
1	C	205	ASN
1	C	219	ILE
1	C	220	GLN
1	C	230	VAL
1	C	235	VAL
1	C	236	ILE
1	C	239	LEU
1	C	244	GLU
1	C	275	SER
1	C	301	PHE

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Mol	Chain	Res	Type
1	C	302	LEU
1	C	304	ASP
1	C	307	ASP
1	C	312	ASP
1	C	315	LEU
1	D	27	THR
1	D	28	SER
1	D	31	VAL
1	D	46	LEU
1	D	59	LEU
1	D	65	THR
1	D	68	GLU
1	D	70	THR
1	D	71	SER
1	D	78	LEU
1	D	98	SER
1	D	104	LEU
1	D	106	ARG
1	D	119	LEU
1	D	121	SER
1	D	122	LYS
1	D	125	ASN
1	D	126	LEU
1	D	150	SER
1	D	211	ARG
1	D	215	SER
1	D	220	GLN
1	D	230	VAL
1	D	239	LEU
1	D	243	ASP
1	D	290	LEU
1	D	301	PHE
1	D	302	LEU
1	D	306	VAL
1	D	308	GLU
1	D	310	SER
1	D	317	SER
1	E	3	LEU
1	E	21	ARG
1	E	27	THR
1	E	28	SER
1	E	57	LYS

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Mol	Chain	Res	Type
1	E	60	LEU
1	E	61	LYS
1	E	64	ASP
1	E	67	VAL
1	E	78	LEU
1	E	85	ARG
1	E	95	ASP
1	E	101	ARG
1	E	104	LEU
1	E	112	LEU
1	E	114	LEU
1	E	119	LEU
1	E	121	SER
1	E	122	LYS
1	E	127	ILE
1	E	129	ASP
1	E	131	LEU
1	E	139	ARG
1	E	141	ARG
1	E	142	GLN
1	E	190	ARG
1	E	195	GLU
1	E	205	ASN
1	E	213	GLU
1	E	215	SER
1	E	220	GLN
1	E	225	ASN
1	E	230	VAL
1	E	233	ARG
1	E	235	VAL
1	E	239	LEU
1	E	254	LEU
1	E	264	ILE
1	E	296	ARG
1	E	299	SER
1	E	301	PHE
1	E	302	LEU
1	E	308	GLU
1	E	311	ASP
1	E	315	LEU
1	E	317	SER
1	E	318	LEU

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Mol	Chain	Res	Type
1	F	3	LEU
1	F	6	SER
1	F	21	ARG
1	F	31	VAL
1	F	33	VAL
1	F	41	SER
1	F	46	LEU
1	F	48	LEU
1	F	61	LYS
1	F	65	THR
1	F	67	VAL
1	F	71	SER
1	F	74	VAL
1	F	78	LEU
1	F	96	THR
1	F	99	VAL
1	F	101	ARG
1	F	102	ARG
1	F	104	LEU
1	F	106	ARG
1	F	112	LEU
1	F	119	LEU
1	F	121	SER
1	F	126	LEU
1	F	130	GLU
1	F	131	LEU
1	F	139	ARG
1	F	204	SER
1	F	220	GLN
1	F	230	VAL
1	F	239	LEU
1	F	244	GLU
1	F	248	ARG
1	F	254	LEU
1	F	278	GLU
1	F	300	THR
1	F	301	PHE
1	F	302	LEU
1	F	308	GLU
1	F	310	SER
1	F	312	ASP
1	F	317	SER

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Mol	Chain	Res	Type
1	G	3	LEU
1	G	18	ARG
1	G	28	SER
1	G	33	VAL
1	G	41	SER
1	G	48	LEU
1	G	57	LYS
1	G	65	THR
1	G	67	VAL
1	G	71	SER
1	G	78	LEU
1	G	85	ARG
1	G	88	ARG
1	G	99	VAL
1	G	104	LEU
1	G	105	ILE
1	G	106	ARG
1	G	119	LEU
1	G	121	SER
1	G	122	LYS
1	G	193	ARG
1	G	202	GLU
1	G	211	ARG
1	G	215	SER
1	G	230	VAL
1	G	252	ARG
1	G	275	SER
1	G	298	LEU
1	G	300	THR
1	G	301	PHE
1	G	302	LEU
1	G	308	GLU
1	G	315	LEU
1	G	318	LEU
1	H	3	LEU
1	H	25	GLU
1	H	27	THR
1	H	28	SER
1	H	46	LEU
1	H	48	LEU
1	H	59	LEU
1	H	65	THR

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Mol	Chain	Res	Type
1	H	67	VAL
1	H	69	CYS
1	H	71	SER
1	H	78	LEU
1	H	92	VAL
1	H	93	MET
1	H	95	ASP
1	H	101	ARG
1	H	104	LEU
1	H	106	ARG
1	H	111	LYS
1	H	112	LEU
1	H	114	LEU
1	H	126	LEU
1	H	131	LEU
1	H	133	GLU
1	H	134	LYS
1	H	139	ARG
1	H	141	ARG
1	H	142	GLN
1	H	190	ARG
1	H	195	GLU
1	H	202	GLU
1	H	243	ASP
1	H	251	SER
1	H	265	SER
1	H	275	SER
1	H	278	GLU
1	H	295	GLU
1	H	296	ARG
1	H	301	PHE
1	H	302	LEU
1	H	304	ASP
1	H	307	ASP
1	H	310	SER
1	H	317	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	220	GLN

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Mol	Chain	Res	Type
1	B	171	HIS
1	D	125	ASN
1	E	171	HIS
1	F	20	GLN
1	F	125	ASN
1	F	220	GLN
1	G	20	GLN
1	G	171	HIS
1	H	20	GLN
1	H	125	ASN
1	H	142	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	PLP	A	401	1	15,15,16	2.28	7 (46%)	21,22,23	1.31	3 (14%)
2	PLP	B	401	1	15,15,16	2.26	6 (40%)	21,22,23	1.37	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PLP	C	401	1	15,15,16	2.33	7 (46%)	21,22,23	1.34	3 (14%)
2	PLP	D	401	1	15,15,16	2.24	6 (40%)	21,22,23	1.39	4 (19%)
2	PLP	E	401	1	15,15,16	2.41	6 (40%)	21,22,23	1.32	3 (14%)
2	PLP	F	401	1	15,15,16	2.29	7 (46%)	21,22,23	1.40	4 (19%)
2	PLP	G	401	1	15,15,16	2.23	6 (40%)	21,22,23	1.36	4 (19%)
2	PLP	H	401	1	15,15,16	2.27	6 (40%)	21,22,23	1.33	4 (19%)

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	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
2	PLP	E	401	1	-	0/6/6/8	0/1/1/1
2	PLP	F	401	1	-	0/6/6/8	0/1/1/1
2	PLP	G	401	1	-	0/6/6/8	0/1/1/1
2	PLP	H	401	1	-	0/6/6/8	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	PLP	C3-C2	-5.88	1.36	1.40
2	C	401	PLP	C3-C2	-5.23	1.37	1.40
2	A	401	PLP	C3-C2	-5.16	1.37	1.40
2	B	401	PLP	C3-C2	-5.11	1.37	1.40
2	H	401	PLP	C3-C2	-5.07	1.37	1.40
2	D	401	PLP	C3-C2	-4.85	1.37	1.40
2	G	401	PLP	C3-C2	-4.81	1.37	1.40
2	F	401	PLP	C3-C2	-4.74	1.37	1.40
2	D	401	PLP	P-O3P	-2.52	1.46	1.54
2	D	401	PLP	P-O2P	-2.52	1.46	1.54
2	E	401	PLP	P-O3P	-2.46	1.46	1.54
2	C	401	PLP	P-O2P	-2.46	1.46	1.54
2	D	401	PLP	C6-C5	-2.45	1.32	1.37
2	B	401	PLP	P-O2P	-2.44	1.46	1.54
2	F	401	PLP	C6-C5	-2.44	1.32	1.37
2	B	401	PLP	C6-C5	-2.44	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	PLP	C6-C5	-2.42	1.32	1.37
2	E	401	PLP	C6-C5	-2.42	1.32	1.37
2	H	401	PLP	P-O2P	-2.40	1.46	1.54
2	A	401	PLP	C6-C5	-2.39	1.32	1.37
2	F	401	PLP	P-O3P	-2.38	1.46	1.54
2	F	401	PLP	P-O2P	-2.38	1.46	1.54
2	B	401	PLP	P-O3P	-2.37	1.46	1.54
2	E	401	PLP	P-O2P	-2.37	1.46	1.54
2	C	401	PLP	P-O3P	-2.35	1.46	1.54
2	C	401	PLP	C6-C5	-2.35	1.32	1.37
2	A	401	PLP	P-O3P	-2.34	1.46	1.54
2	H	401	PLP	P-O3P	-2.32	1.46	1.54
2	G	401	PLP	P-O2P	-2.30	1.46	1.54
2	G	401	PLP	P-O3P	-2.29	1.46	1.54
2	A	401	PLP	P-O2P	-2.25	1.47	1.54
2	H	401	PLP	C6-C5	-2.25	1.32	1.37
2	A	401	PLP	C5-C4	2.10	1.43	1.40
2	C	401	PLP	C5-C4	2.15	1.43	1.40
2	F	401	PLP	C5-C4	2.70	1.43	1.40
2	D	401	PLP	C4A-C4	3.38	1.58	1.51
2	A	401	PLP	C2-N1	3.40	1.40	1.33
2	B	401	PLP	C2-N1	3.44	1.40	1.33
2	B	401	PLP	C4A-C4	3.47	1.58	1.51
2	F	401	PLP	C2-N1	3.50	1.40	1.33
2	E	401	PLP	C2-N1	3.53	1.40	1.33
2	G	401	PLP	C4A-C4	3.55	1.59	1.51
2	H	401	PLP	C4A-C4	3.56	1.59	1.51
2	C	401	PLP	C2-N1	3.59	1.40	1.33
2	H	401	PLP	C2-N1	3.65	1.40	1.33
2	F	401	PLP	C4A-C4	3.68	1.59	1.51
2	D	401	PLP	C2-N1	3.68	1.40	1.33
2	C	401	PLP	C4A-C4	3.72	1.59	1.51
2	E	401	PLP	C4A-C4	3.73	1.59	1.51
2	A	401	PLP	C4A-C4	3.74	1.59	1.51
2	G	401	PLP	C2-N1	3.76	1.41	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	PLP	C3-C2-N1	-2.83	117.14	120.69
2	F	401	PLP	C3-C2-N1	-2.79	117.19	120.69
2	G	401	PLP	C3-C2-N1	-2.76	117.23	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	PLP	C3-C2-N1	-2.72	117.28	120.69
2	D	401	PLP	C3-C2-N1	-2.69	117.32	120.69
2	E	401	PLP	C3-C2-N1	-2.69	117.32	120.69
2	A	401	PLP	C3-C2-N1	-2.68	117.33	120.69
2	H	401	PLP	C3-C2-N1	-2.67	117.35	120.69
2	D	401	PLP	C5-C6-N1	-2.26	119.92	123.86
2	H	401	PLP	C5-C6-N1	-2.23	119.97	123.86
2	C	401	PLP	C5-C6-N1	-2.17	120.06	123.86
2	G	401	PLP	C5-C6-N1	-2.12	120.16	123.86
2	E	401	PLP	C5-C6-N1	-2.09	120.22	123.86
2	B	401	PLP	C5-C6-N1	-2.07	120.25	123.86
2	F	401	PLP	C5-C6-N1	-2.06	120.25	123.86
2	A	401	PLP	C5-C6-N1	-2.00	120.36	123.86
2	B	401	PLP	O3-C3-C2	2.08	120.58	117.53
2	H	401	PLP	O3-C3-C2	2.15	120.68	117.53
2	F	401	PLP	C5A-C5-C4	2.20	124.60	121.63
2	E	401	PLP	C6-N1-C2	2.31	123.90	119.26
2	A	401	PLP	C6-N1-C2	2.33	123.94	119.26
2	G	401	PLP	C6-N1-C2	2.34	123.96	119.26
2	H	401	PLP	C6-N1-C2	2.39	124.05	119.26
2	D	401	PLP	O3-C3-C2	2.40	121.04	117.53
2	D	401	PLP	C6-N1-C2	2.40	124.08	119.26
2	G	401	PLP	O3-C3-C2	2.42	121.07	117.53
2	C	401	PLP	C6-N1-C2	2.44	124.17	119.26
2	B	401	PLP	C6-N1-C2	2.51	124.29	119.26
2	F	401	PLP	C6-N1-C2	2.54	124.36	119.26

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	316/332 (95%)	0.08	13 (4%) 41 44	23, 44, 86, 103	0
1	B	319/332 (96%)	0.09	20 (6%) 23 25	26, 46, 102, 114	0
1	C	317/332 (95%)	0.20	21 (6%) 22 24	22, 48, 89, 110	0
1	D	316/332 (95%)	0.01	20 (6%) 23 25	22, 39, 97, 119	0
1	E	317/332 (95%)	0.49	39 (12%) 5 5	23, 52, 106, 126	0
1	F	316/332 (95%)	-0.14	3 (0%) 85 87	23, 41, 80, 93	0
1	G	317/332 (95%)	0.33	22 (6%) 20 22	27, 49, 90, 107	0
1	H	316/332 (95%)	0.25	31 (9%) 10 10	27, 47, 111, 132	0
All	All	2534/2656 (95%)	0.17	169 (6%) 21 23	22, 46, 99, 132	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	119	LEU	10.6
1	B	96	THR	8.5
1	D	119	LEU	8.3
1	H	313	ALA	7.3
1	E	118	HIS	6.6
1	G	306	VAL	6.5
1	B	116	PRO	6.3
1	B	95	ASP	6.0
1	G	307	ASP	5.7
1	H	118	HIS	5.4
1	E	119	LEU	5.3
1	H	122	LYS	5.2
1	C	306	VAL	5.2
1	B	119	LEU	5.1
1	B	93	MET	5.1
1	D	118	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	316	ALA	4.9
1	E	121	SER	4.8
1	H	115	PHE	4.7
1	B	118	HIS	4.7
1	B	115	PHE	4.5
1	E	279	HIS	4.5
1	C	309	GLY	4.3
1	E	313	ALA	4.2
1	B	114	LEU	4.2
1	E	116	PRO	4.1
1	E	112	LEU	4.1
1	C	315	LEU	4.0
1	H	315	LEU	4.0
1	H	114	LEU	4.0
1	G	313	ALA	3.9
1	A	313	ALA	3.9
1	B	97	TYR	3.9
1	E	311	ASP	3.8
1	E	314	TRP	3.8
1	E	315	LEU	3.7
1	H	69	CYS	3.7
1	H	97	TYR	3.7
1	H	126	LEU	3.7
1	C	314	TRP	3.7
1	H	121	SER	3.6
1	E	115	PHE	3.6
1	G	225	ASN	3.6
1	G	136	GLY	3.5
1	E	316	ALA	3.5
1	H	312	ASP	3.5
1	H	123	GLY	3.4
1	A	307	ASP	3.4
1	A	310	SER	3.4
1	C	311	ASP	3.4
1	G	119	LEU	3.4
1	B	120	GLY	3.4
1	G	126	LEU	3.4
1	C	214	TRP	3.3
1	G	133	GLU	3.3
1	G	118	HIS	3.3
1	D	316	ALA	3.3
1	D	307	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	96	THR	3.3
1	D	116	PRO	3.2
1	H	116	PRO	3.2
1	H	135	TYR	3.2
1	B	131	LEU	3.2
1	C	211	ARG	3.2
1	D	113	VAL	3.1
1	G	122	LYS	3.1
1	E	117	GLY	3.1
1	D	312	ASP	3.1
1	G	318	LEU	3.1
1	A	293	THR	3.1
1	E	293	THR	3.0
1	H	314	TRP	3.0
1	E	95	ASP	3.0
1	C	310	SER	3.0
1	H	95	ASP	3.0
1	E	318	LEU	2.9
1	E	262	ALA	2.9
1	H	279	HIS	2.9
1	G	210	ALA	2.9
1	B	135	TYR	2.9
1	E	304	ASP	2.9
1	D	306	VAL	2.9
1	B	117	GLY	2.8
1	D	315	LEU	2.8
1	G	215	SER	2.8
1	G	314	TRP	2.8
1	C	122	LYS	2.8
1	E	135	TYR	2.8
1	C	225	ASN	2.8
1	B	134	LYS	2.7
1	E	120	GLY	2.7
1	F	118	HIS	2.7
1	H	316	ALA	2.7
1	H	113	VAL	2.7
1	D	95	ASP	2.6
1	E	225	ASN	2.6
1	E	245	VAL	2.6
1	A	27	THR	2.6
1	B	320	THR	2.6
1	A	309	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	40	GLY	2.6
1	D	126	LEU	2.5
1	C	317	SER	2.5
1	G	309	GLY	2.5
1	E	306	VAL	2.5
1	E	35	SER	2.5
1	D	94	GLY	2.5
1	D	114	LEU	2.5
1	C	215	SER	2.5
1	D	309	GLY	2.5
1	G	305	GLY	2.5
1	E	94	GLY	2.4
1	C	312	ASP	2.4
1	H	305	GLY	2.4
1	A	35	SER	2.4
1	E	309	GLY	2.4
1	E	307	ASP	2.4
1	C	308	GLU	2.4
1	D	308	GLU	2.4
1	E	310	SER	2.4
1	A	304	ASP	2.3
1	B	279	HIS	2.3
1	C	313	ALA	2.3
1	E	42	VAL	2.3
1	A	25	GLU	2.3
1	C	133	GLU	2.3
1	H	304	ASP	2.3
1	D	96	THR	2.3
1	F	96	THR	2.3
1	G	310	SER	2.3
1	E	278	GLU	2.2
1	D	122	LYS	2.2
1	C	208	MET	2.2
1	D	121	SER	2.2
1	C	307	ASP	2.2
1	D	115	PHE	2.2
1	H	96	THR	2.2
1	B	112	LEU	2.2
1	F	114	LEU	2.2
1	H	134	LYS	2.2
1	H	93	MET	2.2
1	A	279	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	211	ARG	2.1
1	C	301	PHE	2.1
1	E	243	ASP	2.1
1	E	41	SER	2.1
1	H	40	GLY	2.1
1	A	316	ALA	2.1
1	G	293	THR	2.1
1	A	294	GLY	2.1
1	E	130	GLU	2.1
1	H	124	GLY	2.1
1	E	133	GLU	2.1
1	H	102	ARG	2.1
1	E	104	LEU	2.1
1	A	306	VAL	2.1
1	G	39	GLY	2.1
1	H	309	GLY	2.1
1	B	319	ASP	2.1
1	E	122	LYS	2.1
1	E	305	GLY	2.1
1	C	118	HIS	2.0
1	E	40	GLY	2.0
1	B	94	GLY	2.0
1	B	98	SER	2.0
1	H	307	ASP	2.0
1	D	97	TYR	2.0
1	H	293	THR	2.0
1	G	316	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å^2)	Q<0.9
2	PLP	B	401	15/16	0.97	0.14	0.71	31,38,41,41	0
2	PLP	C	401	15/16	0.97	0.16	0.62	37,42,45,46	0
2	PLP	G	401	15/16	0.98	0.17	0.27	36,39,43,46	0
2	PLP	F	401	15/16	0.99	0.15	0.24	27,30,33,34	0
2	PLP	E	401	15/16	0.98	0.17	0.04	43,45,48,49	0
2	PLP	A	401	15/16	0.98	0.16	0.03	30,34,36,38	0
2	PLP	D	401	15/16	0.99	0.13	-0.09	28,32,34,34	0
2	PLP	H	401	15/16	0.97	0.11	-0.16	36,41,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.