Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:19 AM GMT

PDB ID	:	3E6G
Title	:	Crystal structure of XometC, a cystathionine c-lyase-like protein from Xanthomonas oryzae pv.oryzae
Authors	:	Ngo, H.P.T.; Kim, J.K.; Kim, H.S.; Jung, J.H.; Ahn, Y.J.; Kim, J.G.; Lee, B.M.; Kang, H.W.; Kang, L.W.
Deposited on	:	2008-08-15
Resolution	:	2.80 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 (i) symbol.

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

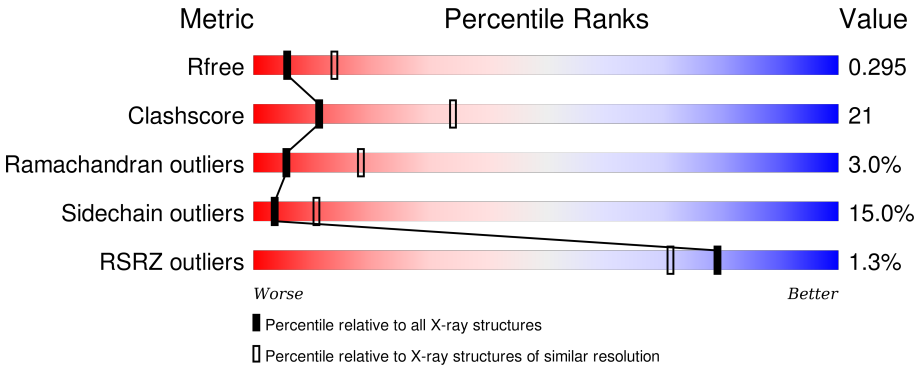
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	400	2% 52% 32% 8% • 8%
1	B	400	54% 24% 7% 16%
1	C	400	2% 54% 32% 6% • 8%
1	D	400	% 53% 23% 7% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10661 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 Cystathionine gamma-lyase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2756	1744	486	511	15			
1	B	336	Total	C	N	O	S	0	0	0
			2525	1601	446	464	14			
1	C	368	Total	C	N	O	S	0	0	0
			2756	1744	486	511	15			
1	D	335	Total	C	N	O	S	0	0	0
			2522	1599	446	463	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q5H4T8
A	-1	SER	-	EXPRESSION TAG	UNP Q5H4T8
A	0	HIS	-	EXPRESSION TAG	UNP Q5H4T8
B	-2	GLY	-	EXPRESSION TAG	UNP Q5H4T8
B	-1	SER	-	EXPRESSION TAG	UNP Q5H4T8
B	0	HIS	-	EXPRESSION TAG	UNP Q5H4T8
C	-2	GLY	-	EXPRESSION TAG	UNP Q5H4T8
C	-1	SER	-	EXPRESSION TAG	UNP Q5H4T8
C	0	HIS	-	EXPRESSION TAG	UNP Q5H4T8
D	-2	GLY	-	EXPRESSION TAG	UNP Q5H4T8
D	-1	SER	-	EXPRESSION TAG	UNP Q5H4T8
D	0	HIS	-	EXPRESSION TAG	UNP Q5H4T8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	28	Total	O	0	0
			28	28		
2	B	24	Total	O	0	0
			24	24		

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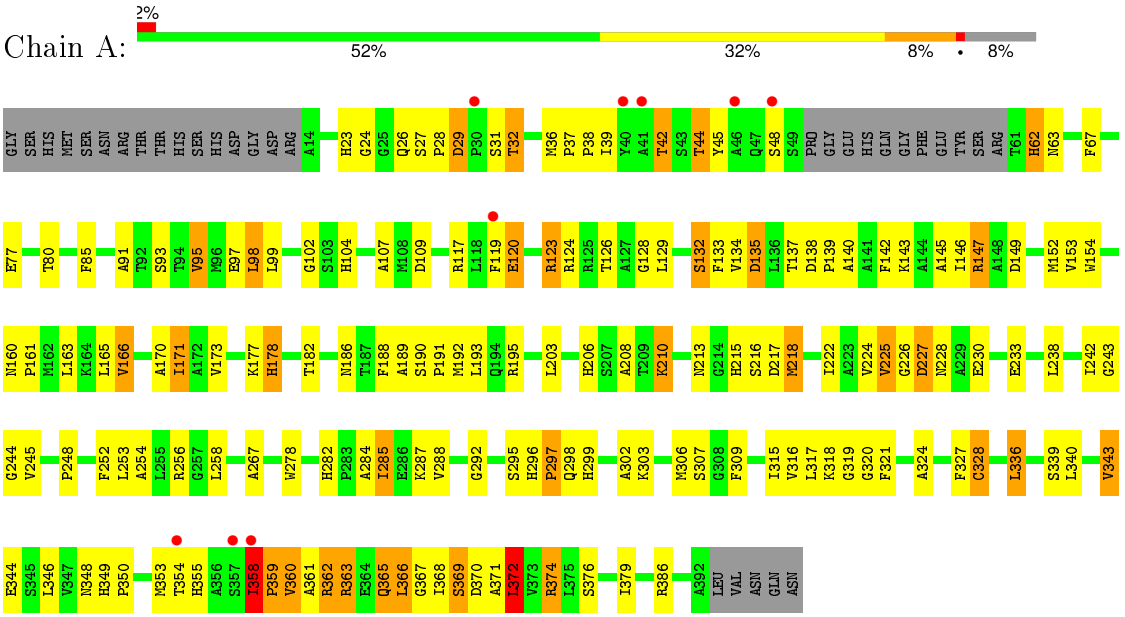
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	21	Total O 21 21	0	0
2	D	29	Total O 29 29	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

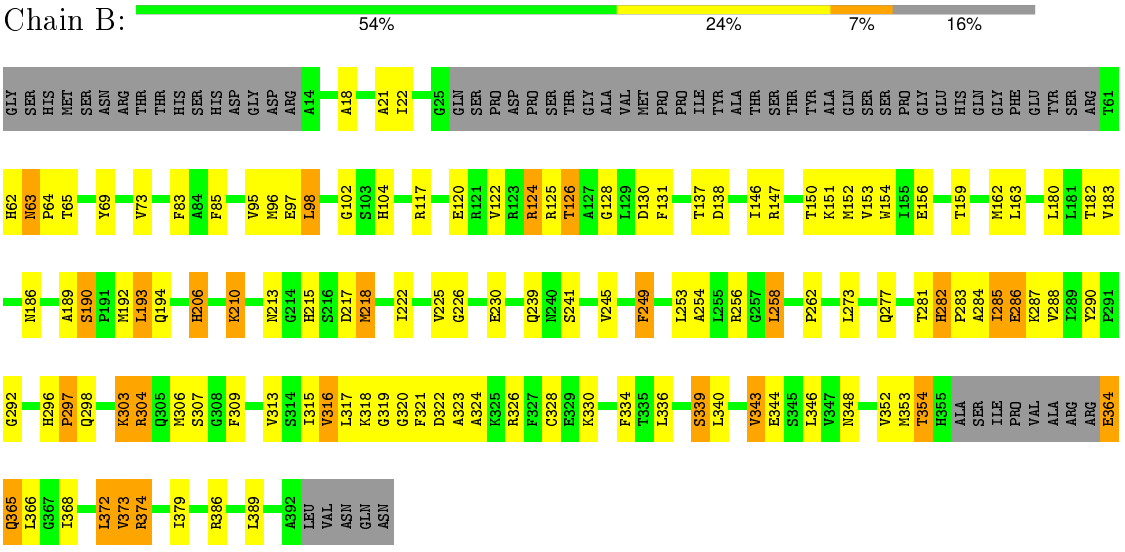
- Molecule 1: Cystathionine gamma-lyase-like protein

Chain A:



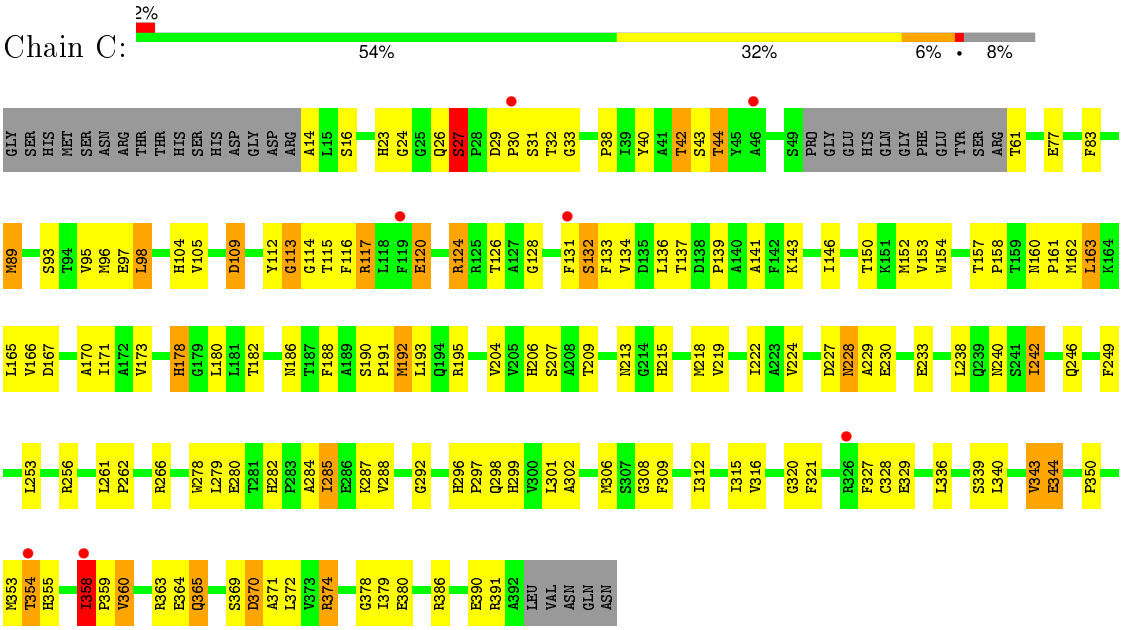
- Molecule 1: Cystathionine gamma-lyase-like protein

Chain B:



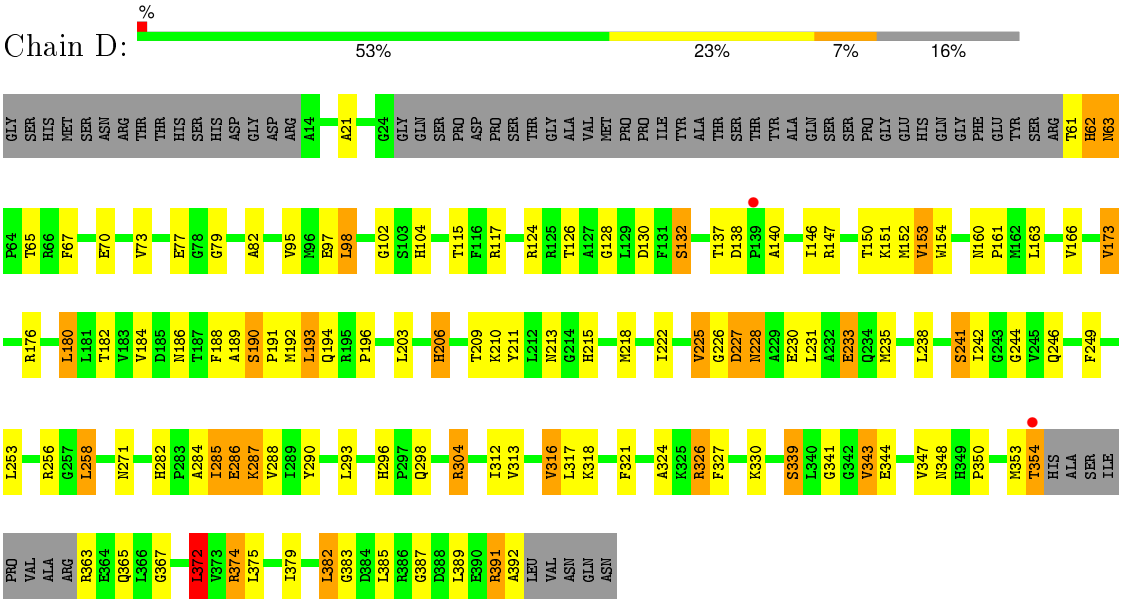
- Molecule 1: Cystathionine gamma-lyase-like protein

Chain C:



• Molecule 1: Cystathionine gamma-lyase-like protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	78.35Å 78.35Å 300.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.26 – 2.80 42.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.26-2.80) 100.0 (42.25-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.295 0.218 , 0.295	Depositor DCC
R_{free} test set	2237 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 20.0	EDS
Estimated twinning fraction	0.489 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	2 of 44392 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10661	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.74	0/2809	0.87	4/3811 (0.1%)
1	B	0.72	0/2570	0.87	1/3479 (0.0%)
1	C	0.77	0/2809	0.87	0/3811
1	D	0.73	0/2566	0.87	2/3473 (0.1%)
All	All	0.74	0/10754	0.87	7/14574 (0.0%)

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	3
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	372	LEU	CA-CB-CG	6.33	129.86	115.30
1	B	372	LEU	CA-CB-CG	6.21	129.59	115.30
1	A	32	THR	CB-CA-C	-6.02	95.34	111.60
1	A	123	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	D	153	VAL	CB-CA-C	-5.67	100.63	111.40
1	A	372	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	258	LEU	CB-CG-CD2	-5.01	102.48	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	HIS	Peptide
1	A	227	ASP	Peptide
1	A	358	ILE	Peptide
1	B	206	HIS	Peptide
1	C	27	SER	Peptide
1	D	206	HIS	Peptide
1	D	391	ARG	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	2756	0	2776	138	0
1	B	2525	0	2548	106	0
1	C	2756	0	2776	126	0
1	D	2522	0	2551	101	0
2	A	28	0	0	1	0
2	B	24	0	0	3	0
2	C	21	0	0	1	0
2	D	29	0	0	0	0
All	All	10661	0	10651	438	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 21.

All (438) 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:C:374:ARG:HG2	1:C:374:ARG:HH11	1.09	1.15
1:B:374:ARG:HG2	1:B:374:ARG:HH11	1.06	1.12
1:A:242:ILE:HD12	1:A:244:GLY:H	1.12	1.11
1:D:242:ILE:HD12	1:D:244:GLY:H	1.15	1.10
1:C:124:ARG:HH11	1:C:124:ARG:HG2	1.04	1.09
1:A:374:ARG:HG2	1:A:374:ARG:HH11	1.00	1.09
1:D:206:HIS:HD2	1:D:222:ILE:HD11	1.20	1.06
1:D:374:ARG:HG2	1:D:374:ARG:HH11	1.17	1.04
1:D:206:HIS:CD2	1:D:222:ILE:HD11	1.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG23	1:A:171:ILE:HD11	1.40	1.03
1:D:228:ASN:N	1:D:228:ASN:HD22	1.62	0.97
1:D:104:HIS:HD1	1:D:150:THR:HG1	1.01	0.96
1:A:374:ARG:HG2	1:A:374:ARG:NH1	1.79	0.95
1:A:287:LYS:HG2	1:A:316:VAL:HG12	1.50	0.94
1:C:124:ARG:NH1	1:C:124:ARG:HG2	1.79	0.93
1:A:256:ARG:HH22	1:D:213:ASN:HD21	1.05	0.93
1:B:374:ARG:NH1	1:B:374:ARG:HG2	1.85	0.90
1:C:287:LYS:HB3	1:C:316:VAL:HG12	1.54	0.89
1:C:124:ARG:HH11	1:C:124:ARG:CG	1.85	0.89
1:A:354:THR:HG23	1:A:355:HIS:ND1	1.88	0.88
1:B:285:ILE:HD11	1:B:288:VAL:HG23	1.56	0.88
1:A:170:ALA:O	1:A:173:VAL:HG12	1.74	0.88
1:A:31:SER:HB2	1:C:31:SER:HB2	1.55	0.87
1:D:203:LEU:HD21	1:D:225:VAL:HG12	1.55	0.87
1:A:256:ARG:NH2	1:D:213:ASN:HD21	1.74	0.85
1:B:213:ASN:HD21	1:C:256:ARG:HH22	1.25	0.85
1:A:242:ILE:CD1	1:A:244:GLY:H	1.90	0.83
1:D:374:ARG:HG2	1:D:374:ARG:NH1	1.92	0.83
1:C:374:ARG:NH1	1:C:374:ARG:HG2	1.88	0.82
1:C:354:THR:HG23	1:C:355:HIS:ND1	1.95	0.82
1:A:350:PRO:HA	1:A:354:THR:HG22	1.62	0.82
1:A:102:GLY:HA2	1:A:128:GLY:O	1.80	0.81
1:A:362:ARG:HH11	1:A:363:ARG:HG2	1.45	0.81
1:C:343:VAL:HG22	1:C:379:ILE:HG12	1.63	0.81
1:D:104:HIS:ND1	1:D:150:THR:OG1	2.08	0.80
1:A:147:ARG:HH21	1:A:149:ASP:HB2	1.46	0.80
1:A:166:VAL:CG2	1:A:171:ILE:HD11	2.12	0.80
1:B:213:ASN:HD21	1:C:256:ARG:NH2	1.80	0.79
1:D:327:PHE:HD1	1:D:392:ALA:HB3	1.47	0.78
1:A:126:THR:HG21	1:B:97:GLU:OE2	1.84	0.77
1:A:242:ILE:HD12	1:A:244:GLY:N	1.94	0.77
1:B:102:GLY:HA2	1:B:128:GLY:O	1.85	0.77
1:B:206:HIS:HD2	1:B:222:ILE:HD11	1.50	0.76
1:A:296:HIS:HD2	1:A:298:GLN:H	1.34	0.76
1:D:213:ASN:O	1:D:215:HIS:HD2	1.68	0.75
1:C:296:HIS:HD2	1:C:298:GLN:H	1.32	0.75
1:C:287:LYS:HB3	1:C:316:VAL:CG1	2.14	0.75
1:C:320:GLY:HA2	1:C:371:ALA:HB2	1.68	0.75
1:C:170:ALA:O	1:C:173:VAL:HG12	1.87	0.74
1:A:95:VAL:O	1:A:98:LEU:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:HG2	1:A:316:VAL:CG1	2.17	0.74
1:A:142:PHE:CD2	1:A:171:ILE:HG22	2.22	0.74
1:C:124:ARG:O	1:C:128:GLY:HA2	1.88	0.73
1:A:344:GLU:HG2	2:A:401:HOH:O	1.88	0.73
1:D:203:LEU:CD2	1:D:225:VAL:HG12	2.18	0.72
1:C:95:VAL:O	1:C:98:LEU:HB2	1.89	0.72
1:D:227:ASP:OD1	1:D:227:ASP:N	2.20	0.72
1:A:256:ARG:HH22	1:D:213:ASN:ND2	1.84	0.72
1:B:62:HIS:HB3	2:B:422:HOH:O	1.90	0.72
1:D:304:ARG:HH11	1:D:304:ARG:HG3	1.54	0.71
1:A:374:ARG:CG	1:A:374:ARG:HH11	1.90	0.70
1:A:31:SER:O	1:A:32:THR:OG1	2.09	0.70
1:D:271:ASN:ND2	1:D:382:LEU:HB2	2.05	0.70
1:B:296:HIS:CD2	1:B:298:GLN:H	2.10	0.70
1:B:73:VAL:HG22	1:B:258:LEU:HD21	1.72	0.70
1:D:102:GLY:HA2	1:D:128:GLY:O	1.91	0.70
1:C:160:ASN:HB2	1:C:188:PHE:CZ	2.26	0.70
1:B:213:ASN:O	1:B:215:HIS:HD2	1.74	0.69
1:A:195:ARG:HH11	1:A:195:ARG:HG3	1.57	0.69
1:D:189:ALA:HA	1:D:193:LEU:HD12	1.73	0.68
1:B:365:GLN:CG	1:B:368:ILE:HB	2.23	0.68
1:D:286:GLU:HB3	1:D:318:LYS:HG2	1.74	0.68
1:B:286:GLU:HB3	1:B:318:LYS:HG3	1.75	0.68
1:D:347:VAL:HG23	1:D:375:LEU:HD23	1.76	0.68
1:D:206:HIS:HD2	1:D:222:ILE:CD1	2.03	0.68
1:A:296:HIS:CD2	1:A:298:GLN:H	2.11	0.68
1:C:143:LYS:HA	1:C:146:ILE:HD12	1.75	0.68
1:C:296:HIS:CD2	1:C:298:GLN:H	2.11	0.67
1:B:189:ALA:O	1:B:190:SER:O	2.13	0.67
1:A:29:ASP:OD2	1:A:32:THR:OG1	2.12	0.66
1:A:44:THR:HG21	1:B:339:SER:H	1.59	0.66
1:B:365:GLN:HG2	1:B:368:ILE:HB	1.78	0.66
1:A:213:ASN:O	1:A:215:HIS:HD2	1.77	0.66
1:D:285:ILE:HD11	1:D:288:VAL:HG23	1.78	0.66
1:C:77:GLU:HG3	1:C:224:VAL:HG21	1.78	0.66
1:D:327:PHE:CD1	1:D:392:ALA:HB3	2.31	0.66
1:C:152:MET:HE1	1:C:154:TRP:HE3	1.61	0.66
1:B:256:ARG:NH2	1:C:213:ASN:HD21	1.94	0.65
1:B:213:ASN:ND2	1:C:256:ARG:HH22	1.91	0.65
1:A:104:HIS:HE2	1:A:132:SER:HG	1.41	0.65
1:D:228:ASN:H	1:D:228:ASN:HD22	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:PRO:HA	1:C:354:THR:HG22	1.79	0.65
1:A:189:ALA:HA	1:A:193:LEU:HD12	1.78	0.64
1:A:296:HIS:O	1:A:298:GLN:N	2.31	0.64
1:C:282:HIS:HE1	1:C:390:GLU:OE2	1.81	0.64
1:C:104:HIS:HE2	1:C:132:SER:HG	1.43	0.64
1:A:104:HIS:NE2	1:A:132:SER:OG	2.29	0.64
1:B:287:LYS:HB3	1:B:316:VAL:HG13	1.80	0.64
1:A:97:GLU:OE2	1:B:126:THR:HG21	1.98	0.63
1:B:206:HIS:CD2	1:B:222:ILE:HD11	2.32	0.63
1:D:296:HIS:CD2	1:D:298:GLN:H	2.15	0.63
1:D:233:GLU:HA	1:D:233:GLU:OE2	1.98	0.63
1:A:165:LEU:HD21	1:A:306:MET:CE	2.28	0.63
1:B:122:VAL:O	1:B:126:THR:HB	1.97	0.63
1:A:137:THR:O	1:A:139:PRO:HD3	1.98	0.63
1:B:63:ASN:HD22	1:B:63:ASN:C	2.02	0.62
1:A:358:ILE:O	1:A:360:VAL:HG22	1.99	0.62
1:B:162:MET:HE2	1:B:368:ILE:HG12	1.81	0.62
1:A:77:GLU:HG3	1:A:224:VAL:HG21	1.81	0.62
1:C:195:ARG:HH11	1:C:195:ARG:HG3	1.63	0.62
1:C:126:THR:HG21	1:D:97:GLU:OE2	2.00	0.61
1:B:365:GLN:HB2	1:B:368:ILE:HD12	1.82	0.61
1:C:213:ASN:O	1:C:215:HIS:HD2	1.83	0.61
1:A:315:ILE:O	1:A:372:LEU:HA	2.00	0.61
1:D:228:ASN:N	1:D:228:ASN:ND2	2.38	0.61
1:B:285:ILE:CD1	1:B:288:VAL:HG23	2.31	0.61
1:B:273:LEU:HD11	1:B:277:GLN:HE21	1.66	0.60
1:A:135:ASP:OD2	1:A:137:THR:HB	2.01	0.60
1:B:296:HIS:HD2	1:B:298:GLN:H	1.49	0.60
1:C:193:LEU:HD22	1:C:308:GLY:HA3	1.83	0.60
1:A:44:THR:HG23	1:B:339:SER:HB2	1.82	0.60
1:D:95:VAL:O	1:D:98:LEU:HB2	2.00	0.60
1:B:156:GLU:O	1:B:159:THR:HG22	2.01	0.60
1:C:152:MET:CE	1:C:154:TRP:HE3	2.14	0.59
1:C:146:ILE:HG21	1:C:178:HIS:HD2	1.68	0.59
1:A:91:ALA:O	1:A:95:VAL:HG12	2.02	0.59
1:A:343:VAL:HG22	1:A:379:ILE:HG12	1.85	0.59
1:B:292:GLY:HA3	1:B:309:PHE:CD2	2.39	0.58
1:B:95:VAL:O	1:B:98:LEU:HB2	2.02	0.58
1:B:328:CYS:HB3	1:B:336:LEU:HD13	1.85	0.58
1:A:28:PRO:O	1:A:29:ASP:HB3	2.02	0.58
1:C:104:HIS:NE2	1:C:132:SER:OG	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASP:HA	1:A:133:PHE:HB3	1.84	0.58
1:D:153:VAL:HG22	1:D:180:LEU:HD12	1.85	0.58
1:D:317:LEU:HD12	1:D:324:ALA:HA	1.86	0.58
1:A:282:HIS:CD2	1:A:284:ALA:H	2.21	0.58
1:C:24:GLY:O	1:C:26:GLN:HG2	2.04	0.58
1:A:362:ARG:NH1	1:A:363:ARG:HG2	2.15	0.57
1:A:282:HIS:HD2	1:A:284:ALA:H	1.52	0.57
1:B:104:HIS:ND1	1:B:150:THR:OG1	2.31	0.57
1:D:124:ARG:HH12	1:D:130:ASP:HA	1.69	0.57
1:D:287:LYS:HB3	1:D:316:VAL:HG13	1.87	0.57
1:C:374:ARG:CG	1:C:374:ARG:HH11	1.98	0.57
1:D:285:ILE:HD11	1:D:288:VAL:CG2	2.34	0.57
1:A:138:ASP:OD1	1:A:140:ALA:HB3	2.05	0.57
1:D:189:ALA:CA	1:D:193:LEU:HD12	2.35	0.56
1:D:327:PHE:HD1	1:D:392:ALA:CB	2.17	0.56
1:A:316:VAL:HA	1:A:371:ALA:O	2.05	0.56
1:B:189:ALA:O	1:B:193:LEU:HD12	2.06	0.56
1:A:186:ASN:O	1:A:189:ALA:O	2.23	0.56
1:A:165:LEU:HD21	1:A:306:MET:HE2	1.88	0.56
1:D:228:ASN:HB2	1:D:231:LEU:H	1.71	0.56
1:B:336:LEU:HD11	1:B:353:MET:CE	2.36	0.56
1:C:116:PHE:HE1	1:C:133:PHE:CE2	2.24	0.56
1:A:296:HIS:O	1:A:297:PRO:C	2.44	0.55
1:C:152:MET:HE1	1:C:154:TRP:CE3	2.42	0.55
1:D:63:ASN:HD22	1:D:63:ASN:C	2.09	0.55
1:D:160:ASN:HB2	1:D:188:PHE:CZ	2.42	0.55
1:D:152:MET:HE3	1:D:154:TRP:HE3	1.71	0.54
1:B:162:MET:CE	1:B:368:ILE:HG12	2.37	0.54
1:A:365:GLN:HG2	1:A:366:LEU:N	2.22	0.54
1:C:89:MET:HG3	1:D:241:SER:O	2.07	0.54
1:A:346:LEU:HB2	1:A:376:SER:HB3	1.89	0.54
1:A:147:ARG:NH2	1:A:149:ASP:HB2	2.19	0.54
1:C:378:GLY:HA3	1:C:380:GLU:OE1	2.07	0.54
1:D:348:ASN:ND2	1:D:353:MET:SD	2.80	0.54
1:C:227:ASP:O	1:C:228:ASN:HB2	2.08	0.54
1:D:286:GLU:HB3	1:D:318:LYS:CG	2.36	0.54
1:B:22:ILE:HG21	1:C:344:GLU:HB3	1.88	0.54
1:C:206:HIS:HD2	1:C:222:ILE:HD11	1.73	0.54
1:A:355:HIS:O	1:A:359:PRO:HB2	2.08	0.53
1:A:165:LEU:HD21	1:A:306:MET:HE1	1.90	0.53
1:C:165:LEU:HD21	1:C:306:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:HG2	1:A:340:LEU:HD12	1.89	0.53
1:D:354:THR:O	1:D:354:THR:CG2	2.56	0.53
1:B:285:ILE:HD11	1:B:288:VAL:CG2	2.35	0.53
1:B:73:VAL:CG2	1:B:258:LEU:HD21	2.39	0.53
1:A:152:MET:HE1	1:A:154:TRP:HE3	1.73	0.53
1:B:193:LEU:O	1:B:306:MET:HA	2.08	0.53
1:B:317:LEU:HD12	1:B:324:ALA:HA	1.90	0.53
1:C:23:HIS:HA	1:C:26:GLN:HB2	1.91	0.53
1:D:271:ASN:HD21	1:D:382:LEU:HB2	1.73	0.52
1:B:18:ALA:HA	1:B:262:PRO:HG2	1.92	0.52
1:A:109:ASP:OD1	1:A:135:ASP:HA	2.09	0.52
1:B:281:THR:O	1:B:282:HIS:HB3	2.09	0.52
1:B:281:THR:O	1:B:282:HIS:CB	2.57	0.52
1:D:206:HIS:HB2	1:D:222:ILE:HG13	1.92	0.52
1:B:213:ASN:HD22	1:B:254:ALA:HA	1.75	0.52
1:C:157:THR:HA	1:C:158:PRO:C	2.30	0.52
1:D:372:LEU:C	1:D:372:LEU:HD12	2.29	0.52
1:C:242:ILE:HD12	1:C:242:ILE:O	2.10	0.52
1:A:324:ALA:O	1:A:327:PHE:HB3	2.09	0.52
1:A:142:PHE:HD2	1:A:171:ILE:HG22	1.71	0.52
1:C:299:HIS:O	1:C:302:ALA:HB3	2.09	0.52
1:A:24:GLY:O	1:A:26:GLN:HG2	2.10	0.52
1:C:146:ILE:HG21	1:C:178:HIS:CD2	2.44	0.52
1:B:256:ARG:HH22	1:C:213:ASN:HD21	1.57	0.52
1:D:211:TYR:CE1	1:D:341:GLY:HA2	2.45	0.52
1:C:109:ASP:HA	1:C:133:PHE:HB3	1.92	0.52
1:D:180:LEU:HD23	1:D:180:LEU:N	2.25	0.52
1:B:124:ARG:NH2	1:B:130:ASP:HA	2.25	0.52
1:A:91:ALA:O	1:A:95:VAL:CG1	2.58	0.51
1:C:336:LEU:HD11	1:C:353:MET:CE	2.40	0.51
1:A:299:HIS:O	1:A:302:ALA:HB3	2.09	0.51
1:A:320:GLY:HA2	1:A:371:ALA:HB2	1.92	0.51
1:A:208:ALA:HB3	1:A:218:MET:HE1	1.93	0.51
1:B:304:ARG:HG3	1:B:304:ARG:HH11	1.74	0.51
1:C:165:LEU:H	1:C:298:GLN:HE22	1.58	0.51
1:B:63:ASN:ND2	1:B:65:THR:H	2.09	0.51
1:A:23:HIS:HA	1:A:26:GLN:HB2	1.93	0.51
1:A:321:PHE:CD1	1:A:321:PHE:C	2.84	0.51
1:B:249:PHE:H	1:B:249:PHE:HD1	1.55	0.50
1:C:365:GLN:HG2	1:C:365:GLN:O	2.11	0.50
1:B:374:ARG:CG	1:B:374:ARG:HH11	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:C	1:A:372:LEU:HD12	2.31	0.50
1:C:186:ASN:HB2	1:C:204:VAL:HG13	1.93	0.50
1:A:107:ALA:O	1:A:133:PHE:HA	2.12	0.50
1:B:336:LEU:HD11	1:B:353:MET:HE3	1.94	0.50
1:C:161:PRO:HB3	1:C:374:ARG:HD3	1.94	0.49
1:A:104:HIS:CE1	1:A:132:SER:HG	2.30	0.49
1:A:285:ILE:HD11	1:A:288:VAL:HG23	1.93	0.49
1:D:290:TYR:CD1	1:D:313:VAL:HG22	2.46	0.49
1:D:350:PRO:O	1:D:354:THR:HB	2.13	0.49
1:D:242:ILE:CD1	1:D:244:GLY:H	2.06	0.49
1:C:114:GLY:HA2	1:C:117:ARG:NH2	2.27	0.49
1:D:382:LEU:HD23	1:D:383:GLY:N	2.28	0.49
1:C:97:GLU:OE2	1:D:126:THR:HG21	2.12	0.49
1:C:43:SER:HB2	1:D:209:THR:HG23	1.95	0.49
1:A:350:PRO:CA	1:A:354:THR:HG22	2.39	0.49
1:C:321:PHE:C	1:C:321:PHE:CD1	2.86	0.49
1:A:161:PRO:HB3	1:A:374:ARG:HD3	1.94	0.49
1:A:195:ARG:HG3	1:A:195:ARG:NH1	2.24	0.49
1:D:296:HIS:HD2	1:D:298:GLN:H	1.58	0.49
1:A:328:CYS:O	1:A:336:LEU:HD22	2.12	0.49
1:D:73:VAL:HG22	1:D:258:LEU:HD21	1.94	0.48
1:C:227:ASP:N	1:C:227:ASP:OD1	2.38	0.48
1:A:317:LEU:C	1:A:319:GLY:H	2.16	0.48
1:C:14:ALA:HB2	2:C:402:HOH:O	2.13	0.48
1:D:186:ASN:HB3	1:D:206:HIS:CE1	2.49	0.48
1:D:104:HIS:HB3	1:D:150:THR:HA	1.95	0.48
1:B:286:GLU:HB3	1:B:318:LYS:CG	2.43	0.48
1:A:213:ASN:HD21	1:D:256:ARG:NH2	2.12	0.48
1:B:348:ASN:ND2	1:B:353:MET:SD	2.86	0.48
1:B:290:TYR:CD1	1:B:313:VAL:HG22	2.48	0.48
1:B:364:GLU:HA	2:B:412:HOH:O	2.14	0.48
1:B:213:ASN:HB2	1:B:218:MET:HE1	1.95	0.48
1:A:340:LEU:HA	1:A:346:LEU:HD12	1.95	0.48
1:C:137:THR:O	1:C:139:PRO:HD3	2.13	0.48
1:B:273:LEU:CD1	1:B:277:GLN:HE21	2.27	0.48
1:D:184:VAL:HG21	1:D:196:PRO:HB3	1.95	0.48
1:D:190:SER:HB2	1:D:191:PRO:HD2	1.95	0.47
1:A:152:MET:CE	1:A:154:TRP:HE3	2.27	0.47
1:A:317:LEU:O	1:A:319:GLY:N	2.45	0.47
1:B:343:VAL:HG22	1:B:379:ILE:HG12	1.96	0.47
1:A:359:PRO:HA	1:A:363:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:THR:CA	1:C:158:PRO:O	2.63	0.47
1:C:157:THR:HA	1:C:158:PRO:O	2.14	0.47
1:A:45:TYR:HD1	1:C:33:GLY:HA3	1.80	0.47
1:D:282:HIS:HD2	1:D:284:ALA:HB3	1.80	0.47
1:A:31:SER:CB	1:A:32:THR:HG23	2.45	0.47
1:C:136:LEU:HD22	1:C:171:ILE:HD12	1.97	0.47
1:B:150:THR:HG22	1:B:180:LEU:HD22	1.96	0.47
1:A:146:ILE:HG21	1:A:178:HIS:HD2	1.79	0.47
1:B:340:LEU:HA	1:B:346:LEU:HD12	1.95	0.47
1:A:368:ILE:O	1:A:369:SER:O	2.32	0.47
1:D:146:ILE:O	1:D:147:ARG:HG3	2.14	0.47
1:B:120:GLU:OE2	1:B:124:ARG:HD2	2.15	0.47
1:B:334:PHE:CE1	1:B:389:LEU:HD21	2.50	0.47
1:B:22:ILE:CG2	1:C:344:GLU:HB3	2.44	0.47
1:A:215:HIS:O	1:A:217:ASP:N	2.48	0.47
1:A:222:ILE:HD11	1:A:224:VAL:HG23	1.97	0.47
1:A:85:PHE:CD2	1:A:91:ALA:HA	2.50	0.46
1:A:321:PHE:HA	1:A:370:ASP:O	2.15	0.46
1:C:282:HIS:HB3	1:C:285:ILE:HG23	1.97	0.46
1:B:162:MET:HE3	1:B:368:ILE:HA	1.97	0.46
1:A:80:THR:HG21	1:A:227:ASP:HB3	1.98	0.46
1:B:326:ARG:O	1:B:330:LYS:HB2	2.14	0.46
1:B:374:ARG:NH1	1:B:374:ARG:CG	2.64	0.46
1:D:233:GLU:CA	1:D:233:GLU:OE2	2.64	0.46
1:B:189:ALA:HA	1:B:193:LEU:HD12	1.98	0.46
1:A:238:LEU:O	1:A:242:ILE:HG13	2.15	0.46
1:A:360:VAL:O	1:A:361:ALA:C	2.54	0.46
1:A:222:ILE:CD1	1:A:224:VAL:HG23	2.46	0.46
1:A:368:ILE:C	1:A:369:SER:O	2.53	0.46
1:C:358:ILE:O	1:C:360:VAL:HG22	2.16	0.46
1:A:242:ILE:HD12	1:A:243:GLY:N	2.31	0.46
1:A:288:VAL:HG22	1:A:315:ILE:HG22	1.97	0.46
1:B:285:ILE:CD1	1:B:288:VAL:CG2	2.94	0.46
1:D:387:GLY:O	1:D:391:ARG:CZ	2.63	0.46
1:C:96:MET:HE3	1:C:105:VAL:HG21	1.96	0.46
1:D:189:ALA:HA	1:D:193:LEU:CD1	2.43	0.46
1:B:124:ARG:HH22	1:B:131:PHE:H	1.64	0.46
1:B:189:ALA:C	1:B:193:LEU:HD12	2.37	0.46
1:A:44:THR:CG2	1:B:339:SER:HB2	2.46	0.46
1:A:267:ALA:HB3	1:A:379:ILE:HG22	1.96	0.46
1:A:365:GLN:C	1:A:367:GLY:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLY:HA2	1:A:309:PHE:CD2	2.51	0.46
1:C:296:HIS:O	1:C:297:PRO:C	2.54	0.45
1:B:154:TRP:CZ3	1:B:183:VAL:HG11	2.51	0.45
1:B:365:GLN:HG2	1:B:368:ILE:CB	2.44	0.45
1:B:104:HIS:HD1	1:B:150:THR:HG1	1.61	0.45
1:B:249:PHE:CD1	1:B:249:PHE:N	2.70	0.45
1:C:150:THR:HG22	1:C:180:LEU:HD22	1.98	0.45
1:C:83:PHE:O	1:C:222:ILE:HA	2.16	0.45
1:C:222:ILE:HD12	1:C:222:ILE:C	2.36	0.45
1:B:146:ILE:O	1:B:147:ARG:HG3	2.17	0.45
1:B:217:ASP:OD2	1:C:256:ARG:NE	2.44	0.45
1:C:206:HIS:HB2	1:C:222:ILE:HG13	1.99	0.45
1:C:38:PRO:HG2	1:C:40:TYR:CE2	2.52	0.45
1:C:120:GLU:O	1:C:124:ARG:HB2	2.15	0.45
1:B:282:HIS:HA	1:B:283:PRO:HD2	1.66	0.45
1:B:206:HIS:HB2	1:B:222:ILE:HG13	1.99	0.45
1:D:326:ARG:O	1:D:330:LYS:HB2	2.17	0.45
1:D:228:ASN:HB2	1:D:231:LEU:HB3	1.98	0.44
1:B:365:GLN:HG2	1:B:368:ILE:H	1.81	0.44
1:D:343:VAL:HG22	1:D:379:ILE:CD1	2.47	0.44
1:A:222:ILE:CD1	1:A:224:VAL:CG2	2.95	0.44
1:C:321:PHE:HD2	1:C:370:ASP:HB2	1.81	0.44
1:D:238:LEU:O	1:D:242:ILE:HG13	2.18	0.44
1:B:69:TYR:O	1:B:73:VAL:HG23	2.17	0.44
1:B:286:GLU:CB	1:B:318:LYS:HG3	2.45	0.44
1:C:44:THR:OG1	1:D:339:SER:HB2	2.17	0.44
1:C:44:THR:HG21	1:D:339:SER:N	2.33	0.44
1:A:349:HIS:H	1:A:353:MET:HE1	1.82	0.44
1:C:282:HIS:CD2	1:C:284:ALA:HB3	2.53	0.44
1:A:213:ASN:HD22	1:A:254:ALA:HA	1.81	0.44
1:A:29:ASP:OD2	1:A:31:SER:O	2.35	0.44
1:A:62:HIS:HD2	1:A:67:PHE:CE2	2.36	0.44
1:C:261:LEU:HB3	1:C:262:PRO:HD3	1.99	0.44
1:B:315:ILE:HG13	1:B:373:VAL:HG22	2.00	0.44
1:C:320:GLY:HA2	1:C:371:ALA:CB	2.42	0.44
1:A:230:GLU:H	1:A:230:GLU:CD	2.21	0.44
1:A:348:ASN:HD21	1:A:354:THR:HB	1.83	0.43
1:D:304:ARG:HH11	1:D:304:ARG:CG	2.24	0.43
1:C:230:GLU:H	1:C:230:GLU:CD	2.21	0.43
1:C:343:VAL:HG22	1:C:379:ILE:CG1	2.39	0.43
1:B:63:ASN:HD22	1:B:64:PRO:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ASN:HB2	1:D:188:PHE:CE2	2.53	0.43
1:C:292:GLY:HA2	1:C:309:PHE:CD2	2.53	0.43
1:A:39:ILE:HD11	1:A:252:PHE:CD2	2.53	0.43
1:C:160:ASN:HB2	1:C:188:PHE:CE2	2.53	0.43
1:C:321:PHE:O	1:C:321:PHE:CD1	2.72	0.43
1:C:162:MET:O	1:C:163:LEU:HB2	2.17	0.43
1:D:62:HIS:CD2	1:D:67:PHE:HE2	2.37	0.43
1:C:98:LEU:HD13	1:C:238:LEU:CD1	2.49	0.43
1:B:152:MET:HE1	1:B:154:TRP:HE3	1.84	0.43
1:C:249:PHE:CB	1:D:249:PHE:CD1	3.01	0.43
1:C:266:ARG:HA	1:C:266:ARG:HD2	1.83	0.43
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.72	0.43
1:C:278:TRP:HZ2	1:C:390:GLU:HB2	1.82	0.43
1:A:134:VAL:HG11	1:A:145:ALA:HB2	2.01	0.43
1:C:190:SER:HB2	1:C:191:PRO:HD2	2.00	0.43
1:A:28:PRO:O	1:A:29:ASP:CB	2.67	0.43
1:C:23:HIS:C	1:C:26:GLN:HB2	2.38	0.43
1:A:120:GLU:OE2	1:A:124:ARG:HD2	2.19	0.43
1:C:114:GLY:HA2	1:C:117:ARG:CZ	2.49	0.43
1:D:282:HIS:CD2	1:D:284:ALA:HB3	2.53	0.43
1:C:209:THR:OG1	1:C:219:VAL:HA	2.19	0.43
1:A:374:ARG:CG	1:A:374:ARG:NH1	2.59	0.43
1:A:363:ARG:HA	1:A:363:ARG:HD3	1.83	0.43
1:C:195:ARG:NH1	1:C:195:ARG:HG3	2.31	0.43
1:C:358:ILE:H	1:C:358:ILE:HG13	1.49	0.43
1:C:288:VAL:HG22	1:C:315:ILE:HG22	2.01	0.43
1:D:63:ASN:ND2	1:D:65:THR:H	2.16	0.42
1:D:188:PHE:CD2	1:D:312:ILE:HD13	2.54	0.42
1:D:354:THR:HG22	1:D:354:THR:O	2.19	0.42
1:A:146:ILE:HG21	1:A:178:HIS:CD2	2.53	0.42
1:B:320:GLY:O	1:B:323:ALA:N	2.48	0.42
1:C:261:LEU:N	1:C:262:PRO:CD	2.82	0.42
1:D:293:LEU:HD23	1:D:293:LEU:HA	1.65	0.42
1:C:134:VAL:CG1	1:C:141:ALA:HB1	2.49	0.42
1:A:359:PRO:HA	1:A:363:ARG:CB	2.49	0.42
1:B:85:PHE:CE1	1:B:239:GLN:HG3	2.55	0.42
1:A:42:THR:HA	1:B:217:ASP:HA	2.01	0.42
1:D:374:ARG:CG	1:D:374:ARG:NH1	2.71	0.42
1:A:62:HIS:HB2	1:A:67:PHE:CZ	2.55	0.42
1:C:279:LEU:HD13	1:C:315:ILE:HG21	2.02	0.42
1:B:319:GLY:HA3	1:B:323:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLU:OE1	1:D:77:GLU:HA	2.20	0.42
1:A:97:GLU:HG2	1:A:123:ARG:NH2	2.35	0.42
1:C:160:ASN:HA	1:C:161:PRO:HA	1.83	0.42
1:A:31:SER:OG	1:A:32:THR:HG23	2.20	0.42
1:A:36:MET:H	1:C:42:THR:CG2	2.33	0.42
1:A:190:SER:OG	1:A:192:MET:HB2	2.20	0.42
1:C:240:ASN:HD22	1:D:117:ARG:HH22	1.68	0.42
1:C:287:LYS:CB	1:C:316:VAL:HG12	2.38	0.41
1:B:213:ASN:O	1:B:215:HIS:CD2	2.65	0.41
1:D:95:VAL:HG12	1:D:235:MET:CE	2.50	0.41
1:B:336:LEU:HD11	1:B:353:MET:HE1	2.03	0.41
1:C:327:PHE:C	1:C:329:GLU:H	2.24	0.41
1:A:63:ASN:HD21	1:A:248:PRO:HG3	1.83	0.41
1:A:31:SER:C	1:A:32:THR:HG23	2.41	0.41
1:B:186:ASN:HB3	1:B:206:HIS:CE1	2.54	0.41
1:A:217:ASP:CG	1:D:256:ARG:HE	2.23	0.41
1:A:190:SER:HB2	1:A:191:PRO:HD2	2.03	0.41
1:B:63:ASN:ND2	1:B:63:ASN:C	2.70	0.41
1:C:89:MET:HE1	1:C:112:TYR:HE2	1.85	0.41
1:B:124:ARG:NH2	1:B:131:PHE:H	2.19	0.41
1:A:349:HIS:H	1:A:353:MET:CE	2.34	0.41
1:D:70:GLU:O	1:D:82:ALA:HB3	2.21	0.41
1:A:37:PRO:HA	1:A:38:PRO:HD2	1.85	0.41
1:B:288:VAL:HG22	1:B:315:ILE:HG22	2.01	0.41
1:B:296:HIS:HA	1:B:297:PRO:HD2	1.80	0.41
1:B:210:LYS:HG2	1:B:340:LEU:CD1	2.50	0.41
1:C:165:LEU:H	1:C:298:GLN:NE2	2.18	0.41
1:D:160:ASN:HA	1:D:161:PRO:HA	1.89	0.41
1:D:146:ILE:CG2	1:D:147:ARG:N	2.83	0.41
1:A:225:VAL:CG2	1:A:226:GLY:N	2.84	0.41
1:C:104:HIS:CE1	1:C:132:SER:HG	2.38	0.41
1:C:190:SER:OG	1:C:192:MET:HB2	2.20	0.41
1:B:18:ALA:HA	1:B:262:PRO:CG	2.51	0.41
1:B:282:HIS:CD2	1:B:284:ALA:H	2.39	0.41
1:C:29:ASP:HA	1:C:30:PRO:HD2	1.91	0.41
1:C:124:ARG:CG	1:C:124:ARG:NH1	2.56	0.41
1:C:282:HIS:HB3	1:C:285:ILE:CG2	2.51	0.41
1:D:189:ALA:O	1:D:190:SER:O	2.39	0.41
1:B:83:PHE:N	1:B:83:PHE:CD1	2.89	0.41
1:D:285:ILE:CD1	1:D:288:VAL:CG2	2.99	0.41
1:A:171:ILE:H	1:A:171:ILE:HG12	1.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASN:O	1:C:229:ALA:C	2.59	0.40
1:D:104:HIS:CE1	1:D:132:SER:OG	2.74	0.40
1:C:113:GLY:O	1:C:116:PHE:HB3	2.20	0.40
1:B:303:LYS:HD3	2:B:406:HOH:O	2.20	0.40
1:A:317:LEU:HD13	1:A:324:ALA:HA	2.03	0.40
1:C:240:ASN:HD22	1:D:117:ARG:NH2	2.19	0.40
1:A:160:ASN:HB2	1:A:188:PHE:CZ	2.55	0.40
1:C:285:ILE:HD11	1:C:287:LYS:C	2.41	0.40
1:C:186:ASN:HB3	1:C:206:HIS:CE1	2.56	0.40
1:C:105:VAL:HB	1:C:131:PHE:CD1	2.56	0.40
1:A:99:LEU:O	1:B:125:ARG:NH1	2.54	0.40
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.93	0.40
1:B:256:ARG:HH22	1:C:213:ASN:ND2	2.18	0.40
1:D:63:ASN:C	1:D:63:ASN:ND2	2.75	0.40
1:D:138:ASP:OD1	1:D:140:ALA:HB3	2.20	0.40
1:C:312:ILE:HD11	1:C:340:LEU:HD13	2.02	0.40
1:C:372:LEU:HD23	1:C:372:LEU:C	2.42	0.40
1:D:385:LEU:HA	1:D:385:LEU:HD23	1.90	0.40
1:D:173:VAL:HA	1:D:176:ARG:NH2	2.36	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	364/400 (91%)	308 (85%)	41 (11%)	15 (4%)	3	11
1	B	330/400 (82%)	298 (90%)	24 (7%)	8 (2%)	7	25
1	C	364/400 (91%)	307 (84%)	47 (13%)	10 (3%)	6	21
1	D	329/400 (82%)	284 (86%)	37 (11%)	8 (2%)	7	25
All	All	1387/1600 (87%)	1197 (86%)	149 (11%)	41 (3%)	5	18

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	358	ILE
1	A	369	SER
1	B	190	SER
1	B	321	PHE
1	B	352	VAL
1	B	354	THR
1	C	27	SER
1	C	228	ASN
1	D	79	GLY
1	A	216	SER
1	A	318	LYS
1	A	359	PRO
1	C	32	THR
1	C	167	ASP
1	D	190	SER
1	D	226	GLY
1	A	119	PHE
1	A	366	LEU
1	C	113	GLY
1	C	120	GLU
1	C	328	CYS
1	C	359	PRO
1	D	21	ALA
1	D	321	PHE
1	A	29	ASP
1	A	135	ASP
1	A	295	SER
1	B	21	ALA
1	B	282	HIS
1	C	358	ILE
1	D	365	GLN
1	A	120	GLU
1	A	297	PRO
1	A	328	CYS
1	C	391	ARG
1	D	62	HIS
1	B	297	PRO
1	D	367	GLY
1	A	27	SER
1	B	226	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	287/315 (91%)	247 (86%)	40 (14%)	4 13
1	B	261/315 (83%)	219 (84%)	42 (16%)	3 9
1	C	287/315 (91%)	246 (86%)	41 (14%)	4 12
1	D	261/315 (83%)	220 (84%)	41 (16%)	3 9
All	All	1096/1260 (87%)	932 (85%)	164 (15%)	3 11

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	44	THR
1	A	48	SER
1	A	62	HIS
1	A	93	SER
1	A	95	VAL
1	A	98	LEU
1	A	117	ARG
1	A	129	LEU
1	A	132	SER
1	A	143	LYS
1	A	147	ARG
1	A	153	VAL
1	A	163	LEU
1	A	166	VAL
1	A	171	ILE
1	A	177	LYS
1	A	178	HIS
1	A	182	THR
1	A	203	LEU
1	A	210	LYS
1	A	218	MET
1	A	225	VAL
1	A	233	GLU

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Mol	Chain	Res	Type
1	A	245	VAL
1	A	253	LEU
1	A	278	TRP
1	A	285	ILE
1	A	303	LYS
1	A	307	SER
1	A	336	LEU
1	A	339	SER
1	A	343	VAL
1	A	360	VAL
1	A	362	ARG
1	A	363	ARG
1	A	365	GLN
1	A	372	LEU
1	A	374	ARG
1	A	386	ARG
1	B	63	ASN
1	B	96	MET
1	B	98	LEU
1	B	117	ARG
1	B	124	ARG
1	B	126	THR
1	B	137	THR
1	B	138	ASP
1	B	151	LYS
1	B	153	VAL
1	B	163	LEU
1	B	182	THR
1	B	192	MET
1	B	193	LEU
1	B	194	GLN
1	B	210	LYS
1	B	218	MET
1	B	225	VAL
1	B	230	GLU
1	B	241	SER
1	B	245	VAL
1	B	249	PHE
1	B	253	LEU
1	B	258	LEU
1	B	285	ILE
1	B	286	GLU

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Mol	Chain	Res	Type
1	B	303	LYS
1	B	304	ARG
1	B	307	SER
1	B	316	VAL
1	B	322	ASP
1	B	339	SER
1	B	343	VAL
1	B	344	GLU
1	B	354	THR
1	B	364	GLU
1	B	365	GLN
1	B	366	LEU
1	B	372	LEU
1	B	373	VAL
1	B	374	ARG
1	B	386	ARG
1	C	16	SER
1	C	27	SER
1	C	42	THR
1	C	44	THR
1	C	61	THR
1	C	89	MET
1	C	93	SER
1	C	98	LEU
1	C	109	ASP
1	C	115	THR
1	C	117	ARG
1	C	124	ARG
1	C	132	SER
1	C	153	VAL
1	C	163	LEU
1	C	166	VAL
1	C	178	HIS
1	C	182	THR
1	C	192	MET
1	C	207	SER
1	C	218	MET
1	C	233	GLU
1	C	242	ILE
1	C	246	GLN
1	C	253	LEU
1	C	280	GLU

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Mol	Chain	Res	Type
1	C	285	ILE
1	C	301	LEU
1	C	339	SER
1	C	343	VAL
1	C	344	GLU
1	C	354	THR
1	C	358	ILE
1	C	360	VAL
1	C	363	ARG
1	C	364	GLU
1	C	365	GLN
1	C	369	SER
1	C	370	ASP
1	C	374	ARG
1	C	386	ARG
1	D	61	THR
1	D	63	ASN
1	D	98	LEU
1	D	115	THR
1	D	132	SER
1	D	137	THR
1	D	151	LYS
1	D	163	LEU
1	D	166	VAL
1	D	173	VAL
1	D	180	LEU
1	D	182	THR
1	D	192	MET
1	D	193	LEU
1	D	194	GLN
1	D	210	LYS
1	D	218	MET
1	D	225	VAL
1	D	227	ASP
1	D	228	ASN
1	D	230	GLU
1	D	233	GLU
1	D	241	SER
1	D	246	GLN
1	D	253	LEU
1	D	258	LEU
1	D	285	ILE

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Mol	Chain	Res	Type
1	D	286	GLU
1	D	287	LYS
1	D	304	ARG
1	D	316	VAL
1	D	326	ARG
1	D	339	SER
1	D	343	VAL
1	D	344	GLU
1	D	354	THR
1	D	363	ARG
1	D	372	LEU
1	D	374	ARG
1	D	382	LEU
1	D	389	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	62	HIS
1	A	213	ASN
1	A	215	HIS
1	A	271	ASN
1	A	282	HIS
1	A	296	HIS
1	A	298	GLN
1	A	348	ASN
1	B	63	ASN
1	B	178	HIS
1	B	206	HIS
1	B	213	ASN
1	B	215	HIS
1	B	271	ASN
1	B	277	GLN
1	B	282	HIS
1	B	296	HIS
1	B	348	ASN
1	C	26	GLN
1	C	213	ASN
1	C	215	HIS
1	C	240	ASN
1	C	271	ASN

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Mol	Chain	Res	Type
1	C	282	HIS
1	C	296	HIS
1	C	298	GLN
1	D	62	HIS
1	D	63	ASN
1	D	213	ASN
1	D	215	HIS
1	D	228	ASN
1	D	240	ASN
1	D	271	ASN
1	D	282	HIS
1	D	296	HIS
1	D	348	ASN

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

There are no ligands in this entry.

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	368/400 (92%)	0.11	9 (2%) 62 50	29, 51, 81, 90	0
1	B	336/400 (84%)	-0.10	0 100 100	27, 50, 72, 86	0
1	C	368/400 (92%)	0.07	7 (1%) 70 59	30, 51, 82, 88	0
1	D	335/400 (83%)	-0.10	2 (0%) 90 86	26, 49, 73, 97	0
All	All	1407/1600 (87%)	-0.00	18 (1%) 79 71	26, 50, 77, 97	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	ILE	3.6
1	C	358	ILE	3.4
1	C	46	ALA	3.2
1	A	354	THR	3.0
1	C	119	PHE	2.8
1	C	131	PHE	2.7
1	A	46	ALA	2.7
1	A	40	TYR	2.7
1	A	41	ALA	2.7
1	A	48	SER	2.4
1	D	354	THR	2.4
1	A	119	PHE	2.4
1	C	30	PRO	2.4
1	C	326	ARG	2.3
1	A	357	SER	2.2
1	C	354	THR	2.2
1	D	139	PRO	2.1
1	A	30	PRO	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.