Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:37 PM GMT

PDB ID	:	1PW4
Title	:	Crystal Structure of the Glycerol-3-Phosphate Transporter from E.Coli
Authors	:	Huang, Y.; Lemieux, M.J.; Song, J.; Auer, M.; Wang, D.N.
Deposited on	:	2003-06-30
Resolution	:	3.30 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:

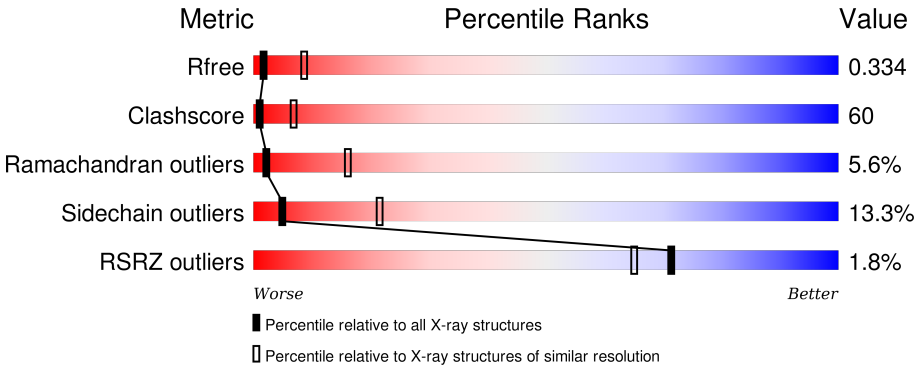
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	451	2% 31% 50% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3403 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 Glycerol-3-phosphate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3403	2275	546	554	28			

There are 5 discrepancies between the modelled and reference sequences:

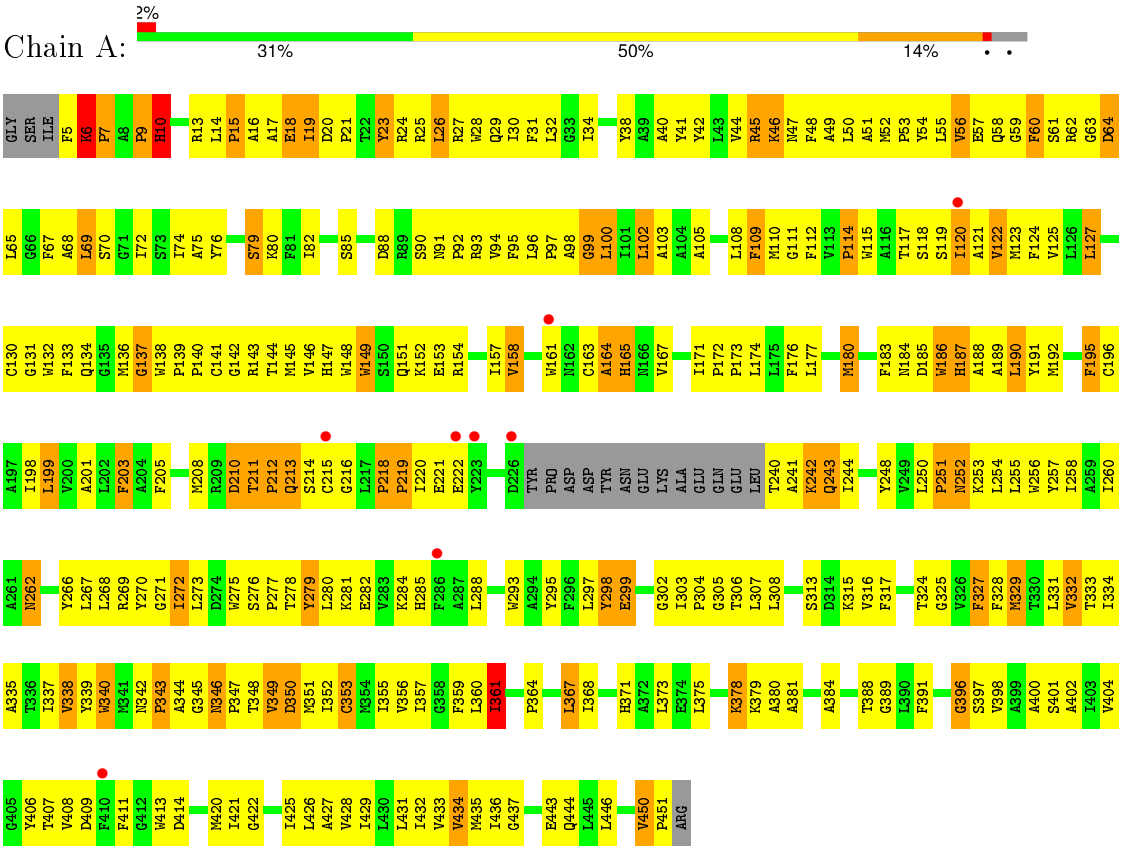
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	CLONING ARTIFACT	UNP P08194
A	449	LEU	-	CLONING ARTIFACT	UNP P08194
A	450	VAL	-	CLONING ARTIFACT	UNP P08194
A	451	PRO	-	CLONING ARTIFACT	UNP P08194
A	452	ARG	-	CLONING ARTIFACT	UNP P08194

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: Glycerol-3-phosphate transporter

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.64Å 97.64Å 175.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.30 14.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (15.00-3.30) 95.4 (14.98-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.296 , 0.325 0.306 , 0.334	Depositor DCC
R_{free} test set	720 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	86.1	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 102.3	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 14843 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	3403	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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	0.58	2/3515 (0.1%)	0.95	19/4781 (0.4%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ALA	C-N	15.29	1.69	1.34
1	A	165	HIS	C-N	-8.11	1.15	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	ARG	C-N-CA	-13.96	86.80	121.70
1	A	164	ALA	C-N-CA	-9.02	99.16	121.70
1	A	57	GLU	N-CA-C	-8.89	87.00	111.00
1	A	63	GLY	N-CA-C	-8.39	92.13	113.10
1	A	165	HIS	O-C-N	-7.87	110.11	122.70
1	A	122	VAL	N-CA-C	-7.73	90.14	111.00
1	A	6	LYS	C-N-CD	-7.28	104.58	120.60
1	A	450	VAL	N-CA-C	6.53	128.62	111.00
1	A	46	LYS	CB-CA-C	6.50	123.39	110.40
1	A	282	GLU	N-CA-C	-5.86	95.19	111.00
1	A	361	ILE	CB-CA-C	-5.80	100.01	111.60
1	A	45	ARG	CA-C-N	5.62	129.56	117.20
1	A	250	LEU	C-N-CD	5.59	140.15	128.40
1	A	218	PRO	N-CA-C	-5.38	98.10	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	GLN	N-CA-C	5.37	125.49	111.00
1	A	165	HIS	CA-C-N	5.30	128.86	117.20
1	A	199	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	6	LYS	C-N-CA	5.22	143.93	122.00
1	A	45	ARG	O-C-N	-5.19	114.39	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	HIS	Mainchain
1	A	298	TYR	Sidechain
1	A	99	GLY	Mainchain

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	3403	0	3421	406	0
All	All	3403	0	3421	406	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 60.

All (406) 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:164:ALA:C	1:A:165:HIS:N	1.69	1.46
1:A:373:LEU:HD23	1:A:381:ALA:HB1	1.34	1.10
1:A:350:ASP:HA	1:A:353:CYS:HB3	1.38	1.04
1:A:7:PRO:HG3	1:A:90:SER:HA	1.38	1.00
1:A:281:LYS:HA	1:A:285:HIS:HB3	1.45	0.98
1:A:55:LEU:HD22	1:A:56:VAL:HG13	1.47	0.96
1:A:157:ILE:HG22	1:A:161:TRP:CD1	2.02	0.93
1:A:55:LEU:O	1:A:56:VAL:HG22	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:HG2	1:A:15:PRO:HD3	1.52	0.90
1:A:157:ILE:HG22	1:A:161:TRP:NE1	1.87	0.90
1:A:164:ALA:C	1:A:165:HIS:CA	2.39	0.89
1:A:255:LEU:HD12	1:A:258:ILE:HD11	1.55	0.89
1:A:55:LEU:HD22	1:A:56:VAL:CG1	2.02	0.89
1:A:145:MET:SD	1:A:157:ILE:HD13	2.12	0.89
1:A:56:VAL:HG12	1:A:60:PHE:HB3	1.55	0.89
1:A:186:TRP:HD1	1:A:187:HIS:H	1.20	0.88
1:A:275:TRP:HZ3	1:A:400:ALA:O	1.56	0.88
1:A:67:PHE:O	1:A:70:SER:HB3	1.75	0.87
1:A:275:TRP:CZ3	1:A:400:ALA:O	2.28	0.87
1:A:351:MET:O	1:A:355:ILE:HG13	1.74	0.86
1:A:157:ILE:CG2	1:A:161:TRP:NE1	2.39	0.86
1:A:267:LEU:HD13	1:A:400:ALA:HA	1.57	0.86
1:A:62:ARG:HE	1:A:64:ASP:HB2	1.40	0.86
1:A:303:ILE:HB	1:A:304:PRO:HD3	1.58	0.85
1:A:45:ARG:C	1:A:46:LYS:HG2	1.98	0.84
1:A:302:GLY:O	1:A:306:THR:HG22	1.77	0.84
1:A:44:VAL:HA	1:A:47:ASN:HD21	1.39	0.84
1:A:353:CYS:O	1:A:357:ILE:HG12	1.76	0.83
1:A:157:ILE:CG2	1:A:161:TRP:HE1	1.91	0.83
1:A:54:TYR:OH	1:A:288:LEU:HD21	1.79	0.81
1:A:281:LYS:HA	1:A:285:HIS:CB	2.10	0.81
1:A:17:ALA:O	1:A:18:GLU:HB2	1.81	0.80
1:A:154:ARG:O	1:A:158:VAL:HG23	1.82	0.80
1:A:56:VAL:HG11	1:A:65:LEU:HD11	1.64	0.79
1:A:53:PRO:HB3	1:A:278:THR:HA	1.65	0.79
1:A:102:LEU:HD22	1:A:133:PHE:CE1	2.17	0.78
1:A:149:TRP:CD2	1:A:152:LYS:HG3	2.19	0.78
1:A:313:SER:HB2	1:A:324:THR:HG21	1.64	0.78
1:A:198:ILE:HD12	1:A:199:LEU:N	1.99	0.78
1:A:7:PRO:HG3	1:A:90:SER:CA	2.11	0.78
1:A:20:ASP:HB2	1:A:21:PRO:HD3	1.64	0.77
1:A:69:LEU:HD23	1:A:72:ILE:HD13	1.66	0.77
1:A:269:ARG:HG3	1:A:361:ILE:HD12	1.67	0.77
1:A:56:VAL:HG11	1:A:61:SER:HB3	1.67	0.76
1:A:373:LEU:CD2	1:A:381:ALA:HB1	2.14	0.76
1:A:340:TRP:HH2	1:A:414:ASP:OD2	1.67	0.76
1:A:272:ILE:HG13	1:A:420:MET:CE	2.17	0.74
1:A:334:ILE:O	1:A:338:VAL:HG12	1.88	0.74
1:A:41:TYR:HB3	1:A:134:GLN:HE21	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HB3	1:A:97:PRO:HD3	1.70	0.74
1:A:328:PHE:O	1:A:332:VAL:HG13	1.87	0.74
1:A:165:HIS:ND1	1:A:165:HIS:O	2.20	0.73
1:A:339:TYR:CD2	1:A:353:CYS:HB2	2.24	0.73
1:A:163:CYS:O	1:A:167:VAL:HG23	1.88	0.73
1:A:7:PRO:CG	1:A:90:SER:HA	2.15	0.73
1:A:171:ILE:O	1:A:174:LEU:HB2	1.89	0.72
1:A:349:VAL:O	1:A:352:ILE:HG22	1.90	0.72
1:A:6:LYS:HD2	1:A:6:LYS:N	2.04	0.72
1:A:119:SER:HB3	1:A:122:VAL:HB	1.71	0.71
1:A:350:ASP:CA	1:A:353:CYS:HB3	2.19	0.70
1:A:123:MET:O	1:A:127:LEU:HB2	1.91	0.70
1:A:165:HIS:CE1	1:A:299:GLU:OE2	2.44	0.70
1:A:145:MET:SD	1:A:157:ILE:CD1	2.80	0.70
1:A:267:LEU:HD12	1:A:267:LEU:O	1.91	0.70
1:A:157:ILE:HG21	1:A:161:TRP:HE1	1.54	0.69
1:A:284:LYS:HE2	1:A:342:ASN:HB3	1.74	0.69
1:A:13:ARG:HG2	1:A:15:PRO:CD	2.22	0.69
1:A:422:GLY:HA2	1:A:425:ILE:HD12	1.73	0.69
1:A:337:ILE:HG22	1:A:421:ILE:HD13	1.74	0.69
1:A:240:THR:HG22	1:A:241:ALA:H	1.57	0.69
1:A:56:VAL:HG12	1:A:60:PHE:CB	2.22	0.69
1:A:262:ASN:ND2	1:A:368:ILE:HD12	2.07	0.69
1:A:339:TYR:CE1	1:A:353:CYS:HA	2.28	0.68
1:A:346:ASN:HD21	1:A:350:ASP:CG	1.96	0.68
1:A:267:LEU:CD1	1:A:400:ALA:HA	2.24	0.68
1:A:40:ALA:CB	1:A:100:LEU:HD11	2.23	0.68
1:A:220:ILE:O	1:A:222:GLU:N	2.27	0.68
1:A:298:TYR:CZ	1:A:361:ILE:HD11	2.29	0.68
1:A:269:ARG:HB2	1:A:361:ILE:HG21	1.76	0.68
1:A:279:TYR:HD1	1:A:413:TRP:NE1	1.93	0.67
1:A:49:ALA:HA	1:A:52:MET:CE	2.25	0.67
1:A:255:LEU:O	1:A:258:ILE:HG13	1.95	0.66
1:A:337:ILE:O	1:A:340:TRP:HB3	1.95	0.66
1:A:255:LEU:HD21	1:A:384:ALA:HB1	1.76	0.66
1:A:41:TYR:HB3	1:A:134:GLN:NE2	2.11	0.66
1:A:149:TRP:CE2	1:A:152:LYS:HG3	2.31	0.65
1:A:284:LYS:HD3	1:A:346:ASN:ND2	2.12	0.65
1:A:103:ALA:HB2	1:A:133:PHE:HB3	1.79	0.65
1:A:50:LEU:HD11	1:A:173:PRO:HA	1.79	0.65
1:A:72:ILE:HD12	1:A:72:ILE:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD22	1:A:298:TYR:CE2	2.33	0.64
1:A:350:ASP:HA	1:A:353:CYS:CB	2.23	0.64
1:A:98:ALA:O	1:A:102:LEU:HB2	1.97	0.64
1:A:258:ILE:HD11	1:A:375:LEU:HD12	1.79	0.64
1:A:210:ASP:HB2	1:A:212:PRO:HD2	1.78	0.64
1:A:40:ALA:HB3	1:A:100:LEU:HD11	1.79	0.64
1:A:138:TRP:O	1:A:141:CYS:HB3	1.98	0.64
1:A:95:PHE:CE2	1:A:136:MET:HB2	2.33	0.63
1:A:272:ILE:HG13	1:A:420:MET:HE3	1.81	0.63
1:A:340:TRP:CE3	1:A:340:TRP:O	2.52	0.63
1:A:364:PRO:O	1:A:368:ILE:HG13	1.97	0.63
1:A:346:ASN:N	1:A:347:PRO:CD	2.61	0.63
1:A:273:LEU:HD22	1:A:298:TYR:HE2	1.64	0.62
1:A:49:ALA:HA	1:A:52:MET:HE3	1.81	0.62
1:A:64:ASP:HA	1:A:406:TYR:CE1	2.35	0.62
1:A:64:ASP:HA	1:A:406:TYR:HE1	1.63	0.62
1:A:52:MET:O	1:A:56:VAL:HG22	1.98	0.62
1:A:44:VAL:HA	1:A:47:ASN:ND2	2.13	0.62
1:A:53:PRO:HB3	1:A:278:THR:CA	2.30	0.62
1:A:60:PHE:CZ	1:A:118:SER:HB3	2.35	0.62
1:A:52:MET:HG2	1:A:65:LEU:HD13	1.81	0.62
1:A:211:THR:N	1:A:212:PRO:CD	2.63	0.62
1:A:191:TYR:CD2	1:A:192:MET:N	2.68	0.62
1:A:195:PHE:O	1:A:198:ILE:HG13	2.00	0.61
1:A:55:LEU:HD23	1:A:56:VAL:H	1.64	0.61
1:A:212:PRO:HG2	1:A:213:GLN:H	1.65	0.61
1:A:103:ALA:HB2	1:A:133:PHE:CB	2.29	0.61
1:A:102:LEU:HD13	1:A:133:PHE:CE2	2.35	0.61
1:A:45:ARG:O	1:A:46:LYS:HG2	2.00	0.61
1:A:103:ALA:HA	1:A:133:PHE:HD1	1.64	0.61
1:A:281:LYS:O	1:A:281:LYS:HG2	2.01	0.61
1:A:408:VAL:HG11	1:A:413:TRP:HE3	1.66	0.61
1:A:298:TYR:OH	1:A:361:ILE:HD11	2.01	0.61
1:A:281:LYS:CA	1:A:285:HIS:HB3	2.27	0.61
1:A:15:PRO:O	1:A:19:ILE:HG12	2.01	0.60
1:A:99:GLY:HA2	1:A:136:MET:SD	2.41	0.60
1:A:408:VAL:HG11	1:A:413:TRP:CE3	2.36	0.60
1:A:220:ILE:C	1:A:222:GLU:H	2.03	0.60
1:A:9:PRO:HG2	1:A:10:HIS:H	1.66	0.60
1:A:298:TYR:OH	1:A:361:ILE:CD1	2.50	0.60
1:A:55:LEU:HD23	1:A:56:VAL:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG22	1:A:205:PHE:HE1	1.64	0.60
1:A:275:TRP:HD1	1:A:278:THR:HG21	1.67	0.59
1:A:99:GLY:CA	1:A:136:MET:SD	2.90	0.59
1:A:198:ILE:HD11	1:A:199:LEU:HD23	1.84	0.59
1:A:407:THR:O	1:A:407:THR:HG22	2.03	0.59
1:A:279:TYR:CD1	1:A:413:TRP:NE1	2.71	0.58
1:A:327:PHE:C	1:A:327:PHE:CD1	2.76	0.58
1:A:82:ILE:HD11	1:A:132:TRP:CZ2	2.38	0.58
1:A:211:THR:N	1:A:212:PRO:HD2	2.18	0.58
1:A:210:ASP:C	1:A:212:PRO:CD	2.72	0.58
1:A:396:GLY:O	1:A:400:ALA:HB2	2.04	0.58
1:A:272:ILE:HG13	1:A:420:MET:HE1	1.86	0.58
1:A:10:HIS:ND1	1:A:10:HIS:O	2.36	0.58
1:A:275:TRP:CH2	1:A:401:SER:HA	2.39	0.58
1:A:384:ALA:O	1:A:388:THR:HG23	2.04	0.58
1:A:108:LEU:HD21	1:A:195:PHE:HD1	1.68	0.58
1:A:198:ILE:CD1	1:A:199:LEU:HD23	2.34	0.58
1:A:165:HIS:HD1	1:A:165:HIS:C	2.07	0.57
1:A:56:VAL:CG1	1:A:65:LEU:HD11	2.33	0.57
1:A:339:TYR:CG	1:A:353:CYS:HB2	2.40	0.57
1:A:340:TRP:CH2	1:A:414:ASP:HA	2.39	0.57
1:A:271:GLY:O	1:A:275:TRP:HE3	1.87	0.57
1:A:97:PRO:HG2	1:A:205:PHE:HB2	1.86	0.57
1:A:157:ILE:O	1:A:158:VAL:C	2.42	0.57
1:A:109:PHE:HD2	1:A:109:PHE:O	1.86	0.57
1:A:258:ILE:CD1	1:A:375:LEU:HD12	2.35	0.57
1:A:450:VAL:O	1:A:451:PRO:C	2.42	0.57
1:A:191:TYR:HD2	1:A:192:MET:N	2.03	0.57
1:A:180:MET:HA	1:A:180:MET:CE	2.35	0.57
1:A:45:ARG:O	1:A:46:LYS:CG	2.53	0.56
1:A:171:ILE:N	1:A:172:PRO:HD2	2.20	0.56
1:A:203:PHE:C	1:A:203:PHE:CD2	2.78	0.56
1:A:335:ALA:O	1:A:338:VAL:HG13	2.05	0.56
1:A:42:TYR:HE2	1:A:45:ARG:CZ	2.17	0.56
1:A:56:VAL:HG23	1:A:56:VAL:O	2.06	0.56
1:A:102:LEU:HD22	1:A:133:PHE:CZ	2.39	0.56
1:A:210:ASP:C	1:A:212:PRO:HD3	2.26	0.56
1:A:255:LEU:HD13	1:A:375:LEU:HB2	1.87	0.55
1:A:122:VAL:CG1	1:A:123:MET:N	2.69	0.55
1:A:186:TRP:HD1	1:A:187:HIS:N	1.98	0.55
1:A:428:VAL:O	1:A:432:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ILE:HG13	1:A:338:VAL:N	2.22	0.55
1:A:262:ASN:CG	1:A:368:ILE:HD12	2.27	0.55
1:A:212:PRO:CG	1:A:213:GLN:H	2.20	0.55
1:A:429:ILE:O	1:A:432:ILE:HB	2.08	0.54
1:A:14:LEU:N	1:A:15:PRO:HD3	2.22	0.54
1:A:108:LEU:HD21	1:A:195:PHE:CD1	2.43	0.54
1:A:244:ILE:CD1	1:A:379:LYS:HD3	2.37	0.54
1:A:70:SER:O	1:A:74:ILE:HG13	2.07	0.54
1:A:325:GLY:O	1:A:329:MET:N	2.26	0.54
1:A:72:ILE:HD11	1:A:127:LEU:HG	1.88	0.54
1:A:50:LEU:O	1:A:53:PRO:HD2	2.08	0.54
1:A:218:PRO:O	1:A:220:ILE:N	2.41	0.54
1:A:14:LEU:O	1:A:15:PRO:C	2.46	0.54
1:A:183:PHE:HB3	1:A:191:TYR:HH	1.72	0.54
1:A:346:ASN:N	1:A:347:PRO:HD3	2.23	0.54
1:A:343:PRO:C	1:A:345:GLY:H	2.11	0.54
1:A:211:THR:HG22	1:A:211:THR:O	2.08	0.54
1:A:186:TRP:CD1	1:A:187:HIS:N	2.74	0.54
1:A:436:ILE:CG2	1:A:437:GLY:N	2.71	0.54
1:A:305:GLY:O	1:A:308:LEU:N	2.41	0.54
1:A:27:ARG:NH2	1:A:149:TRP:CE2	2.76	0.53
1:A:119:SER:HB3	1:A:122:VAL:CB	2.39	0.53
1:A:121:ALA:HA	1:A:124:PHE:H	1.73	0.53
1:A:13:ARG:HG3	1:A:216:GLY:HA3	1.90	0.53
1:A:111:GLY:HA2	1:A:190:LEU:HD21	1.90	0.53
1:A:183:PHE:O	1:A:185:ASP:N	2.40	0.53
1:A:275:TRP:CH2	1:A:401:SER:O	2.62	0.53
1:A:183:PHE:HB3	1:A:191:TYR:OH	2.08	0.53
1:A:93:ARG:HA	1:A:208:MET:HE2	1.89	0.53
1:A:58:GLN:O	1:A:60:PHE:N	2.42	0.53
1:A:41:TYR:OH	1:A:137:GLY:HA2	2.09	0.53
1:A:339:TYR:CE2	1:A:353:CYS:HB2	2.44	0.53
1:A:62:ARG:HB2	1:A:64:ASP:HB3	1.90	0.53
1:A:76:TYR:O	1:A:79:SER:HB3	2.09	0.53
1:A:240:THR:HG22	1:A:241:ALA:N	2.23	0.53
1:A:55:LEU:O	1:A:56:VAL:CG2	2.51	0.52
1:A:56:VAL:HB	1:A:61:SER:H	1.74	0.52
1:A:275:TRP:HH2	1:A:401:SER:O	1.92	0.52
1:A:40:ALA:HB1	1:A:100:LEU:HD11	1.91	0.52
1:A:275:TRP:HD1	1:A:278:THR:CG2	2.23	0.52
1:A:275:TRP:CD1	1:A:278:THR:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:SER:HB3	1:A:122:VAL:CG1	2.40	0.52
1:A:50:LEU:HD11	1:A:173:PRO:CA	2.39	0.52
1:A:327:PHE:HE1	1:A:331:LEU:HD12	1.75	0.52
1:A:45:ARG:CB	1:A:46:LYS:HG2	2.40	0.52
1:A:345:GLY:C	1:A:347:PRO:HD2	2.30	0.52
1:A:212:PRO:O	1:A:216:GLY:N	2.42	0.52
1:A:380:ALA:O	1:A:384:ALA:N	2.42	0.52
1:A:55:LEU:HD22	1:A:56:VAL:HG12	1.88	0.52
1:A:127:LEU:O	1:A:130:CYS:HB3	2.10	0.52
1:A:82:ILE:HD11	1:A:132:TRP:HZ2	1.75	0.52
1:A:198:ILE:O	1:A:201:ALA:HB3	2.10	0.51
1:A:348:THR:HG22	1:A:348:THR:O	2.10	0.51
1:A:56:VAL:HG21	1:A:61:SER:HB3	1.91	0.51
1:A:41:TYR:CE2	1:A:137:GLY:HA3	2.45	0.51
1:A:280:LEU:O	1:A:281:LYS:HB3	2.11	0.51
1:A:23:TYR:HE2	1:A:211:THR:CG2	2.24	0.51
1:A:324:THR:HB	1:A:367:LEU:HD21	1.93	0.51
1:A:99:GLY:HA3	1:A:136:MET:SD	2.51	0.51
1:A:157:ILE:HG22	1:A:161:TRP:HE1	1.59	0.51
1:A:105:ALA:O	1:A:108:LEU:HB2	2.11	0.51
1:A:10:HIS:CG	1:A:10:HIS:O	2.64	0.51
1:A:327:PHE:CE1	1:A:331:LEU:HD12	2.45	0.51
1:A:352:ILE:O	1:A:356:VAL:HG23	2.11	0.51
1:A:52:MET:O	1:A:55:LEU:O	2.28	0.51
1:A:327:PHE:C	1:A:327:PHE:HD1	2.13	0.51
1:A:315:LYS:HD2	1:A:315:LYS:O	2.11	0.51
1:A:335:ALA:O	1:A:339:TYR:CD1	2.64	0.50
1:A:18:GLU:C	1:A:21:PRO:HD2	2.32	0.50
1:A:48:PHE:O	1:A:51:ALA:HB3	2.12	0.50
1:A:55:LEU:CD2	1:A:56:VAL:HG13	2.29	0.50
1:A:213:GLN:OE1	1:A:214:SER:HB2	2.11	0.50
1:A:251:PRO:O	1:A:256:TRP:CD1	2.65	0.50
1:A:94:VAL:O	1:A:97:PRO:HD2	2.11	0.50
1:A:325:GLY:O	1:A:329:MET:HB2	2.11	0.50
1:A:13:ARG:HG2	1:A:15:PRO:CG	2.41	0.50
1:A:429:ILE:O	1:A:433:VAL:HG23	2.11	0.50
1:A:257:TYR:HA	1:A:260:ILE:HG22	1.93	0.50
1:A:218:PRO:O	1:A:219:PRO:C	2.49	0.50
1:A:6:LYS:HD2	1:A:6:LYS:H	1.77	0.50
1:A:242:LYS:O	1:A:243:GLN:C	2.50	0.50
1:A:317:PHE:CE1	1:A:324:THR:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HG21	1:A:161:TRP:NE1	2.21	0.49
1:A:212:PRO:HG2	1:A:213:GLN:N	2.27	0.49
1:A:91:ASN:OD1	1:A:210:ASP:OD2	2.30	0.49
1:A:62:ARG:HE	1:A:64:ASP:CB	2.16	0.49
1:A:38:TYR:CE1	1:A:138:TRP:HB2	2.48	0.49
1:A:252:ASN:O	1:A:254:LEU:N	2.46	0.49
1:A:275:TRP:HA	1:A:278:THR:CG2	2.42	0.49
1:A:277:PRO:HG2	1:A:278:THR:H	1.78	0.49
1:A:339:TYR:HE2	1:A:349:VAL:HG12	1.78	0.49
1:A:431:LEU:O	1:A:434:VAL:HG23	2.12	0.49
1:A:284:LYS:HD3	1:A:346:ASN:CB	2.43	0.49
1:A:324:THR:HB	1:A:367:LEU:CD2	2.42	0.49
1:A:13:ARG:C	1:A:15:PRO:HD3	2.33	0.48
1:A:144:THR:O	1:A:147:HIS:N	2.41	0.48
1:A:120:ILE:O	1:A:121:ALA:HB3	2.13	0.48
1:A:51:ALA:O	1:A:55:LEU:N	2.41	0.48
1:A:443:GLU:O	1:A:446:LEU:HB2	2.13	0.48
1:A:211:THR:HA	1:A:213:GLN:HE21	1.78	0.48
1:A:27:ARG:NH2	1:A:149:TRP:NE1	2.62	0.48
1:A:279:TYR:C	1:A:279:TYR:CD2	2.86	0.48
1:A:210:ASP:CB	1:A:212:PRO:HD2	2.44	0.48
1:A:7:PRO:HG3	1:A:90:SER:CB	2.42	0.47
1:A:20:ASP:HB3	1:A:24:ARG:HH21	1.78	0.47
1:A:284:LYS:HD3	1:A:346:ASN:HD22	1.79	0.47
1:A:267:LEU:HD13	1:A:400:ALA:CA	2.37	0.47
1:A:285:HIS:ND1	1:A:285:HIS:N	2.60	0.47
1:A:64:ASP:O	1:A:67:PHE:N	2.46	0.47
1:A:49:ALA:HA	1:A:52:MET:HE2	1.95	0.47
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.77	0.47
1:A:40:ALA:HB3	1:A:100:LEU:CD1	2.45	0.47
1:A:14:LEU:N	1:A:15:PRO:CD	2.77	0.47
1:A:268:LEU:O	1:A:268:LEU:HD13	2.14	0.47
1:A:20:ASP:HB2	1:A:21:PRO:CD	2.40	0.47
1:A:28:TRP:O	1:A:32:LEU:HD13	2.15	0.47
1:A:165:HIS:ND1	1:A:165:HIS:C	2.67	0.46
1:A:45:ARG:C	1:A:46:LYS:CG	2.68	0.46
1:A:112:PHE:O	1:A:114:PRO:HD3	2.15	0.46
1:A:198:ILE:C	1:A:198:ILE:HD12	2.34	0.46
1:A:55:LEU:CD2	1:A:56:VAL:CG1	2.86	0.46
1:A:23:TYR:HE2	1:A:211:THR:HG21	1.79	0.46
1:A:345:GLY:C	1:A:347:PRO:CD	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ILE:O	1:A:425:ILE:HG13	2.15	0.46
1:A:18:GLU:OE1	1:A:21:PRO:HG2	2.15	0.46
1:A:41:TYR:CZ	1:A:137:GLY:CA	2.99	0.46
1:A:293:TRP:O	1:A:297:LEU:HG	2.14	0.46
1:A:110:MET:O	1:A:117:THR:HB	2.16	0.46
1:A:56:VAL:CG1	1:A:61:SER:H	2.28	0.46
1:A:210:ASP:N	1:A:210:ASP:OD1	2.48	0.46
1:A:65:LEU:O	1:A:68:ALA:HB3	2.15	0.46
1:A:13:ARG:CG	1:A:15:PRO:HD3	2.36	0.46
1:A:133:PHE:O	1:A:136:MET:HG2	2.16	0.46
1:A:268:LEU:O	1:A:272:ILE:HB	2.16	0.46
1:A:102:LEU:HD13	1:A:133:PHE:CZ	2.50	0.46
1:A:136:MET:O	1:A:139:PRO:HD2	2.16	0.46
1:A:404:VAL:O	1:A:408:VAL:HG23	2.15	0.46
1:A:444:GLN:C	1:A:446:LEU:N	2.70	0.46
1:A:346:ASN:ND2	1:A:350:ASP:HB2	2.30	0.46
1:A:34:ILE:HD13	1:A:144:THR:HG21	1.98	0.46
1:A:244:ILE:HD11	1:A:379:LYS:HD3	1.97	0.45
1:A:328:PHE:CD2	1:A:360:LEU:HD22	2.51	0.45
1:A:340:TRP:CH2	1:A:414:ASP:OD2	2.58	0.45
1:A:120:ILE:H	1:A:123:MET:CE	2.29	0.45
1:A:190:LEU:HD23	1:A:191:TYR:N	2.32	0.45
1:A:41:TYR:CZ	1:A:137:GLY:HA2	2.52	0.45
1:A:58:GLN:C	1:A:60:PHE:H	2.20	0.45
1:A:149:TRP:CG	1:A:152:LYS:HG3	2.51	0.45
1:A:269:ARG:HD3	1:A:270:TYR:CE2	2.52	0.45
1:A:273:LEU:HA	1:A:276:SER:OG	2.17	0.45
1:A:176:PHE:CE1	1:A:190:LEU:N	2.85	0.45
1:A:183:PHE:CB	1:A:191:TYR:HH	2.29	0.44
1:A:398:VAL:O	1:A:402:ALA:HB3	2.17	0.44
1:A:42:TYR:CD1	1:A:165:HIS:HA	2.52	0.44
1:A:335:ALA:HB1	1:A:339:TYR:CE1	2.53	0.44
1:A:357:ILE:O	1:A:361:ILE:HG12	2.17	0.44
1:A:212:PRO:CG	1:A:213:GLN:N	2.80	0.44
1:A:53:PRO:HB3	1:A:278:THR:CB	2.48	0.44
1:A:368:ILE:O	1:A:371:HIS:N	2.50	0.44
1:A:45:ARG:NE	1:A:134:GLN:HG2	2.33	0.44
1:A:306:THR:HG23	1:A:307:LEU:N	2.31	0.44
1:A:427:ALA:O	1:A:431:LEU:HB2	2.18	0.44
1:A:26:LEU:HA	1:A:26:LEU:HD22	1.86	0.44
1:A:69:LEU:CD2	1:A:72:ILE:HD13	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:O	1:A:14:LEU:HG	2.18	0.43
1:A:339:TYR:CE2	1:A:349:VAL:HG12	2.53	0.43
1:A:339:TYR:CZ	1:A:353:CYS:HA	2.52	0.43
1:A:335:ALA:HB1	1:A:339:TYR:HE1	1.82	0.43
1:A:275:TRP:CH2	1:A:404:VAL:HB	2.53	0.43
1:A:44:VAL:O	1:A:47:ASN:ND2	2.51	0.43
1:A:218:PRO:O	1:A:220:ILE:HG12	2.17	0.43
1:A:114:PRO:O	1:A:115:TRP:C	2.56	0.43
1:A:269:ARG:HB2	1:A:361:ILE:CG2	2.46	0.43
1:A:346:ASN:HD21	1:A:350:ASP:CB	2.31	0.43
1:A:25:ARG:O	1:A:29:GLN:HB2	2.18	0.43
1:A:356:VAL:O	1:A:357:ILE:C	2.57	0.43
1:A:408:VAL:O	1:A:411:PHE:O	2.36	0.43
1:A:188:ALA:O	1:A:191:TYR:CE1	2.72	0.43
1:A:252:ASN:OD1	1:A:255:LEU:HB2	2.19	0.43
1:A:75:ALA:HB3	1:A:131:GLY:HA3	2.01	0.43
1:A:269:ARG:HG3	1:A:361:ILE:CD1	2.45	0.42
1:A:450:VAL:HG12	1:A:451:PRO:N	2.33	0.42
1:A:52:MET:CE	1:A:69:LEU:HD12	2.50	0.42
1:A:32:LEU:N	1:A:32:LEU:HD12	2.34	0.42
1:A:52:MET:HE2	1:A:69:LEU:HD12	2.01	0.42
1:A:30:ILE:HG23	1:A:31:PHE:N	2.34	0.42
1:A:251:PRO:O	1:A:252:ASN:C	2.58	0.42
1:A:241:ALA:HB3	1:A:243:GLN:HE21	1.84	0.42
1:A:16:ALA:O	1:A:17:ALA:HB3	2.19	0.42
1:A:100:LEU:O	1:A:103:ALA:N	2.53	0.42
1:A:50:LEU:HD11	1:A:173:PRO:HB3	2.01	0.42
1:A:303:ILE:HB	1:A:304:PRO:CD	2.39	0.42
1:A:142:GLY:O	1:A:146:VAL:HG23	2.20	0.42
1:A:136:MET:O	1:A:140:PRO:HD2	2.19	0.41
1:A:275:TRP:HA	1:A:278:THR:HG22	2.01	0.41
1:A:120:ILE:H	1:A:123:MET:HE2	1.84	0.41
1:A:15:PRO:HA	1:A:19:ILE:HG13	2.02	0.41
1:A:279:TYR:HD1	1:A:413:TRP:CE2	2.38	0.41
1:A:367:LEU:HA	1:A:367:LEU:HD12	1.58	0.41
1:A:176:PHE:CZ	1:A:189:ALA:HB3	2.54	0.41
1:A:436:ILE:HG22	1:A:437:GLY:N	2.35	0.41
1:A:79:SER:OG	1:A:80:LYS:N	2.53	0.41
1:A:335:ALA:HA	1:A:338:VAL:CG1	2.50	0.41
1:A:332:VAL:CG2	1:A:333:THR:N	2.84	0.41
1:A:328:PHE:CE2	1:A:360:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:O	1:A:427:ALA:C	2.58	0.41
1:A:122:VAL:HG13	1:A:123:MET:N	2.35	0.41
1:A:153:GLU:O	1:A:154:ARG:C	2.59	0.41
1:A:212:PRO:O	1:A:216:GLY:HA2	2.20	0.41
1:A:53:PRO:HB3	1:A:278:THR:HB	2.01	0.41
1:A:220:ILE:C	1:A:222:GLU:N	2.71	0.41
1:A:141:CYS:O	1:A:145:MET:HG3	2.21	0.41
1:A:388:THR:OG1	1:A:389:GLY:N	2.53	0.41
1:A:123:MET:O	1:A:124:PHE:C	2.57	0.41
1:A:397:SER:HA	1:A:400:ALA:HB3	2.01	0.41
1:A:108:LEU:CD2	1:A:112:PHE:HE1	2.33	0.41
1:A:56:VAL:HG21	1:A:61:SER:CB	2.50	0.41
1:A:140:PRO:C	1:A:142:GLY:N	2.72	0.41
1:A:328:PHE:O	1:A:332:VAL:CG1	2.64	0.41
1:A:85:SER:O	1:A:88:ASP:HB3	2.21	0.41
1:A:74:ILE:HG13	1:A:74:ILE:H	1.55	0.41
1:A:248:TYR:CD1	1:A:248:TYR:N	2.89	0.41
1:A:269:ARG:CB	1:A:361:ILE:HG21	2.49	0.40
1:A:252:ASN:HA	1:A:252:ASN:HD22	1.60	0.40
1:A:62:ARG:O	1:A:409:ASP:OD2	2.39	0.40
1:A:316:VAL:HG12	1:A:317:PHE:N	2.36	0.40
1:A:15:PRO:HA	1:A:19:ILE:CG1	2.51	0.40
1:A:355:ILE:O	1:A:359:PHE:HB2	2.21	0.40
1:A:88:ASP:O	1:A:143:ARG:NE	2.53	0.40
1:A:378:LYS:HG3	1:A:378:LYS:H	1.55	0.40
1:A:334:ILE:CG2	1:A:335:ALA:N	2.84	0.40
1:A:177:LEU:C	1:A:177:LEU:HD13	2.42	0.40
1:A:19:ILE:HG23	1:A:215:CYS:SG	2.62	0.40
1:A:211:THR:HA	1:A:213:GLN:NE2	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	430/451 (95%)	356 (83%)	50 (12%)	24 (6%)	2 16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	211	THR
1	A	221	GLU
1	A	18	GLU
1	A	59	GLY
1	A	100	LEU
1	A	251	PRO
1	A	253	LYS
1	A	9	PRO
1	A	212	PRO
1	A	242	LYS
1	A	243	GLN
1	A	15	PRO
1	A	137	GLY
1	A	344	ALA
1	A	346	ASN
1	A	378	LYS
1	A	120	ILE
1	A	114	PRO
1	A	158	VAL
1	A	56	VAL
1	A	219	PRO
1	A	396	GLY
1	A	7	PRO

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	345/360 (96%)	299 (87%)	46 (13%)	5 21

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	6	LYS
1	A	10	HIS
1	A	19	ILE
1	A	23	TYR
1	A	26	LEU
1	A	60	PHE
1	A	64	ASP
1	A	69	LEU
1	A	79	SER
1	A	102	LEU
1	A	109	PHE
1	A	125	VAL
1	A	127	LEU
1	A	148	TRP
1	A	149	TRP
1	A	151	GLN
1	A	180	MET
1	A	186	TRP
1	A	187	HIS
1	A	190	LEU
1	A	195	PHE
1	A	196	CYS
1	A	203	PHE
1	A	210	ASP
1	A	252	ASN
1	A	262	ASN
1	A	266	TYR
1	A	272	ILE
1	A	279	TYR
1	A	295	TYR
1	A	299	GLU
1	A	327	PHE
1	A	329	MET
1	A	332	VAL
1	A	338	VAL
1	A	340	TRP
1	A	343	PRO
1	A	349	VAL
1	A	350	ASP
1	A	353	CYS
1	A	361	ILE
1	A	367	LEU

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Mol	Chain	Res	Type
1	A	391	PHE
1	A	434	VAL
1	A	435	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	91	ASN
1	A	134	GLN
1	A	243	GLN
1	A	262	ASN
1	A	346	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	434/451 (96%)	-0.31	8 (1%) 71 65	14, 74, 159, 200	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	3.5
1	A	410	PHE	3.5
1	A	223	TYR	3.1
1	A	286	PHE	2.7
1	A	161	TRP	2.2
1	A	226	ASP	2.2
1	A	215	CYS	2.2
1	A	120	ILE	2.1

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.