Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 01:45 PM EST

PDB ID	:	4MGR
Title	:	The crystal structure of Bacillus subtilis GabR, an autorepressor and PLP- and GABA-dependent transcriptional activator of gabT
Authors	:	Wu, R.; Edayathumangalam, R.; Garcia, R.; Wang, Y.; Wang, W.; Kreinbring, C.A.; Bach, A.; Liao, J.; Stone, T.; Terwilliger, T.; Hoang, Q.Q.; Belitsky, B.R.; Petsko, G.A.; Ringe, D.; Liu, D.
Deposited on	:	2013-08-28
Resolution	:	2.55 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

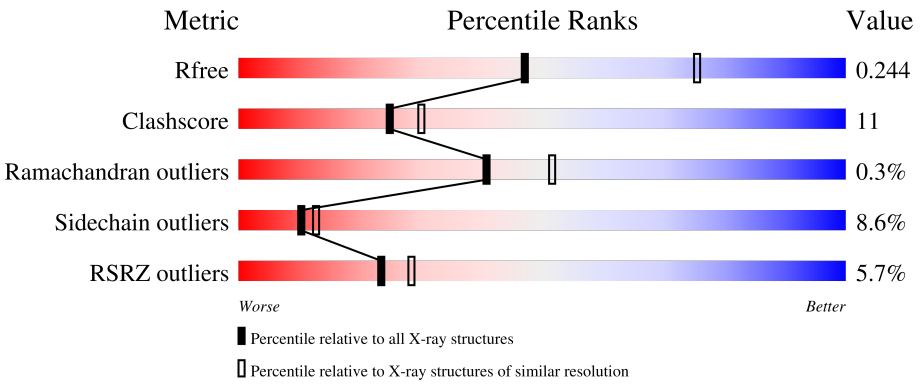
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	485	8% 67% 25% • •
1	B	485	6% 68% 24% • 5%
1	C	485	4% 72% 23% • •
1	D	485	5% 71% 24% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	B	503	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15770 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 HTH-type transcriptional regulatory protein GabR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3800	2413	656	714	17	0	0	0
1	B	463	3757	2383	652	705	17	0	0	0
1	C	475	3855	2449	667	721	18	0	0	0
1	D	472	3831	2432	663	718	18	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	480	HIS	-	expression tag	UNP P94426
A	481	HIS	-	expression tag	UNP P94426
A	482	HIS	-	expression tag	UNP P94426
A	483	HIS	-	expression tag	UNP P94426
A	484	HIS	-	expression tag	UNP P94426
A	485	HIS	-	expression tag	UNP P94426
B	480	HIS	-	expression tag	UNP P94426
B	481	HIS	-	expression tag	UNP P94426
B	482	HIS	-	expression tag	UNP P94426
B	483	HIS	-	expression tag	UNP P94426
B	484	HIS	-	expression tag	UNP P94426
B	485	HIS	-	expression tag	UNP P94426
C	480	HIS	-	expression tag	UNP P94426
C	481	HIS	-	expression tag	UNP P94426
C	482	HIS	-	expression tag	UNP P94426
C	483	HIS	-	expression tag	UNP P94426
C	484	HIS	-	expression tag	UNP P94426
C	485	HIS	-	expression tag	UNP P94426
D	480	HIS	-	expression tag	UNP P94426
D	481	HIS	-	expression tag	UNP P94426
D	482	HIS	-	expression tag	UNP P94426

Continued on next page...

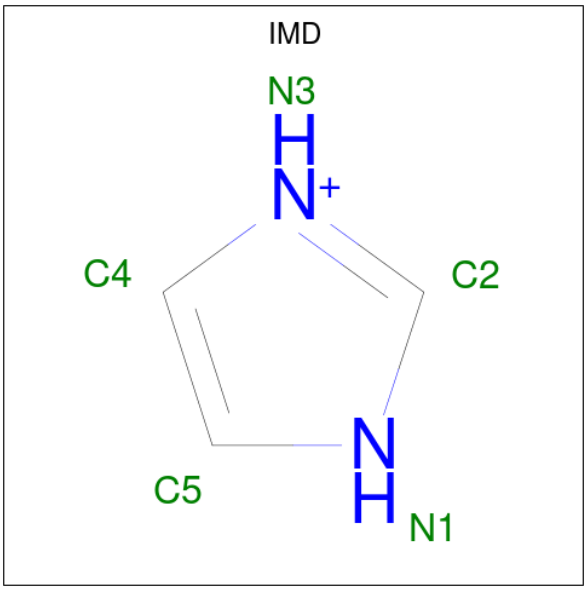
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	483	HIS	-	expression tag	UNP P94426
D	484	HIS	-	expression tag	UNP P94426
D	485	HIS	-	expression tag	UNP P94426

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

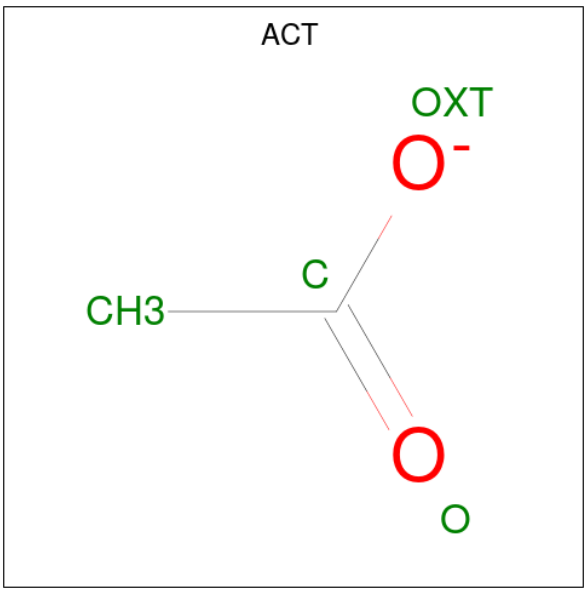
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	5	3	2	0	0
3	B	1	5	3	2	0	0
3	C	1	5	3	2	0	0
3	D	1	5	3	2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
4	B	1	4	2	2	0	0
4	B	1	4	2	2	0	0
4	B	1	4	2	2	0	0
4	B	1	4	2	2	0	0
4	C	1	4	2	2	0	0
4	C	1	4	2	2	0	0
4	D	1	4	2	2	0	0
4	D	1	4	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	101	101	101	0	0
5	B	102	102	102	0	0

Continued on next page...

Continued from previous page...

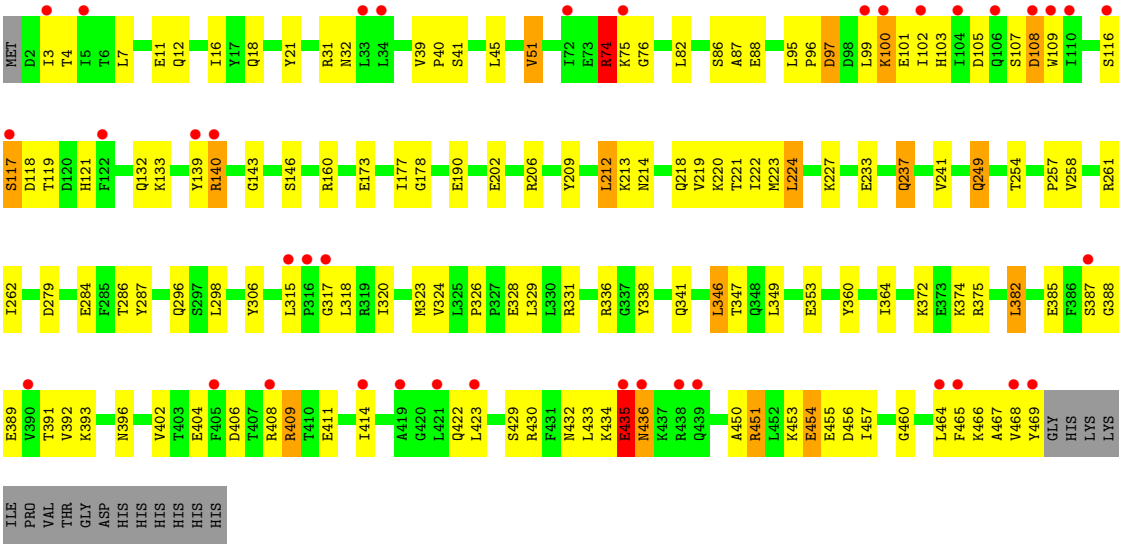
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	134	134	134	0	0
			Total	O		
5	D	130	130	130	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

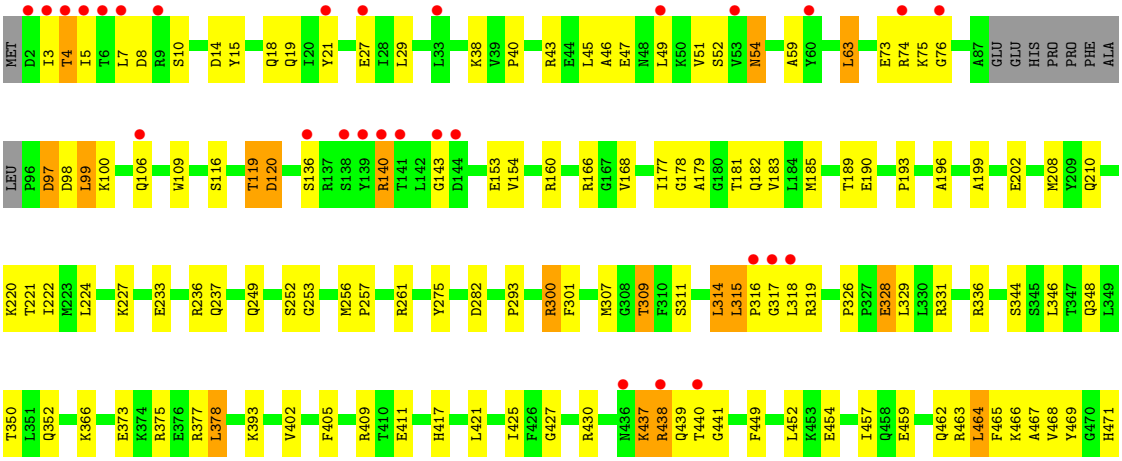
• Molecule 1: HTH-type transcriptional regulatory protein GabR

Chain A:

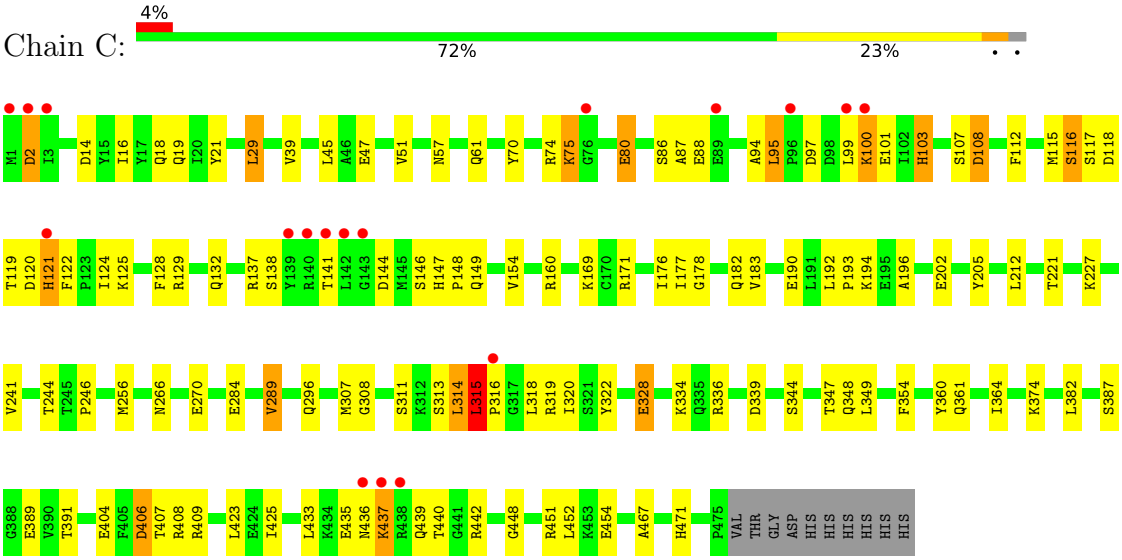


• Molecule 1: HTH-type transcriptional regulatory protein GabR

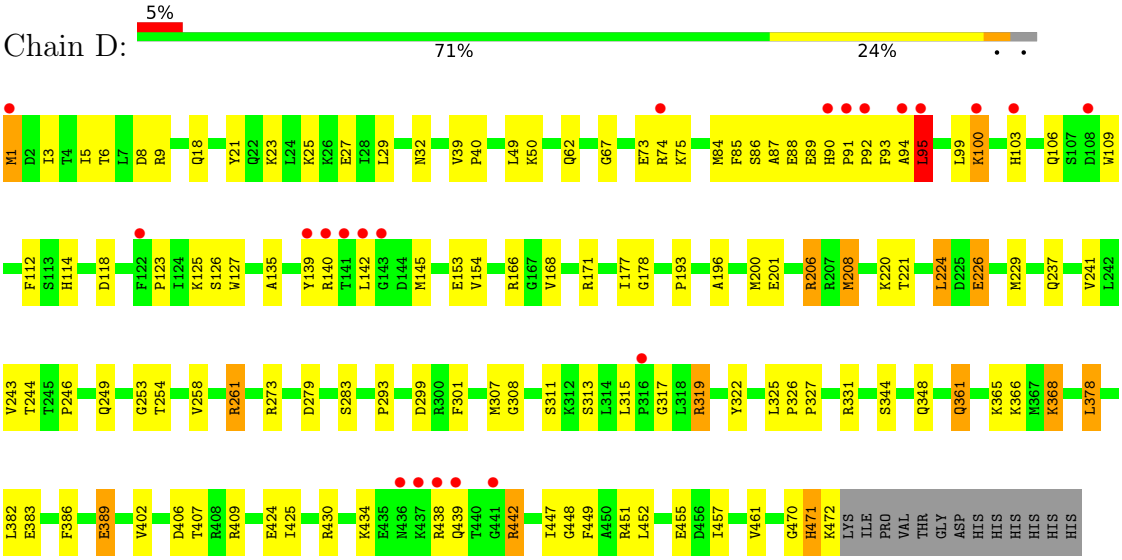
Chain B:



• Molecule 1: HTH-type transcriptional regulatory protein GabR



• Molecule 1: HTH-type transcriptional regulatory protein GabR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.93Å 101.36Å 213.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 2.55 49.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.30-2.55) 87.7 (49.31-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.194 , 0.244 0.194 , 0.244	Depositor DCC
R_{free} test set	4245 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15770	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IMD, ACT

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	0.27	0/3876	0.55	2/5227 (0.0%)
1	B	0.26	0/3829	0.52	0/5157
1	C	0.27	0/3933	0.54	1/5302 (0.0%)
1	D	0.26	0/3908	0.52	1/5268 (0.0%)
All	All	0.26	0/15546	0.53	4/20954 (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	2
1	B	0	3
1	C	0	6
All	All	0	11

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	A	74	ARG	N-CA-C	-5.88	95.14	111.00
1	A	435	GLU	N-CA-C	5.71	126.40	111.00
1	D	95	LEU	CA-CB-CG	5.66	128.32	115.30
1	C	315	LEU	C-N-CD	5.03	138.96	128.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	435	GLU	Peptide
1	A	436	ASN	Peptide
1	B	314	LEU	Peptide
1	B	97	ASP	Peptide
1	B	99	LEU	Peptide
1	C	108	ASP	Peptide
1	C	314	LEU	Peptide
1	C	315	LEU	Peptide
1	C	387	SER	Peptide
1	C	439	GLN	Peptide
1	C	75	LYS	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	3800	0	3810	96	0
1	B	3757	0	3774	88	0
1	C	3855	0	3876	89	0
1	D	3831	0	3845	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	5	0	0
3	B	5	0	5	0	0
3	C	5	0	5	1	0
3	D	5	0	5	0	0
4	A	4	0	3	0	0
4	B	16	0	12	3	0
4	C	8	0	6	1	0
4	D	8	0	6	0	0
5	A	101	0	0	12	0
5	B	102	0	0	11	0
5	C	134	0	0	19	0
5	D	130	0	0	18	0
All	All	15770	0	15352	331	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 11.

All (331) 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:86:SER:O	5:A:664:HOH:O	1.90	0.91
1:C:171:ARG:NH1	5:C:730:HOH:O	2.03	0.90
4:B:503:ACT:O	5:B:663:HOH:O	1.91	0.88
1:B:75:LYS:HB3	1:B:76:GLY:HA2	1.54	0.88
1:C:284:GLU:O	5:C:606:HOH:O	1.91	0.88
1:B:51:VAL:O	5:B:700:HOH:O	1.93	0.86
1:C:137:ARG:NH2	5:C:718:HOH:O	2.02	0.86
1:A:434:LYS:HA	1:A:435:GLU:HB2	1.58	0.84
4:B:503:ACT:OXT	5:B:689:HOH:O	1.95	0.83
1:C:328:GLU:OE2	5:C:726:HOH:O	1.95	0.83
1:C:101:GLU:OE1	5:C:601:HOH:O	1.98	0.81
1:C:146:SER:O	5:C:614:HOH:O	1.98	0.80
1:D:407:THR:O	5:D:645:HOH:O	2.00	0.80
1:A:105:ASP:OD1	1:D:171:ARG:NH1	2.16	0.79
1:A:338:TYR:O	5:A:647:HOH:O	1.99	0.78
1:A:101:GLU:OE2	5:A:686:HOH:O	2.02	0.78
1:A:190:GLU:OE1	1:A:336:ARG:NH2	2.17	0.78
1:C:108:ASP:OD2	5:C:710:HOH:O	2.01	0.77
1:C:16:ILE:HG21	1:C:51:VAL:HG21	1.66	0.77
1:B:315:LEU:HD21	1:B:319:ARG:H	1.47	0.77
1:C:74:ARG:HG2	1:C:75:LYS:HE2	1.66	0.77
1:C:316:PRO:HG2	1:D:142:LEU:HD13	1.67	0.77
1:C:182:GLN:OE1	5:C:660:HOH:O	2.04	0.76
1:B:314:LEU:O	5:B:691:HOH:O	2.03	0.76
1:D:67:GLY:O	5:D:646:HOH:O	2.03	0.75
1:B:439:GLN:HG2	1:B:440:THR:HG22	1.69	0.74
1:C:120:ASP:OD2	5:C:646:HOH:O	2.06	0.73
1:D:279:ASP:OD1	5:D:607:HOH:O	2.06	0.73
1:C:227:LYS:NZ	5:C:721:HOH:O	2.20	0.73
1:D:442:ARG:NH1	5:D:715:HOH:O	2.20	0.73
1:A:96:PRO:HA	1:A:99:LEU:HB3	1.71	0.72
1:A:86:SER:HA	1:A:87:ALA:HB3	1.70	0.72
1:D:8:ASP:OD2	5:D:718:HOH:O	2.07	0.72
1:A:454:GLU:HA	1:A:457:ILE:HG13	1.71	0.72
1:A:323:MET:SD	5:A:685:HOH:O	2.47	0.71
1:D:50:LYS:NZ	5:D:631:HOH:O	2.21	0.71
1:A:109:TRP:H	1:A:422:GLN:HB3	1.55	0.71
1:B:314:LEU:HB2	1:B:315:LEU:HA	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LEU:O	5:C:694:HOH:O	2.08	0.70
1:B:160:ARG:HB3	1:D:140:ARG:HH22	1.56	0.70
1:B:311:SER:HA	1:B:315:LEU:HD22	1.71	0.70
1:C:315:LEU:HD12	1:C:315:LEU:H	1.56	0.70
1:B:430:ARG:NH2	5:B:668:HOH:O	2.24	0.70
1:D:243:VAL:O	5:D:637:HOH:O	2.09	0.69
1:C:94:ALA:HB1	1:C:95:LEU:HA	1.74	0.68
1:A:389:GLU:HB3	1:A:406:ASP:HB2	1.74	0.68
1:A:116:SER:HB3	1:A:117:SER:HB3	1.75	0.67
1:A:284:GLU:O	5:A:682:HOH:O	2.14	0.66
1:B:282:ASP:OD1	5:B:661:HOH:O	2.12	0.66
1:A:31:ARG:NH2	1:A:82:LEU:O	2.27	0.65
1:D:438:ARG:HB3	1:D:439:GLN:HG3	1.77	0.65
1:C:311:SER:O	1:C:315:LEU:HD11	1.96	0.64
1:B:378:LEU:HD12	1:B:449:PHE:HB3	1.79	0.64
1:D:9:ARG:NH2	1:D:49:LEU:O	2.30	0.64
1:A:177:ILE:HG22	1:A:178:GLY:HA3	1.80	0.64
1:D:1:MET:HG3	1:D:40:PRO:HD3	1.79	0.63
1:C:86:SER:HA	1:C:87:ALA:HB3	1.78	0.63
3:C:502:IMD:N3	5:C:702:HOH:O	2.14	0.63
1:A:97:ASP:OD1	1:A:97:ASP:N	2.30	0.63
1:A:40:PRO:HB2	1:A:45:LEU:HB2	1.80	0.63
1:A:146:SER:O	5:A:602:HOH:O	2.16	0.62
1:C:129:ARG:NH1	5:C:653:HOH:O	2.33	0.62
1:D:311:SER:OG	5:D:640:HOH:O	2.16	0.62
1:B:154:VAL:HG21	1:B:348:GLN:HB3	1.82	0.62
1:A:456:ASP:O	1:A:460:GLY:N	2.30	0.61
1:C:190:GLU:OE1	1:C:336:ARG:NH2	2.32	0.61
1:A:391:THR:HB	1:A:404:GLU:HB2	1.82	0.61
1:B:190:GLU:OE2	1:B:336:ARG:NH2	2.32	0.61
1:A:375:ARG:NH1	5:A:688:HOH:O	2.34	0.61
1:B:439:GLN:N	1:B:439:GLN:OE1	2.34	0.60
1:D:94:ALA:HA	1:D:95:LEU:HB3	1.82	0.60
1:B:182:GLN:OE1	5:B:627:HOH:O	2.15	0.60
1:C:409:ARG:NH1	1:C:467:ALA:O	2.34	0.60
1:C:316:PRO:HB2	1:D:142:LEU:HD22	1.84	0.60
1:A:220:LYS:HD3	1:A:237:GLN:HB2	1.84	0.60
1:A:432:ASN:HB3	1:A:435:GLU:CD	2.22	0.60
1:B:3:ILE:HG22	1:B:4:THR:H	1.66	0.60
1:C:86:SER:HB3	1:C:87:ALA:O	2.01	0.59
1:D:154:VAL:HG21	1:D:348:GLN:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:MET:SD	5:C:635:HOH:O	2.57	0.59
1:C:86:SER:HB2	1:D:301:PHE:CZ	2.37	0.59
1:B:275:TYR:OH	1:B:328:GLU:OE2	2.13	0.59
1:B:326:PRO:HD2	1:B:329:LEU:HD12	1.84	0.59
1:C:122:PHE:O	1:D:139:TYR:OH	2.20	0.59
1:C:318:LEU:HD11	1:C:347:THR:HG23	1.85	0.59
1:C:154:VAL:HG21	1:C:348:GLN:HB3	1.85	0.58
1:D:261:ARG:NH2	1:D:293:PRO:O	2.37	0.58
1:D:409:ARG:NH2	1:D:470:GLY:O	2.36	0.58
1:B:120:ASP:OD1	1:B:120:ASP:N	2.36	0.57
1:B:437:LYS:HA	1:B:438:ARG:C	2.23	0.57
1:A:434:LYS:CA	1:A:435:GLU:HB2	2.32	0.57
1:A:326:PRO:HD2	1:A:329:LEU:HD12	1.86	0.57
1:D:258:VAL:HA	1:D:261:ARG:HG3	1.85	0.57
1:C:244:THR:HG23	1:C:246:PRO:HD3	1.86	0.57
1:A:320:ILE:HD11	1:A:347:THR:HG22	1.87	0.57
1:C:99:LEU:HD13	1:D:171:ARG:HH21	1.71	0.56
1:A:103:HIS:HB2	1:C:103:HIS:HB3	1.86	0.56
1:D:177:ILE:HG22	1:D:178:GLY:HA3	1.88	0.56
1:B:315:LEU:HG	1:B:318:LEU:HB3	1.88	0.55
1:C:336:ARG:NH1	1:C:339:ASP:OD2	2.39	0.55
1:C:146:SER:HB3	5:C:648:HOH:O	2.06	0.55
1:B:315:LEU:HD21	1:B:319:ARG:N	2.18	0.55
1:A:393:LYS:NZ	5:A:698:HOH:O	2.39	0.55
1:D:299:ASP:O	5:D:653:HOH:O	2.18	0.55
1:A:341:GLN:O	1:B:319:ARG:NH1	2.40	0.55
1:B:153:GLU:HB3	1:B:352:GLN:HE22	1.71	0.55
1:D:25:LYS:NZ	5:D:726:HOH:O	2.39	0.55
1:C:407:THR:HG22	1:C:409:ARG:H	1.72	0.55
1:B:300:ARG:NH1	5:B:682:HOH:O	2.39	0.55
1:B:261:ARG:NH2	1:B:293:PRO:O	2.41	0.54
1:C:2:ASP:OD1	1:C:2:ASP:N	2.40	0.54
1:A:143:GLY:O	1:B:116:SER:HB2	2.07	0.54
1:A:74:ARG:O	1:A:76:GLY:HA3	2.08	0.54
1:A:119:THR:HB	1:B:143:GLY:HA3	1.90	0.54
1:B:46:ALA:HB1	5:B:700:HOH:O	2.07	0.54
1:B:40:PRO:HB2	1:B:45:LEU:HB2	1.90	0.54
1:B:43:ARG:O	1:B:46:ALA:HB3	2.08	0.54
1:C:149:GLN:HG2	1:C:176:ILE:HG12	1.90	0.54
1:A:12:GLN:HE22	1:C:125:LYS:H	1.54	0.53
1:C:70:TYR:HD2	1:C:80:GLU:HG2	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:TYR:HB3	1:A:372:LYS:HG3	1.89	0.53
1:D:3:ILE:O	5:D:628:HOH:O	2.19	0.53
1:A:466:LYS:N	1:A:468:VAL:O	2.27	0.53
1:C:95:LEU:O	1:C:99:LEU:HG	2.08	0.53
1:C:160:ARG:NH2	5:C:604:HOH:O	2.40	0.53
1:C:108:ASP:OD1	5:C:654:HOH:O	2.19	0.53
1:D:224:LEU:HD12	1:D:229:MET:HA	1.91	0.53
1:D:94:ALA:HB1	1:D:95:LEU:O	2.09	0.52
1:A:86:SER:HB2	1:B:301:PHE:CZ	2.43	0.52
1:A:375:ARG:NE	1:A:396:ASN:OD1	2.42	0.52
1:B:315:LEU:CD2	1:B:319:ARG:H	2.18	0.52
1:B:106:GLN:O	1:B:109:TRP:N	2.34	0.52
1:A:86:SER:HB3	1:A:88:GLU:N	2.25	0.52
1:A:11:GLU:HG3	1:A:12:GLN:HG2	1.92	0.52
1:C:315:LEU:HB2	1:C:318:LEU:H	1.74	0.52
1:A:18:GLN:HA	1:A:21:TYR:CE2	2.45	0.52
1:C:194:LYS:NZ	5:C:659:HOH:O	2.31	0.52
1:A:119:THR:HG22	1:A:451:ARG:HH22	1.75	0.51
1:B:166:ARG:HB2	1:B:168:VAL:HG23	1.91	0.51
1:B:177:ILE:HG22	1:B:178:GLY:HA3	1.92	0.51
1:B:311:SER:HA	1:B:315:LEU:HD13	1.92	0.51
1:A:393:LYS:HB2	1:A:402:VAL:HB	1.92	0.51
1:C:18:GLN:HA	1:C:21:TYR:CE2	2.45	0.51
1:A:173:GLU:HG2	1:B:100:LYS:HA	1.92	0.51
1:B:220:LYS:HD3	1:B:237:GLN:HB3	1.93	0.51
1:D:86:SER:HB2	1:D:87:ALA:HA	1.92	0.51
1:A:227:LYS:HG2	1:A:257:PRO:HG2	1.93	0.51
1:D:112:PHE:HD2	1:D:425:ILE:HD12	1.75	0.51
1:C:266:ASN:O	1:C:270:GLU:HG2	2.11	0.51
1:B:153:GLU:HB3	1:B:352:GLN:NE2	2.26	0.50
1:B:5:ILE:HB	1:B:49:LEU:HD21	1.92	0.50
1:C:202:GLU:HB2	1:C:221:THR:OG1	2.11	0.50
1:A:132:GLN:NE2	5:A:615:HOH:O	2.43	0.50
1:D:424:GLU:OE1	1:D:451:ARG:NH1	2.45	0.50
1:B:202:GLU:HB2	1:B:221:THR:OG1	2.11	0.50
1:C:374:LYS:NZ	1:C:452:LEU:O	2.40	0.50
1:A:409:ARG:HD3	1:A:414:ILE:HG12	1.93	0.50
1:B:440:THR:OG1	1:B:441:GLY:N	2.45	0.50
1:A:109:TRP:HA	1:A:422:GLN:O	2.12	0.50
1:D:244:THR:HG23	1:D:246:PRO:HD3	1.94	0.50
1:B:199:ALA:HB1	1:B:222:ILE:HD12	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLN:HA	1:B:21:TYR:CE2	2.47	0.49
1:C:389:GLU:HB3	1:C:406:ASP:OD1	2.13	0.49
1:B:185:MET:HG3	1:B:208:MET:SD	2.52	0.49
1:C:360:TYR:O	1:C:364:ILE:HG12	2.13	0.49
1:A:464:LEU:O	1:A:468:VAL:N	2.45	0.49
1:B:317:GLY:N	5:B:642:HOH:O	2.34	0.49
1:D:5:ILE:HG12	1:D:23:LYS:HG2	1.94	0.49
1:C:315:LEU:H	1:C:315:LEU:CD1	2.23	0.49
1:D:39:VAL:O	5:D:679:HOH:O	2.20	0.49
1:A:387:SER:N	1:A:388:GLY:HA3	2.28	0.49
1:B:8:ASP:OD2	1:B:10:SER:OG	2.28	0.49
1:A:160:ARG:NH2	5:A:663:HOH:O	2.45	0.48
1:D:18:GLN:HA	1:D:21:TYR:CE2	2.48	0.48
1:D:103:HIS:HD2	5:D:727:HOH:O	1.96	0.48
1:B:185:MET:O	1:B:189:THR:HG23	2.13	0.48
1:B:471:HIS:O	1:B:472:LYS:HB2	2.13	0.48
1:D:193:PRO:HG2	1:D:196:ALA:HB2	1.95	0.48
1:A:467:ALA:HB3	5:A:679:HOH:O	2.13	0.48
1:C:146:SER:CB	5:C:648:HOH:O	2.62	0.48
1:D:438:ARG:HB3	1:D:439:GLN:CG	2.43	0.48
1:B:430:ARG:NH2	4:B:505:ACT:O	2.45	0.48
1:D:226:GLU:H	1:D:226:GLU:HG3	1.34	0.47
1:D:430:ARG:NH2	5:D:629:HOH:O	2.37	0.47
1:D:206:ARG:HG3	1:D:430:ARG:O	2.14	0.47
1:B:177:ILE:CG2	1:B:178:GLY:HA3	2.45	0.47
1:B:466:LYS:HA	1:B:469:TYR:O	2.13	0.47
1:A:139:TYR:HA	1:A:140:ARG:HA	1.67	0.47
1:A:453:LYS:HE3	1:A:456:ASP:OD2	2.14	0.47
1:C:117:SER:OG	1:C:118:ASP:N	2.47	0.47
1:C:141:THR:HG23	1:C:144:ASP:HA	1.96	0.47
1:D:382:LEU:HD23	1:D:461:VAL:HG13	1.97	0.47
1:B:314:LEU:HB2	1:B:315:LEU:CA	2.43	0.46
1:A:206:ARG:NH1	1:A:433:LEU:O	2.39	0.46
1:B:249:GLN:O	1:B:253:GLY:N	2.46	0.46
1:C:315:LEU:HD13	1:C:315:LEU:O	2.16	0.46
1:A:119:THR:HG22	1:A:451:ARG:NH2	2.30	0.46
1:A:95:LEU:HD21	1:B:331:ARG:HH12	1.80	0.46
1:A:16:ILE:HG21	1:A:51:VAL:HG21	1.97	0.46
1:D:114:HIS:HA	1:D:448:GLY:HA3	1.98	0.46
1:A:433:LEU:N	1:A:435:GLU:OE1	2.49	0.46
1:B:73:GLU:OE2	1:B:74:ARG:HG3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:HB2	5:B:681:HOH:O	2.15	0.46
1:C:177:ILE:HG22	1:C:178:GLY:HA3	1.98	0.46
1:D:438:ARG:HA	1:D:439:GLN:HA	1.80	0.46
1:C:193:PRO:HB2	1:C:196:ALA:HB2	1.98	0.45
1:D:177:ILE:CG2	1:D:178:GLY:HA3	2.46	0.45
1:A:202:GLU:HB2	1:A:221:THR:HB	1.98	0.45
1:D:123:PRO:HB2	1:D:126:SER:HB3	1.97	0.45
1:A:212:LEU:HB3	1:A:219:VAL:HG21	1.98	0.45
1:A:258:VAL:O	1:A:262:ILE:HG12	2.16	0.45
1:B:366:LYS:HE3	1:B:366:LYS:HB2	1.76	0.45
1:B:227:LYS:HG2	1:B:257:PRO:HG3	1.99	0.45
1:B:393:LYS:HB2	1:B:402:VAL:HB	1.98	0.45
1:A:177:ILE:CG2	1:A:178:GLY:HA3	2.47	0.45
1:B:193:PRO:HB2	1:B:196:ALA:HB2	1.99	0.45
1:A:107:SER:HA	1:A:108:ASP:HA	1.49	0.45
1:A:454:GLU:HG2	1:A:455:GLU:OE2	2.17	0.45
1:A:100:LYS:HE3	1:A:102:ILE:HG12	1.98	0.45
1:B:179:ALA:HA	1:B:319:ARG:O	2.17	0.45
1:B:454:GLU:HA	1:B:457:ILE:HG13	1.98	0.45
1:D:92:PRO:HA	1:D:93:PHE:HB2	1.99	0.45
1:B:427:GLY:O	1:B:430:ARG:HG2	2.17	0.45
1:C:320:ILE:HD11	1:C:347:THR:HG22	1.98	0.45
1:D:201:GLU:HB3	1:D:224:LEU:HD11	1.98	0.45
1:A:432:ASN:HB3	1:A:435:GLU:CG	2.46	0.44
1:C:57:ASN:O	1:C:61:GLN:HG2	2.17	0.44
1:D:365:LYS:HA	1:D:365:LYS:HD3	1.78	0.44
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.88	0.44
1:B:373:GLU:O	1:B:377:ARG:HG2	2.17	0.44
1:D:200:MET:HE1	1:D:208:MET:HB3	1.98	0.44
1:C:94:ALA:HB1	1:C:95:LEU:CA	2.44	0.44
1:D:368:LYS:NZ	5:D:658:HOH:O	2.38	0.44
1:B:405:PHE:CD2	1:B:468:VAL:HG11	2.53	0.44
1:C:437:LYS:HB2	1:C:437:LYS:HE3	1.77	0.44
1:C:177:ILE:CG2	1:C:178:GLY:HA3	2.47	0.44
1:A:287:TYR:HB2	1:A:396:ASN:ND2	2.31	0.44
1:B:409:ARG:HH21	1:B:467:ALA:HB2	1.82	0.44
1:D:254:THR:OG1	5:D:680:HOH:O	2.05	0.44
1:D:307:MET:HB3	1:D:307:MET:HE2	1.71	0.44
1:A:143:GLY:HA3	1:B:119:THR:HG23	2.00	0.43
1:A:360:TYR:O	1:A:364:ILE:HG12	2.18	0.43
1:C:70:TYR:CD2	1:C:80:GLU:HG2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLU:OE2	1:A:429:SER:OG	2.33	0.43
1:C:344:SER:HA	1:D:317:GLY:O	2.19	0.43
1:B:14:ASP:O	1:B:19:GLN:NE2	2.42	0.43
1:C:14:ASP:O	1:C:19:GLN:NE2	2.49	0.43
1:C:112:PHE:HB2	1:C:425:ILE:HG22	2.01	0.43
1:C:115:MET:O	1:C:451:ARG:NE	2.51	0.43
1:C:334:LYS:HA	4:C:503:ACT:H1	2.01	0.43
1:D:73:GLU:C	1:D:75:LYS:H	2.20	0.43
1:A:360:TYR:CZ	1:A:364:ILE:HD11	2.54	0.43
1:B:309:THR:HG23	1:B:311:SER:H	1.83	0.43
1:C:128:PHE:O	1:C:132:GLN:HG2	2.19	0.43
1:C:308:GLY:HA3	1:C:322:TYR:CE1	2.54	0.43
1:D:106:GLN:O	1:D:109:TRP:HB2	2.19	0.43
1:A:117:SER:OG	1:A:118:ASP:N	2.51	0.43
1:A:133:LYS:HD2	1:A:353:GLU:OE1	2.19	0.43
1:C:29:LEU:HD12	1:C:29:LEU:HA	1.88	0.42
1:C:284:GLU:CD	1:C:284:GLU:H	2.23	0.42
1:A:306:TYR:HB3	1:A:324:VAL:HB	2.01	0.42
1:C:406:ASP:OD1	1:C:406:ASP:N	2.42	0.42
1:A:86:SER:HB3	1:A:88:GLU:H	1.82	0.42
1:D:386:PHE:O	1:D:389:GLU:HG2	2.18	0.42
1:B:233:GLU:OE2	1:B:236:ARG:NH2	2.28	0.42
1:A:212:LEU:HA	1:A:212:LEU:HD12	1.83	0.42
1:A:279:ASP:OD1	5:A:630:HOH:O	2.22	0.42
1:C:406:ASP:HB3	1:C:442:ARG:NH1	2.34	0.42
1:A:99:LEU:HD23	1:A:99:LEU:O	2.20	0.42
1:C:147:HIS:HA	1:C:148:PRO:HD3	1.80	0.42
1:C:391:THR:HB	1:C:404:GLU:HG2	2.01	0.42
1:D:361:GLN:OE1	5:D:617:HOH:O	2.22	0.42
1:B:311:SER:CA	1:B:315:LEU:HD22	2.44	0.42
1:D:471:HIS:O	1:D:472:LYS:HB2	2.20	0.42
1:A:223:MET:HG2	1:A:224:LEU:N	2.34	0.42
1:C:95:LEU:HD11	1:D:331:ARG:HH21	1.85	0.42
1:C:112:PHE:O	1:C:448:GLY:N	2.45	0.42
1:A:374:LYS:HZ1	1:A:450:ALA:HA	1.84	0.42
1:C:311:SER:HA	1:C:315:LEU:HG	2.02	0.42
1:B:464:LEU:O	1:B:465:PHE:HB3	2.20	0.42
1:C:119:THR:HG22	1:D:142:LEU:HB2	2.01	0.42
1:D:127:TRP:CD2	1:D:315:LEU:HD11	2.55	0.41
1:D:308:GLY:HA3	1:D:322:TYR:CZ	2.55	0.41
1:B:15:TYR:O	1:B:19:GLN:HG3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:VAL:HG22	1:D:62:GLN:OE1	2.19	0.41
1:C:389:GLU:H	1:C:389:GLU:HG2	1.69	0.41
1:D:112:PHE:O	1:D:448:GLY:N	2.50	0.41
1:A:249:GLN:HB3	1:A:254:THR:O	2.19	0.41
1:B:459:GLU:O	1:B:463:ARG:N	2.53	0.41
1:D:27:GLU:OE1	1:D:32:ASN:ND2	2.50	0.41
1:D:319:ARG:HA	5:D:640:HOH:O	2.21	0.41
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.92	0.41
1:B:439:GLN:HG2	1:B:440:THR:N	2.35	0.41
1:C:116:SER:HA	1:C:117:SER:HA	1.82	0.41
1:D:90:HIS:HA	1:D:91:PRO:HD3	1.87	0.41
1:D:135:ALA:O	1:D:139:TYR:HB2	2.21	0.41
1:D:220:LYS:HD3	1:D:237:GLN:HB3	2.01	0.41
1:D:378:LEU:HD12	1:D:449:PHE:HB3	2.01	0.41
1:A:233:GLU:O	1:A:237:GLN:HG2	2.19	0.41
1:B:464:LEU:HD23	1:B:464:LEU:HA	1.88	0.41
1:C:435:GLU:HA	1:C:436:ASN:HB3	2.01	0.41
1:D:452:LEU:HD21	1:D:457:ILE:HG12	2.02	0.41
1:A:222:ILE:HD13	1:A:237:GLN:HE21	1.86	0.41
1:A:434:LYS:NZ	1:A:436:ASN:H	2.19	0.41
1:B:38:LYS:HE2	1:B:76:GLY:HA3	2.02	0.41
1:B:411:GLU:CD	1:B:427:GLY:HA3	2.40	0.41
1:D:166:ARG:HB2	1:D:168:VAL:HG23	2.03	0.41
1:C:118:ASP:O	1:C:121:HIS:HD2	2.03	0.41
1:A:100:LYS:HG2	1:A:102:ILE:HG12	2.03	0.41
1:A:119:THR:HG21	1:B:140:ARG:O	2.21	0.41
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.93	0.41
1:A:318:LEU:HD11	1:A:347:THR:HG23	2.03	0.41
1:B:54:ASN:OD1	1:B:54:ASN:N	2.53	0.41
1:C:138:SER:HB2	1:C:349:LEU:HD13	2.01	0.41
1:B:346:LEU:O	1:B:350:THR:OG1	2.27	0.41
1:C:99:LEU:HD13	1:D:171:ARG:NH2	2.36	0.40
1:C:314:LEU:HD21	1:C:354:PHE:CE2	2.57	0.40
1:C:334:LYS:HZ1	1:D:100:LYS:HD2	1.86	0.40
1:D:326:PRO:HA	1:D:327:PRO:HD3	1.95	0.40
1:D:425:ILE:HD11	1:D:447:ILE:HD13	2.02	0.40
1:A:209:TYR:CZ	1:A:213:LYS:HD2	2.56	0.40
1:A:317:GLY:O	1:B:344:SER:HA	2.22	0.40
1:C:100:LYS:HD2	1:C:100:LYS:HA	1.68	0.40
1:A:75:LYS:HE2	1:A:75:LYS:HB2	1.81	0.40
1:B:59:ALA:O	1:B:63:LEU:HD22	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:HG23	1:B:307:MET:SD	2.62	0.40
1:B:256:MET:SD	1:B:261:ARG:HG3	2.61	0.40
1:B:316:PRO:HA	1:B:317:GLY:HA2	1.90	0.40
1:A:257:PRO:O	1:A:261:ARG:HG3	2.22	0.40
1:A:315:LEU:HB2	1:A:318:LEU:HB2	2.04	0.40
1:D:249:GLN:O	1:D:253:GLY:N	2.43	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	466/485 (96%)	434 (93%)	30 (6%)	2 (0%)	34	46
1	B	459/485 (95%)	425 (93%)	33 (7%)	1 (0%)	47	60
1	C	473/485 (98%)	443 (94%)	29 (6%)	1 (0%)	47	60
1	D	470/485 (97%)	435 (93%)	34 (7%)	1 (0%)	47	60
All	All	1868/1940 (96%)	1737 (93%)	126 (7%)	5 (0%)	41	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	ASP
1	A	435	GLU
1	A	74	ARG
1	C	88	GLU
1	D	95	LEU

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	416/431 (96%)	378 (91%)	38 (9%)	9 11
1	B	411/431 (95%)	380 (92%)	31 (8%)	13 17
1	C	422/431 (98%)	386 (92%)	36 (8%)	10 13
1	D	419/431 (97%)	380 (91%)	39 (9%)	9 10
All	All	1668/1724 (97%)	1524 (91%)	144 (9%)	10 13

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	4	THR
1	A	7	LEU
1	A	32	ASN
1	A	39	VAL
1	A	41	SER
1	A	51	VAL
1	A	97	ASP
1	A	100	LYS
1	A	108	ASP
1	A	117	SER
1	A	121	HIS
1	A	140	ARG
1	A	212	LEU
1	A	214	ASN
1	A	218	GLN
1	A	224	LEU
1	A	237	GLN
1	A	241	VAL
1	A	249	GLN
1	A	286	THR
1	A	296	GLN
1	A	328	GLU
1	A	331	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	346	LEU
1	A	349	LEU
1	A	382	LEU
1	A	385	GLU
1	A	392	VAL
1	A	408	ARG
1	A	409	ARG
1	A	423	LEU
1	A	430	ARG
1	A	435	GLU
1	A	451	ARG
1	A	454	GLU
1	A	465	PHE
1	A	469	TYR
1	B	4	THR
1	B	7	LEU
1	B	27	GLU
1	B	29	LEU
1	B	47	GLU
1	B	52	SER
1	B	54	ASN
1	B	63	LEU
1	B	97	ASP
1	B	99	LEU
1	B	119	THR
1	B	120	ASP
1	B	136	SER
1	B	140	ARG
1	B	183	VAL
1	B	210	GLN
1	B	224	LEU
1	B	252	SER
1	B	300	ARG
1	B	309	THR
1	B	315	LEU
1	B	328	GLU
1	B	375	ARG
1	B	378	LEU
1	B	417	HIS
1	B	421	LEU
1	B	425	ILE
1	B	437	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	438	ARG
1	B	462	GLN
1	B	464	LEU
1	C	2	ASP
1	C	29	LEU
1	C	39	VAL
1	C	45	LEU
1	C	47	GLU
1	C	80	GLU
1	C	95	LEU
1	C	97	ASP
1	C	100	LYS
1	C	103	HIS
1	C	107	SER
1	C	116	SER
1	C	121	HIS
1	C	124	ILE
1	C	169	LYS
1	C	183	VAL
1	C	205	TYR
1	C	212	LEU
1	C	241	VAL
1	C	289	VAL
1	C	296	GLN
1	C	307	MET
1	C	313	SER
1	C	315	LEU
1	C	319	ARG
1	C	328	GLU
1	C	361	GLN
1	C	382	LEU
1	C	406	ASP
1	C	408	ARG
1	C	423	LEU
1	C	433	LEU
1	C	437	LYS
1	C	440	THR
1	C	454	GLU
1	C	471	HIS
1	D	1	MET
1	D	6	THR
1	D	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	74	ARG
1	D	84	MET
1	D	85	PHE
1	D	88	GLU
1	D	89	GLU
1	D	99	LEU
1	D	100	LYS
1	D	118	ASP
1	D	125	LYS
1	D	145	MET
1	D	153	GLU
1	D	206	ARG
1	D	208	MET
1	D	221	THR
1	D	224	LEU
1	D	226	GLU
1	D	241	VAL
1	D	261	ARG
1	D	273	ARG
1	D	283	SER
1	D	313	SER
1	D	319	ARG
1	D	325	LEU
1	D	344	SER
1	D	361	GLN
1	D	366	LYS
1	D	368	LYS
1	D	378	LEU
1	D	383	GLU
1	D	389	GLU
1	D	402	VAL
1	D	406	ASP
1	D	434	LYS
1	D	442	ARG
1	D	455	GLU
1	D	471	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	B	352	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	182	GLN
1	C	369	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

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	$\#\|Z\| > 2$
3	IMD	C	502	-	3,5,5	0.41	0	4,5,5	0.60	0
3	IMD	D	502	-	3,5,5	0.40	0	4,5,5	0.60	0
4	ACT	C	504	-	3,3,3	0.76	0	3,3,3	1.37	0
4	ACT	D	504	-	3,3,3	0.75	0	3,3,3	1.37	0
4	ACT	B	503	-	3,3,3	0.78	0	3,3,3	1.40	0
4	ACT	A	503	-	3,3,3	0.78	0	3,3,3	1.36	0
4	ACT	D	503	-	3,3,3	0.77	0	3,3,3	1.34	0
3	IMD	B	502	-	3,5,5	0.40	0	4,5,5	0.59	0
4	ACT	B	505	-	3,3,3	0.76	0	3,3,3	1.35	0
4	ACT	C	503	-	3,3,3	0.76	0	3,3,3	1.35	0
4	ACT	B	504	-	3,3,3	0.78	0	3,3,3	1.31	0
3	IMD	A	502	-	3,5,5	0.40	0	4,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	B	506	-	3,3,3	0.75	0	3,3,3	1.36	0

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
3	IMD	C	502	-	-	-	0/1/1/1
3	IMD	A	502	-	-	-	0/1/1/1
3	IMD	B	502	-	-	-	0/1/1/1
3	IMD	D	502	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	IMD	1	0
4	B	503	ACT	2	0
4	B	505	ACT	1	0
4	C	503	ACT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	468/485 (96%)	0.28	38 (8%)	12	15	20, 49, 102, 126	0
1	B	463/485 (95%)	0.21	29 (6%)	20	23	15, 42, 98, 143	0
1	C	475/485 (97%)	0.02	18 (3%)	40	47	16, 36, 93, 137	0
1	D	472/485 (97%)	0.04	22 (4%)	31	38	13, 36, 91, 123	0
All	All	1878/1940 (96%)	0.14	107 (5%)	23	28	13, 40, 97, 143	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	LEU	8.6
1	A	387	SER	8.0
1	D	141	THR	7.8
1	A	99	LEU	7.0
1	B	139	TYR	5.4
1	B	144	ASP	5.4
1	C	139	TYR	5.3
1	D	92	PRO	5.3
1	B	76	GLY	5.1
1	D	438	ARG	4.9
1	A	436	ASN	4.8
1	B	106	GLN	4.7
1	C	99	LEU	4.6
1	D	140	ARG	4.6
1	B	440	THR	4.5
1	D	142	LEU	4.5
1	A	438	ARG	4.4
1	C	1	MET	4.2
1	D	90	HIS	4.1
1	B	438	ARG	4.1
1	B	49	LEU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	7	LEU	4.0
1	A	423	LEU	3.9
1	B	436	ASN	3.9
1	A	390	VAL	3.9
1	A	469	TYR	3.9
1	D	143	GLY	3.9
1	A	408	ARG	3.8
1	D	91	PRO	3.8
1	D	316	PRO	3.8
1	A	435	GLU	3.8
1	C	89	GLU	3.6
1	D	441	GLY	3.6
1	D	94	ALA	3.6
1	B	140	ARG	3.6
1	A	139	TYR	3.4
1	C	437	LYS	3.4
1	B	5	ILE	3.4
1	A	110	ILE	3.3
1	C	100	LYS	3.3
1	A	100	LYS	3.2
1	A	315	LEU	3.2
1	C	141	THR	3.1
1	B	317	GLY	3.1
1	D	139	TYR	3.1
1	A	72	ILE	3.1
1	D	437	LYS	3.1
1	A	419	ALA	3.0
1	C	3	ILE	3.0
1	A	468	VAL	3.0
1	B	318	LEU	3.0
1	D	95	LEU	2.9
1	C	121	HIS	2.9
1	D	74	ARG	2.9
1	A	109	TRP	2.8
1	C	436	ASN	2.8
1	D	436	ASN	2.8
1	A	108	ASP	2.8
1	A	106	GLN	2.8
1	A	421	LEU	2.8
1	A	5	ILE	2.8
1	B	316	PRO	2.8
1	A	140	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	439	GLN	2.7
1	A	439	GLN	2.7
1	B	143	GLY	2.7
1	B	33	LEU	2.7
1	B	53	VAL	2.7
1	A	102	ILE	2.7
1	B	141	THR	2.7
1	A	316	PRO	2.7
1	A	117	SER	2.7
1	B	3	ILE	2.7
1	D	108	ASP	2.7
1	B	27	GLU	2.6
1	D	103	HIS	2.6
1	D	1	MET	2.6
1	D	100	LYS	2.6
1	A	3	ILE	2.5
1	A	405	PHE	2.5
1	C	316	PRO	2.5
1	B	4	THR	2.5
1	D	122	PHE	2.5
1	C	438	ARG	2.4
1	B	136	SER	2.4
1	C	143	GLY	2.4
1	B	6	THR	2.4
1	A	34	LEU	2.4
1	A	116	SER	2.4
1	A	33	LEU	2.4
1	B	60	TYR	2.3
1	A	104	ILE	2.3
1	A	465	PHE	2.3
1	A	75	LYS	2.3
1	C	2	ASP	2.3
1	A	122	PHE	2.2
1	A	414	ILE	2.2
1	A	464	LEU	2.2
1	B	2	ASP	2.2
1	B	9	ARG	2.2
1	B	21	TYR	2.2
1	C	96	PRO	2.2
1	B	74	ARG	2.1
1	B	138	SER	2.1
1	C	140	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	317	GLY	2.1
1	C	76	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	D	504	4/4	0.53	0.26	55,62,62,65	0
2	ZN	C	501	1/1	0.78	0.14	78,78,78,78	0
4	ACT	B	505	4/4	0.85	0.20	45,57,58,63	0
2	ZN	B	501	1/1	0.86	0.18	88,88,88,88	0
4	ACT	C	504	4/4	0.88	0.14	51,58,58,61	0
4	ACT	B	504	4/4	0.88	0.13	24,42,43,50	0
3	IMD	A	502	5/5	0.89	0.15	41,41,43,43	0
4	ACT	A	503	4/4	0.91	0.15	28,29,33,44	0
4	ACT	B	503	4/4	0.91	0.30	27,29,37,49	0
3	IMD	C	502	5/5	0.93	0.13	27,31,37,40	0
4	ACT	C	503	4/4	0.93	0.15	26,38,42,44	0
2	ZN	D	501	1/1	0.94	0.11	81,81,81,81	0
4	ACT	D	503	4/4	0.95	0.13	38,42,43,44	0
3	IMD	B	502	5/5	0.96	0.11	17,20,22,26	0
4	ACT	B	506	4/4	0.96	0.14	60,61,62,64	0
3	IMD	D	502	5/5	0.98	0.13	28,29,37,38	0
2	ZN	A	501	1/1	0.99	0.09	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.