



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 06:34 pm GMT

PDB ID : 4A3R
Title : Crystal structure of Enolase from *Bacillus subtilis*.
Authors : Newman, J.A.; Hewitt, L.; Rodrigues, C.; Solovyova, A.S.; Harwood, C.R.;
Lewis, R.J.
Deposited on : 2011-10-04
Resolution : 2.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, 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

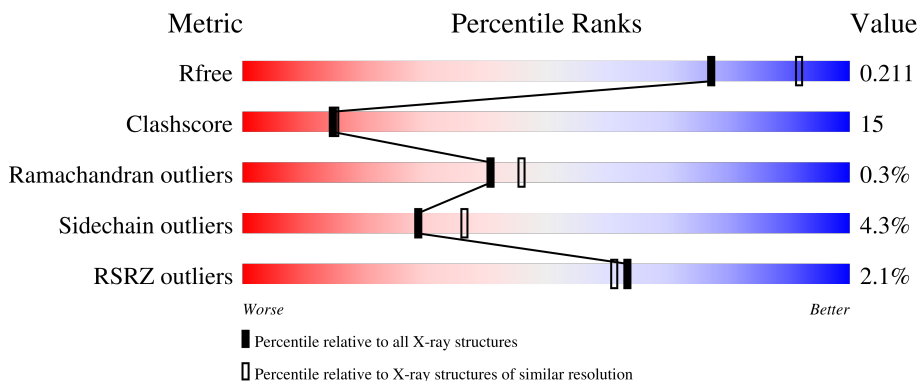
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	 78% 20% .
1	B	430	 4% 75% 21% .
1	C	430	 3% 76% 21% .
1	D	430	 83% 14% .

2 Entry composition [i](#)

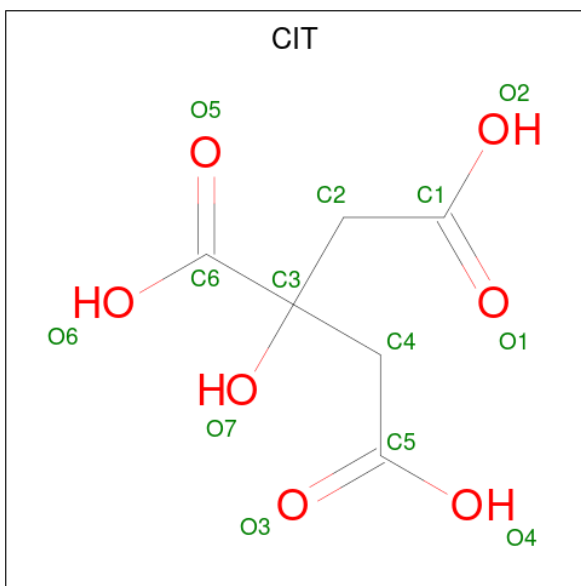
There are 4 unique types of molecules in this entry. The entry contains 13840 atoms, of which 5 are hydrogens and 0 are deuteriums.

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 ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	428	Total 3258	C 2044	N 547	O 656	S 11	0	0	0
1	B	428	Total 3258	C 2044	N 547	O 656	S 11	0	0	0
1	C	428	Total 3258	C 2044	N 547	O 656	S 11	0	0	0
1	D	428	Total 3258	C 2044	N 547	O 656	S 11	0	0	0

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	D	1	Total 18	C 6	H 5	O 7	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	Na 2	0	0

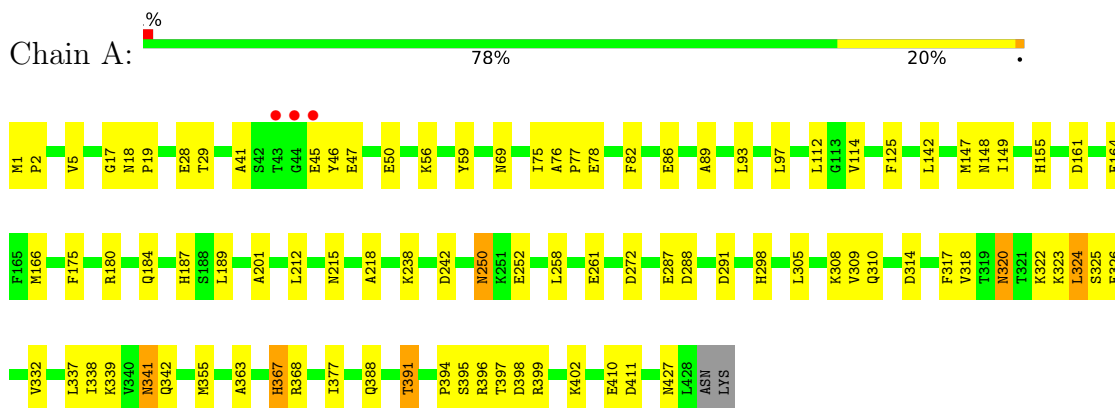
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	229	Total 229	O 229	0	0
4	B	154	Total 154	O 154	0	0
4	C	204	Total 204	O 204	0	0
4	D	201	Total 201	O 201	0	0

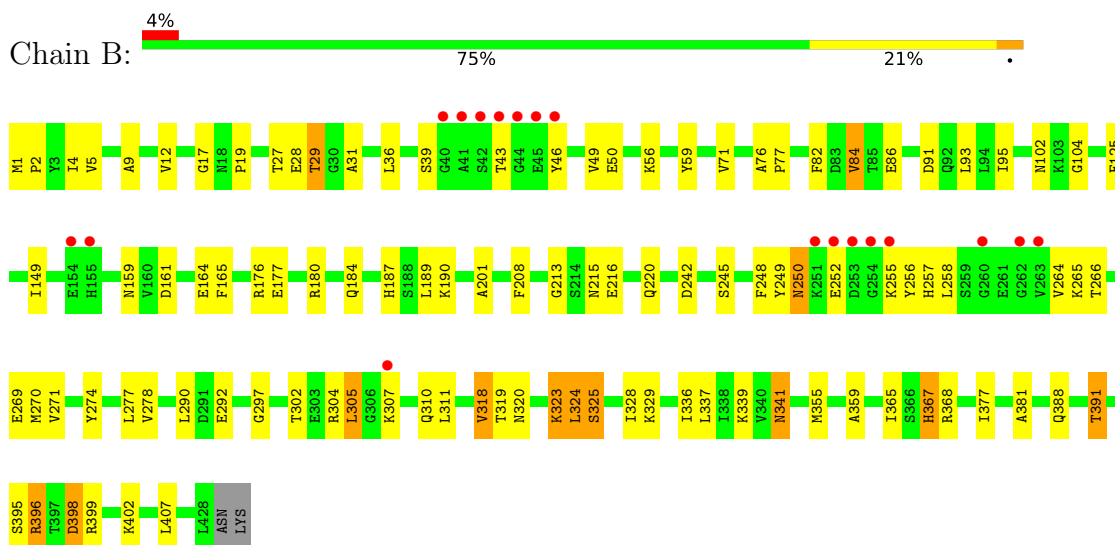
3 Residue-property plots [i](#)

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.

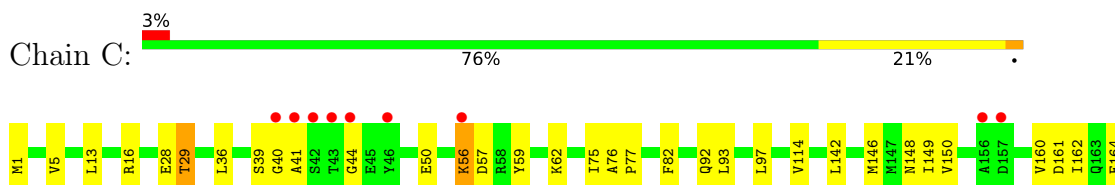
- Molecule 1: ENOLASE

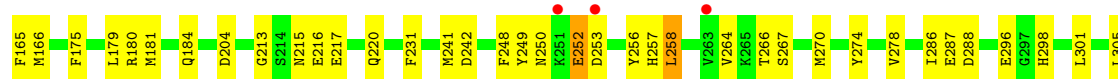


- Molecule 1: ENOLASE

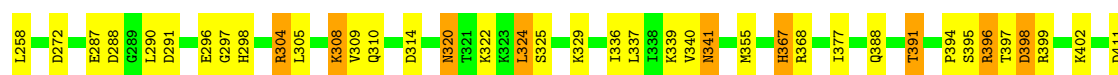
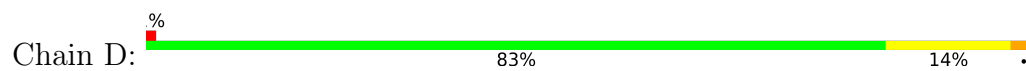


- Molecule 1: ENOLASE





• Molecule 1: ENOLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	187.07Å 187.07Å 56.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.20 19.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.83-2.20) 90.1 (19.83-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.19Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.174 , 0.218 0.169 , 0.211	Depositor DCC
R_{free} test set	4822 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtrriage
Anisotropy	0.517	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13840	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/3308	0.55	0/4478
1	B	0.39	0/3308	0.53	0/4478
1	C	0.39	0/3308	0.54	0/4478
1	D	0.41	0/3308	0.56	1/4478 (0.0%)
All	All	0.40	0/13232	0.55	1/17912 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	LEU	CA-CB-CG	-5.68	102.24	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3258	0	3211	98	0
1	B	3258	0	3211	108	0
1	C	3258	0	3211	110	0
1	D	3258	0	3211	90	0
2	D	13	5	5	3	0
3	D	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	229	0	0	8	0
4	B	154	0	0	4	0
4	C	204	0	0	8	0
4	D	201	0	0	5	0
All	All	13835	5	12849	393	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 15.

All (393) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:LEU:HB3	1:D:355:MET:CE	1.74	1.16
1:D:324:LEU:HB3	1:D:355:MET:HE2	1.14	1.12
1:A:324:LEU:HB3	1:A:355:MET:HE2	1.28	1.11
1:A:142:LEU:HD21	1:A:410:GLU:HB2	1.10	1.10
1:A:147:MET:HE2	1:A:394:PRO:HD3	1.30	1.10
1:B:324:LEU:HB3	1:B:355:MET:HE2	1.28	1.08
1:C:142:LEU:HD21	1:C:410:GLU:HB2	1.35	1.04
1:C:324:LEU:HB3	1:C:355:MET:HE1	1.40	1.00
1:A:310:GLN:HE22	1:A:388:GLN:HE22	1.03	0.98
1:B:161:ASP:H	1:B:215:ASN:HD21	1.12	0.98
1:D:310:GLN:HE22	1:D:388:GLN:HE22	1.05	0.98
1:A:341:ASN:HD21	1:A:368:ARG:HH11	1.07	0.97
1:A:391:THR:HG21	1:A:402:LYS:HG2	1.47	0.95
1:A:142:LEU:CD2	1:A:410:GLU:HB2	1.97	0.94
1:C:310:GLN:HE22	1:C:388:GLN:HE22	1.13	0.93
1:D:314:ASP:OD2	4:D:2161:HOH:O	1.88	0.91
1:D:147:MET:CE	1:D:394:PRO:HD3	2.00	0.90
1:A:324:LEU:HB3	1:A:355:MET:CE	2.02	0.90
1:D:325:SER:N	1:D:355:MET:HE1	1.87	0.90
1:D:308:LYS:HG3	1:D:309:VAL:HG23	1.54	0.88
1:C:324:LEU:HB3	1:C:355:MET:CE	2.02	0.88
1:B:310:GLN:HE22	1:B:388:GLN:HE22	1.18	0.87
1:B:341:ASN:HD21	1:B:368:ARG:HH11	1.24	0.86
1:D:161:ASP:H	1:D:215:ASN:HD21	1.24	0.85
1:D:5:VAL:CG1	1:D:28:GLU:HG3	2.07	0.85
1:B:271:VAL:HG11	1:B:304:ARG:HG3	1.59	0.85
1:B:324:LEU:HB3	1:B:355:MET:CE	2.07	0.84
1:D:1:MET:SD	4:D:2001:HOH:O	2.36	0.84
1:D:367:HIS:CD2	1:D:399:ARG:HH11	1.96	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:LEU:HD13	1:D:355:MET:HG2	1.59	0.83
1:B:164:GLU:HG3	1:B:242:ASP:HB3	1.59	0.83
1:A:142:LEU:HD21	1:A:410:GLU:CB	2.03	0.82
1:B:255:LYS:HE2	1:B:266:THR:HG22	1.60	0.81
1:A:341:ASN:HD21	1:A:368:ARG:NH1	1.79	0.81
1:B:250:ASN:HB2	1:B:257:HIS:CD2	2.16	0.81
1:A:250:ASN:HD21	1:A:252:GLU:HB3	1.46	0.81
1:D:30:GLY:O	4:D:2023:HOH:O	1.98	0.81
1:D:324:LEU:CB	1:D:355:MET:HE2	2.07	0.80
1:C:320:ASN:HD22	1:C:323:LYS:H	1.28	0.80
1:C:142:LEU:CD2	1:C:410:GLU:HB2	2.12	0.79
1:B:1:MET:HG2	1:B:125:PHE:HE1	1.47	0.79
1:C:318:VAL:HG13	1:C:318:VAL:O	1.81	0.78
1:B:1:MET:HG3	1:B:29:THR:HB	1.66	0.77
1:D:391:THR:HG21	1:D:402:LYS:HG2	1.65	0.76
1:B:318:VAL:O	1:B:318:VAL:HG13	1.85	0.76
1:A:147:MET:CE	1:A:394:PRO:HD3	2.12	0.75
1:B:161:ASP:H	1:B:215:ASN:ND2	1.82	0.75
1:B:250:ASN:HB2	1:B:257:HIS:HD2	1.48	0.75
1:C:161:ASP:H	1:C:215:ASN:HD21	1.34	0.74
1:C:296:GLU:HB2	4:C:2152:HOH:O	1.87	0.74
1:A:341:ASN:ND2	1:A:368:ARG:HH11	1.83	0.74
1:C:391:THR:HG21	1:C:402:LYS:HG2	1.70	0.73
1:A:5:VAL:CG1	1:A:28:GLU:HG2	2.18	0.73
1:C:318:VAL:O	1:C:318:VAL:CG1	2.36	0.73
1:C:1:MET:HG3	1:C:29:THR:HB	1.69	0.73
1:A:180:ARG:HH11	1:A:184:GLN:HE22	1.33	0.73
1:A:272:ASP:OD2	4:A:2159:HOH:O	2.06	0.73
1:C:288:ASP:OD2	1:C:314:ASP:HB3	1.89	0.73
1:B:161:ASP:N	1:B:215:ASN:HD21	1.86	0.72
1:D:147:MET:HE2	1:D:394:PRO:HD3	1.71	0.72
1:D:147:MET:HE3	1:D:394:PRO:HD3	1.71	0.72
1:A:59:TYR:H	1:B:184:GLN:HE21	1.37	0.72
1:A:59:TYR:H	1:B:184:GLN:NE2	1.86	0.72
1:B:249:TYR:CD1	1:B:256:TYR:CE1	2.77	0.71
1:A:1:MET:HG2	1:A:29:THR:HG21	1.72	0.71
1:C:184:GLN:HE21	1:D:59:TYR:H	1.38	0.71
1:D:377:ILE:HD11	1:D:391:THR:CG2	2.21	0.71
1:D:1:MET:HG3	1:D:29:THR:HB	1.72	0.71
1:A:45:GLU:HG3	1:A:46:TYR:CD2	2.26	0.70
1:B:318:VAL:O	1:B:318:VAL:CG1	2.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LEU:HD23	1:D:339:LYS:HE3	1.73	0.70
1:C:250:ASN:HD22	1:C:253:ASP:H	1.38	0.70
1:A:142:LEU:HD23	1:A:175:PHE:HB3	1.73	0.70
1:B:329:LYS:NZ	1:B:329:LYS:CB	2.54	0.70
1:C:324:LEU:HD13	1:C:355:MET:HE2	1.73	0.70
1:B:149:ILE:HG12	1:B:189:LEU:CD2	2.22	0.69
1:D:161:ASP:N	1:D:215:ASN:HD21	1.90	0.69
1:A:337:LEU:HD23	1:A:339:LYS:HE3	1.74	0.69
1:C:5:VAL:HG13	1:C:28:GLU:HG3	1.74	0.69
1:A:147:MET:HE2	1:A:394:PRO:CD	2.17	0.69
1:A:161:ASP:H	1:A:215:ASN:HD21	1.39	0.69
1:A:250:ASN:ND2	1:A:252:GLU:HB3	2.07	0.69
1:B:329:LYS:HZ3	1:B:329:LYS:HB3	1.58	0.69
1:A:69:ASN:HB3	4:A:2049:HOH:O	1.93	0.69
1:D:250:ASN:HD21	1:D:252:GLU:HB2	1.58	0.68
1:B:325:SER:N	1:B:355:MET:HE1	2.08	0.68
1:D:325:SER:N	1:D:355:MET:CE	2.56	0.68
1:B:324:LEU:HD13	1:B:355:MET:HG2	1.76	0.68
1:C:59:TYR:H	1:D:184:GLN:NE2	1.91	0.68
1:B:249:TYR:HD1	1:B:256:TYR:CE1	2.12	0.68
1:A:287:GLU:OE2	4:A:2144:HOH:O	2.10	0.67
1:C:184:GLN:NE2	1:D:59:TYR:H	1.92	0.67
1:C:367:HIS:CD2	1:C:399:ARG:HH11	2.12	0.67
1:A:184:GLN:NE2	1:B:59:TYR:H	1.93	0.67
1:A:310:GLN:NE2	1:A:388:GLN:HE22	1.86	0.67
1:A:1:MET:HG3	1:A:29:THR:HB	1.76	0.67
1:B:1:MET:HG3	1:B:29:THR:CB	2.24	0.67
1:A:164:GLU:HG2	4:A:2095:HOH:O	1.94	0.66
1:C:274:TYR:O	1:C:278:VAL:HG23	1.95	0.66
1:D:377:ILE:HD11	1:D:391:THR:HG23	1.77	0.66
1:A:310:GLN:HE22	1:A:388:GLN:NE2	1.86	0.66
1:C:59:TYR:H	1:D:184:GLN:HE21	1.43	0.66
1:A:142:LEU:HD23	1:A:175:PHE:CB	2.26	0.65
1:B:86:GLU:OE2	4:B:2042:HOH:O	2.14	0.65
1:D:250:ASN:HB3	1:D:253:ASP:OD1	1.95	0.65
1:D:5:VAL:HG13	1:D:28:GLU:HG3	1.79	0.64
1:B:341:ASN:HD21	1:B:368:ARG:NH1	1.96	0.64
1:B:367:HIS:CD2	1:B:399:ARG:HH11	2.16	0.64
1:C:162:ILE:H	1:C:215:ASN:ND2	1.95	0.64
1:A:377:ILE:HD11	1:A:391:THR:CG2	2.28	0.63
1:C:161:ASP:N	1:C:215:ASN:HD21	1.94	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:ARG:HE	2:D:1429:CIT:C1	2.12	0.63
1:C:5:VAL:CG1	1:C:28:GLU:HG3	2.28	0.63
1:C:324:LEU:HD13	1:C:355:MET:HG2	1.79	0.63
1:B:395:SER:O	1:B:396:ARG:HB2	1.97	0.62
1:C:146:MET:HG2	1:C:166:MET:SD	2.39	0.62
1:A:308:LYS:HG3	1:A:309:VAL:HG23	1.79	0.62
1:B:93:LEU:C	1:B:93:LEU:HD23	2.20	0.62
1:D:147:MET:CE	1:D:394:PRO:CD	2.77	0.62
4:C:2053:HOH:O	1:D:177:GLU:OE2	2.16	0.62
1:A:250:ASN:HD21	1:A:252:GLU:CB	2.12	0.62
1:C:320:ASN:HD21	1:C:322:LYS:HB2	1.64	0.62
1:D:287:GLU:OE2	1:D:337:LEU:HD22	2.00	0.62
1:A:112:LEU:HD22	1:A:341:ASN:HA	1.82	0.61
1:B:325:SER:N	1:B:355:MET:CE	2.63	0.61
1:B:76:ALA:HB3	1:B:77:PRO:HD3	1.81	0.61
1:C:56:LYS:CE	4:C:2050:HOH:O	2.48	0.61
1:C:5:VAL:CG1	1:C:28:GLU:CG	2.78	0.61
1:C:248:PHE:CE1	1:C:258:LEU:HD11	2.36	0.61
1:D:367:HIS:HD2	1:D:399:ARG:HH11	1.48	0.61
1:A:180:ARG:HH11	1:A:184:GLN:NE2	1.99	0.60
1:C:142:LEU:HD23	1:C:175:PHE:CB	2.31	0.60
1:B:341:ASN:ND2	1:B:368:ARG:HH11	1.97	0.60
1:A:5:VAL:HG11	1:A:28:GLU:HA	1.83	0.60
1:A:325:SER:HB3	1:A:355:MET:HE1	1.83	0.60
1:B:325:SER:CB	1:B:355:MET:HE1	2.31	0.60
1:D:1:MET:HG2	1:D:125:PHE:HE1	1.67	0.60
1:B:329:LYS:NZ	1:B:329:LYS:HB3	2.15	0.59
1:B:49:VAL:HG23	1:B:104:GLY:HA2	1.84	0.59
1:C:62:LYS:NZ	4:C:2022:HOH:O	2.35	0.59
1:A:142:LEU:HD22	1:A:410:GLU:OE2	2.01	0.59
1:B:245:SER:HA	1:B:248:PHE:CE1	2.37	0.59
1:B:391:THR:HG21	1:B:402:LYS:HG2	1.83	0.59
1:A:149:ILE:HG12	1:A:189:LEU:CD2	2.33	0.59
1:A:324:LEU:HD13	1:A:355:MET:HG2	1.85	0.59
1:B:149:ILE:HG12	1:B:189:LEU:HD22	1.84	0.59
1:C:162:ILE:H	1:C:215:ASN:HD21	1.50	0.59
1:D:325:SER:CA	1:D:355:MET:HE1	2.33	0.58
1:C:161:ASP:H	1:C:215:ASN:ND2	2.01	0.58
1:B:216:GLU:O	1:B:220:GLN:HG3	2.03	0.58
1:D:341:ASN:HD21	1:D:368:ARG:HH11	1.52	0.58
1:C:318:VAL:HG12	1:C:320:ASN:HB2	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASN:HD22	1:A:323:LYS:H	1.51	0.58
1:D:161:ASP:H	1:D:215:ASN:ND2	1.98	0.58
1:A:367:HIS:HB3	1:A:391:THR:HG22	1.86	0.57
1:B:180:ARG:HH11	1:B:184:GLN:NE2	2.02	0.57
1:C:5:VAL:HG11	1:C:28:GLU:HA	1.87	0.57
1:C:325:SER:N	1:C:355:MET:CE	2.67	0.57
1:D:40:GLY:HA2	2:D:1429:CIT:O2	2.04	0.57
1:C:377:ILE:HD11	1:C:391:THR:HG23	1.86	0.57
1:D:5:VAL:CG1	1:D:28:GLU:CG	2.82	0.57
1:C:248:PHE:CD1	1:C:258:LEU:CD1	2.88	0.56
1:B:318:VAL:HG12	1:B:320:ASN:HB2	1.87	0.56
1:D:1:MET:HG3	1:D:29:THR:CB	2.35	0.56
1:A:149:ILE:HG12	1:A:189:LEU:HD22	1.87	0.56
1:A:367:HIS:CD2	1:A:399:ARG:HH11	2.23	0.56
1:C:248:PHE:CD1	1:C:258:LEU:HD12	2.40	0.56
1:C:1:MET:HG3	1:C:29:THR:CB	2.34	0.56
1:C:257:HIS:CE1	1:C:264:VAL:HG21	2.40	0.56
1:C:329:LYS:HB3	1:C:329:LYS:NZ	2.21	0.56
1:B:325:SER:CA	1:B:355:MET:HE1	2.36	0.56
1:B:5:VAL:CG1	1:B:28:GLU:HG2	2.36	0.56
1:D:325:SER:H	1:D:355:MET:HE1	1.70	0.55
1:A:325:SER:N	1:A:355:MET:HE1	2.22	0.55
1:A:318:VAL:HG23	1:A:342:GLN:NE2	2.22	0.55
1:D:288:ASP:OD2	1:D:314:ASP:HB3	2.06	0.55
1:D:290:LEU:HD13	1:D:297:GLY:C	2.27	0.55
1:B:248:PHE:HE2	1:B:270:MET:HE2	1.73	0.54
1:C:149:ILE:HG23	1:C:150:VAL:HG23	1.89	0.54
1:C:40:GLY:CA	1:C:341:ASN:HD21	2.20	0.54
1:D:324:LEU:HB3	1:D:355:MET:HE3	1.83	0.54
1:B:248:PHE:HE2	1:B:270:MET:CE	2.20	0.54
1:C:298:HIS:HB3	1:C:332:VAL:HG13	1.90	0.54
1:D:367:HIS:HB3	1:D:391:THR:HG22	1.87	0.54
1:C:395:SER:O	1:C:396:ARG:HB2	2.08	0.54
1:D:180:ARG:HH11	1:D:184:GLN:HE22	1.56	0.54
1:A:161:ASP:N	1:A:215:ASN:HD21	2.07	0.53
1:C:249:TYR:HB2	1:C:256:TYR:CE1	2.44	0.53
4:C:2010:HOH:O	1:D:411:ASP:HB2	2.08	0.53
1:D:291:ASP:O	1:D:298:HIS:HE1	1.91	0.53
1:B:265:LYS:HB3	1:B:269:GLU:HB2	1.91	0.53
1:A:93:LEU:C	1:A:93:LEU:HD23	2.30	0.53
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:VAL:HG13	1:A:318:VAL:O	2.09	0.52
1:B:49:VAL:CG2	1:B:104:GLY:HA2	2.39	0.52
1:B:5:VAL:HG13	1:B:28:GLU:HG3	1.90	0.52
1:C:16:ARG:HD3	1:C:204:ASP:CG	2.30	0.52
1:D:5:VAL:HG11	1:D:28:GLU:HA	1.90	0.52
1:A:78:GLU:HG3	1:A:97:LEU:HD11	1.91	0.52
1:D:341:ASN:ND2	1:D:368:ARG:HH11	2.07	0.52
1:C:324:LEU:HD13	1:C:355:MET:CE	2.39	0.52
1:C:397:THR:OG1	1:D:398:ASP:HB3	2.10	0.51
1:B:36:LEU:N	1:B:36:LEU:HD12	2.24	0.51
1:B:304:ARG:O	1:B:305:LEU:HD12	2.10	0.51
1:B:5:VAL:CG1	1:B:28:GLU:CG	2.89	0.51
1:B:290:LEU:HD13	1:B:297:GLY:C	2.31	0.51
1:A:250:ASN:ND2	1:A:252:GLU:CB	2.72	0.51
1:A:314:ASP:OD2	4:A:2144:HOH:O	2.19	0.51
1:B:329:LYS:HB2	1:B:329:LYS:HZ2	1.76	0.51
1:C:250:ASN:HB3	1:C:253:ASP:OD1	2.10	0.51
1:D:27:THR:CG2	1:D:31:ALA:HB3	2.41	0.51
1:A:320:ASN:HD21	1:A:322:LYS:HB2	1.74	0.51
1:A:291:ASP:O	1:A:298:HIS:HE1	1.92	0.51
1:B:328:ILE:HD13	1:B:359:ALA:HB2	1.93	0.51
1:A:201:ALA:HB3	1:B:201:ALA:HB3	1.92	0.50
1:B:176:ARG:HG3	1:B:407:LEU:HD22	1.92	0.50
1:D:395:SER:O	1:D:396:ARG:HB2	2.10	0.50
1:B:320:ASN:HD22	1:B:323:LYS:H	1.58	0.50
1:C:249:TYR:HD1	1:C:256:TYR:CE1	2.29	0.50
1:A:1:MET:HG3	1:A:29:THR:CB	2.42	0.50
1:D:272:ASP:OD1	1:D:304:ARG:NH2	2.44	0.50
1:D:377:ILE:CD1	1:D:391:THR:HG23	2.42	0.50
1:D:308:LYS:NZ	1:D:308:LYS:HB3	2.27	0.50
1:B:329:LYS:NZ	1:B:329:LYS:HB2	2.27	0.50
1:C:44:GLY:C	4:C:2037:HOH:O	2.50	0.50
1:C:180:ARG:HH11	1:C:184:GLN:NE2	2.09	0.50
1:D:148:ASN:HA	1:D:166:MET:HG2	1.94	0.49
1:A:1:MET:HG2	1:A:125:PHE:HE1	1.77	0.49
1:D:101:GLU:OE1	4:D:2078:HOH:O	2.18	0.49
1:A:325:SER:N	1:A:355:MET:CE	2.76	0.49
1:D:180:ARG:HH11	1:D:184:GLN:NE2	2.08	0.49
1:C:391:THR:HG21	1:C:402:LYS:CG	2.41	0.49
1:D:367:HIS:CD2	1:D:399:ARG:NH1	2.73	0.49
1:A:5:VAL:HG12	1:A:28:GLU:HG2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:SER:CA	1:C:355:MET:HE3	2.43	0.49
1:A:397:THR:OG1	1:B:398:ASP:HB3	2.13	0.48
1:B:49:VAL:HG22	1:B:102:ASN:O	2.13	0.48
1:D:324:LEU:HD13	1:D:355:MET:CE	2.43	0.48
1:A:148:ASN:HA	1:A:166:MET:HG2	1.95	0.48
1:B:377:ILE:HD11	1:B:391:THR:HG23	1.95	0.48
1:A:180:ARG:NH1	1:A:184:GLN:HE22	2.09	0.48
1:A:161:ASP:H	1:A:215:ASN:ND2	2.09	0.48
1:B:149:ILE:HG22	1:B:165:PHE:O	2.14	0.48
1:C:16:ARG:HD3	1:C:204:ASP:OD2	2.13	0.48
1:C:256:TYR:CD2	1:C:270:MET:HG3	2.49	0.48
1:C:377:ILE:HD11	1:C:391:THR:CG2	2.43	0.48
1:A:317:PHE:O	1:A:318:VAL:HG12	2.14	0.47
1:C:56:LYS:HE3	4:C:2050:HOH:O	2.11	0.47
1:D:147:MET:HE1	1:D:394:PRO:HG3	1.97	0.47
1:B:250:ASN:CB	1:B:257:HIS:CD2	2.92	0.47
1:C:179:LEU:HD21	1:D:13:LEU:HD22	1.97	0.47
1:C:249:TYR:CD1	1:C:256:TYR:CE1	3.02	0.47
1:A:5:VAL:CG1	1:A:28:GLU:CG	2.90	0.47
1:B:180:ARG:HH11	1:B:184:GLN:HE22	1.62	0.47
1:B:249:TYR:HB2	1:B:256:TYR:CE1	2.50	0.47
1:D:320:ASN:HD22	1:D:322:LYS:H	1.62	0.47
1:B:1:MET:HG2	1:B:125:PHE:CE1	2.38	0.47
1:B:325:SER:HB3	1:B:355:MET:HE1	1.96	0.47
1:A:212:LEU:HD13	1:A:218:ALA:HA	1.95	0.47
1:B:337:LEU:HD23	1:B:339:LYS:HE3	1.95	0.47
1:C:142:LEU:HD23	1:C:175:PHE:HB3	1.97	0.47
1:B:274:TYR:O	1:B:278:VAL:HG23	2.15	0.47
1:C:93:LEU:C	1:C:93:LEU:HD23	2.36	0.47
1:D:337:LEU:CD2	1:D:339:LYS:HE3	2.43	0.47
1:D:341:ASN:HD21	1:D:368:ARG:NH1	2.13	0.46
1:B:395:SER:O	1:B:396:ARG:CB	2.63	0.46
1:D:324:LEU:HD13	1:D:355:MET:HE3	1.97	0.46
1:C:142:LEU:CD2	1:C:175:PHE:HB3	2.45	0.46
1:D:250:ASN:C	1:D:250:ASN:HD22	2.18	0.46
1:B:391:THR:HG21	1:B:402:LYS:CG	2.45	0.46
1:C:367:HIS:HD2	1:C:399:ARG:HH11	1.62	0.46
1:A:187:HIS:HE1	1:B:17:GLY:O	1.99	0.46
1:D:324:LEU:CD1	1:D:355:MET:HG2	2.40	0.46
1:B:328:ILE:HD13	1:B:359:ALA:CB	2.46	0.46
1:C:180:ARG:HH11	1:C:184:GLN:HE22	1.62	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HD23	1:B:93:LEU:O	2.15	0.45
1:C:310:GLN:NE2	1:C:388:GLN:HE22	1.95	0.45
1:D:1:MET:HE3	1:D:2:PRO:HD3	1.97	0.45
1:B:341:ASN:ND2	4:B:2123:HOH:O	2.30	0.45
1:A:411:ASP:HB2	4:A:2213:HOH:O	2.16	0.45
1:B:5:VAL:HG13	1:B:28:GLU:CG	2.47	0.45
1:C:241:MET:HE2	1:C:286:ILE:HG12	1.98	0.45
1:C:181:MET:HG2	1:C:231:PHE:CE1	2.51	0.45
1:A:75:ILE:HG21	1:A:114:VAL:HG21	1.99	0.45
1:C:242:ASP:HA	1:C:287:GLU:HB3	1.99	0.45
1:C:325:SER:N	1:C:355:MET:HE1	2.32	0.45
1:D:64:VAL:HA	4:D:2044:HOH:O	2.17	0.45
1:D:177:GLU:O	1:D:181:MET:HG3	2.17	0.45
1:A:298:HIS:HB3	1:A:332:VAL:HG13	1.99	0.45
1:C:310:GLN:HE22	1:C:388:GLN:NE2	1.96	0.45
1:C:41:ALA:C	1:C:50:GLU:HG2	2.37	0.45
1:C:320:ASN:ND2	1:C:323:LYS:H	2.06	0.45
1:B:324:LEU:HG	1:B:336:ILE:HD12	1.99	0.45
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.78	0.44
1:B:257:HIS:ND1	1:B:264:VAL:CG2	2.81	0.44
1:B:257:HIS:ND1	1:B:264:VAL:HG21	2.32	0.44
1:C:142:LEU:CD2	1:C:175:PHE:CB	2.96	0.44
1:D:367:HIS:CG	1:D:391:THR:HA	2.52	0.44
1:A:391:THR:O	1:A:399:ARG:HB3	2.17	0.44
1:B:46:TYR:CG	1:B:323:LYS:HE3	2.53	0.44
1:C:160:VAL:HG13	1:C:215:ASN:ND2	2.32	0.44
1:A:427:ASN:OD1	1:A:427:ASN:N	2.51	0.44
1:B:161:ASP:OD2	1:B:258:LEU:HB3	2.17	0.44
1:A:17:GLY:O	1:B:187:HIS:HE1	2.01	0.44
1:C:328:ILE:HD13	1:C:359:ALA:HB2	1.99	0.44
1:B:29:THR:O	1:B:29:THR:HG23	2.17	0.44
1:D:320:ASN:HD22	1:D:320:ASN:C	2.21	0.44
1:C:36:LEU:HD12	1:C:36:LEU:N	2.32	0.43
1:C:39:SER:HB3	1:C:370:GLY:HA3	1.99	0.43
1:D:146:MET:HG2	1:D:166:MET:SD	2.58	0.43
1:D:258:LEU:N	1:D:258:LEU:HD12	2.33	0.43
1:B:9:ALA:HB2	1:B:71:VAL:HG11	2.01	0.43
1:B:91:ASP:O	1:B:95:ILE:HG13	2.17	0.43
1:B:319:THR:O	1:B:319:THR:HG22	2.18	0.43
1:D:367:HIS:HB3	1:D:391:THR:CG2	2.49	0.43
1:A:325:SER:CB	1:A:355:MET:HE1	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASP:HA	1:A:287:GLU:HB3	1.99	0.43
1:A:258:LEU:CD1	1:A:258:LEU:N	2.81	0.43
1:B:27:THR:OG1	1:B:31:ALA:HB3	2.18	0.43
1:C:324:LEU:O	1:C:328:ILE:HG13	2.19	0.43
1:A:1:MET:CG	1:A:29:THR:HG21	2.47	0.43
1:B:177:GLU:HA	1:B:177:GLU:OE1	2.19	0.43
1:C:5:VAL:CG1	1:C:28:GLU:HG2	2.48	0.43
1:C:92:GLN:OE1	4:C:2073:HOH:O	2.20	0.43
1:B:255:LYS:HE2	1:B:266:THR:CG2	2.41	0.43
1:C:213:GLY:N	1:C:217:GLU:OE1	2.42	0.43
1:D:147:MET:CE	1:D:394:PRO:CG	2.97	0.43
1:A:1:MET:O	1:A:29:THR:HG22	2.18	0.42
1:B:4:ILE:HD11	1:B:84:VAL:HG23	2.00	0.42
1:B:1:MET:SD	4:B:2001:HOH:O	2.62	0.42
1:C:148:ASN:HA	1:C:166:MET:HG2	2.00	0.42
1:B:159:ASN:HB3	1:B:213:GLY:O	2.19	0.42
1:C:164:GLU:HB2	1:C:242:ASP:HB3	2.01	0.42
1:C:216:GLU:O	1:C:220:GLN:HG3	2.19	0.42
1:A:5:VAL:CG1	1:A:28:GLU:HA	2.46	0.42
1:B:258:LEU:HD12	1:B:258:LEU:N	2.34	0.42
1:B:265:LYS:NZ	4:B:2113:HOH:O	2.51	0.42
2:D:1429:CIT:C1	2:D:1429:CIT:C5	2.98	0.42
1:C:266:THR:O	1:C:267:SER:C	2.57	0.42
1:C:325:SER:N	1:C:355:MET:HE3	2.34	0.42
1:A:1:MET:HB3	1:A:2:PRO:CD	2.50	0.42
1:C:405:GLN:O	1:C:409:ILE:HG13	2.19	0.42
1:A:341:ASN:ND2	1:A:368:ARG:NH1	2.55	0.42
1:B:12:VAL:O	1:B:19:PRO:HA	2.20	0.42
1:C:248:PHE:CE1	1:C:258:LEU:CD1	3.01	0.42
1:B:1:MET:O	1:B:27:THR:HB	2.20	0.41
1:B:190:LYS:HB2	1:B:208:PHE:CZ	2.55	0.41
1:B:365:ILE:HG13	1:B:381:ALA:HB2	2.02	0.41
1:C:56:LYS:NZ	1:C:56:LYS:HB3	2.35	0.41
1:C:301:LEU:CD1	1:C:305:LEU:HD22	2.50	0.41
1:C:418:GLN:NE2	1:C:420:HIS:NE2	2.68	0.41
1:D:148:ASN:CA	1:D:166:MET:HG2	2.50	0.41
1:B:266:THR:OG1	1:B:269:GLU:HG3	2.20	0.41
1:C:75:ILE:HG21	1:C:114:VAL:HG21	2.02	0.41
1:C:76:ALA:HB3	1:C:77:PRO:HD3	2.01	0.41
1:D:324:LEU:HG	1:D:336:ILE:HD12	2.01	0.41
1:D:329:LYS:NZ	1:D:329:LYS:CB	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HA	1:A:19:PRO:HD3	1.89	0.41
1:A:320:ASN:ND2	1:A:322:LYS:H	2.18	0.41
1:A:338:ILE:HG13	1:A:363:ALA:HB1	2.02	0.41
1:C:250:ASN:HD21	1:C:252:GLU:HB2	1.85	0.41
1:A:86:GLU:HB3	1:A:89:ALA:HB3	2.03	0.41
1:B:1:MET:N	1:B:2:PRO:HD2	2.35	0.41
1:B:302:THR:HA	1:B:311:LEU:CD1	2.50	0.41
1:C:391:THR:O	1:C:399:ARG:HB3	2.21	0.41
1:D:1:MET:HE2	1:D:1:MET:HB3	1.94	0.41
1:A:47:GLU:HB3	1:A:318:VAL:HG22	2.02	0.41
1:D:13:LEU:HD12	1:D:13:LEU:HA	1.90	0.41
1:D:250:ASN:ND2	1:D:252:GLU:HB2	2.32	0.41
1:A:288:ASP:OD2	1:A:314:ASP:HB3	2.21	0.41
1:B:149:ILE:CG1	1:B:189:LEU:HD22	2.51	0.41
1:D:250:ASN:ND2	1:D:252:GLU:H	2.19	0.41
1:D:296:GLU:H	1:D:296:GLU:HG2	1.75	0.41
1:A:1:MET:HG2	1:A:29:THR:CG2	2.48	0.41
1:B:39:SER:O	1:B:39:SER:OG	2.34	0.41
1:B:250:ASN:HD22	1:B:250:ASN:C	2.24	0.41
1:D:395:SER:O	1:D:396:ARG:CB	2.69	0.41
1:C:142:LEU:HD22	1:C:410:GLU:OE2	2.21	0.41
1:C:149:ILE:HG22	1:C:165:PHE:O	2.21	0.41
1:C:249:TYR:HB2	1:C:256:TYR:HE1	1.85	0.41
1:A:147:MET:CE	1:A:394:PRO:CD	2.90	0.40
1:C:324:LEU:HB3	1:C:355:MET:HE2	1.94	0.40
1:C:324:LEU:HD22	1:C:328:ILE:HG13	2.02	0.40
1:A:155:HIS:ND1	4:A:2095:HOH:O	2.37	0.40
1:A:377:ILE:HD11	1:A:391:THR:HG23	2.02	0.40
1:C:40:GLY:HA2	1:C:341:ASN:HD21	1.86	0.40
1:C:56:LYS:HG3	1:C:57:ASP:N	2.35	0.40
1:A:41:ALA:C	1:A:50:GLU:HG2	2.41	0.40
1:A:76:ALA:HB3	1:A:77:PRO:HD3	2.02	0.40
1:A:238:LYS:NZ	4:A:2142:HOH:O	2.36	0.40
1:C:250:ASN:HB2	1:C:257:HIS:CD2	2.56	0.40
1:C:325:SER:HA	1:C:355:MET:HE3	2.02	0.40
1:C:398:ASP:HB3	1:D:397:THR:OG1	2.21	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	426/430 (99%)	414 (97%)	11 (3%)	1 (0%)	47	55
1	B	426/430 (99%)	408 (96%)	16 (4%)	2 (0%)	29	31
1	C	426/430 (99%)	409 (96%)	16 (4%)	1 (0%)	47	55
1	D	426/430 (99%)	414 (97%)	11 (3%)	1 (0%)	47	55
All	All	1704/1720 (99%)	1645 (96%)	54 (3%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	ARG
1	B	292	GLU
1	B	396	ARG
1	C	396	ARG
1	D	396	ARG

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	345/347 (99%)	332 (96%)	13 (4%)	33	42
1	B	345/347 (99%)	327 (95%)	18 (5%)	23	28
1	C	345/347 (99%)	332 (96%)	13 (4%)	33	42
1	D	345/347 (99%)	329 (95%)	16 (5%)	27	34
All	All	1380/1388 (99%)	1320 (96%)	60 (4%)	29	36

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	82	PHE
1	A	250	ASN
1	A	261	GLU
1	A	305	LEU
1	A	320	ASN
1	A	324	LEU
1	A	326	GLU
1	A	341	ASN
1	A	367	HIS
1	A	391	THR
1	A	395	SER
1	A	398	ASP
1	B	29	THR
1	B	43	THR
1	B	50	GLU
1	B	56	LYS
1	B	82	PHE
1	B	84	VAL
1	B	250	ASN
1	B	252	GLU
1	B	305	LEU
1	B	307	LYS
1	B	318	VAL
1	B	323	LYS
1	B	324	LEU
1	B	325	SER
1	B	341	ASN
1	B	367	HIS
1	B	391	THR
1	B	398	ASP
1	C	13	LEU
1	C	29	THR
1	C	56	LYS
1	C	82	PHE
1	C	97	LEU
1	C	252	GLU
1	C	258	LEU
1	C	307	LYS
1	C	318	VAL
1	C	324	LEU
1	C	367	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	391	THR
1	C	398	ASP
1	D	43	THR
1	D	49	VAL
1	D	56	LYS
1	D	82	PHE
1	D	250	ASN
1	D	252	GLU
1	D	304	ARG
1	D	305	LEU
1	D	308	LYS
1	D	320	ASN
1	D	324	LEU
1	D	340	VAL
1	D	341	ASN
1	D	367	HIS
1	D	391	THR
1	D	398	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	187	HIS
1	A	215	ASN
1	A	250	ASN
1	A	298	HIS
1	A	320	ASN
1	A	341	ASN
1	A	367	HIS
1	A	388	GLN
1	A	418	GLN
1	B	127	GLN
1	B	132	GLN
1	B	155	HIS
1	B	163	GLN
1	B	184	GLN
1	B	187	HIS
1	B	215	ASN
1	B	250	ASN
1	B	298	HIS
1	B	320	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	341	ASN
1	B	367	HIS
1	B	388	GLN
1	B	418	GLN
1	C	92	GLN
1	C	148	ASN
1	C	151	ASN
1	C	184	GLN
1	C	187	HIS
1	C	215	ASN
1	C	250	ASN
1	C	298	HIS
1	C	320	ASN
1	C	367	HIS
1	C	388	GLN
1	C	418	GLN
1	D	132	GLN
1	D	148	ASN
1	D	151	ASN
1	D	184	GLN
1	D	187	HIS
1	D	215	ASN
1	D	250	ASN
1	D	298	HIS
1	D	320	ASN
1	D	341	ASN
1	D	367	HIS
1	D	388	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

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
2	CIT	D	1429	3	12,12,12	1.11	0	17,17,17	1.73	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	D	1429	3	-	7/16/16/16	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1429	CIT	O6-C6-C3	3.93	119.88	113.05
2	D	1429	CIT	C3-C2-C1	-2.53	107.70	113.81
2	D	1429	CIT	O4-C5-O3	-2.48	117.12	123.30
2	D	1429	CIT	O2-C1-O1	-2.12	118.02	123.30
2	D	1429	CIT	O4-C5-C4	2.02	120.85	114.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1429	CIT	O7-C3-C6-O5
2	D	1429	CIT	O7-C3-C6-O6
2	D	1429	CIT	C4-C3-C6-O5
2	D	1429	CIT	C4-C3-C6-O6
2	D	1429	CIT	C6-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1429	CIT	C2-C3-C4-C5
2	D	1429	CIT	O7-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1429	CIT	3	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

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, 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	428/430 (99%)	-0.61	3 (0%) 87 86	18, 29, 43, 63	0
1	B	428/430 (99%)	-0.28	18 (4%) 36 34	19, 31, 66, 88	0
1	C	428/430 (99%)	-0.39	12 (2%) 53 51	20, 31, 60, 84	0
1	D	428/430 (99%)	-0.60	3 (0%) 87 86	19, 28, 43, 66	0
All	All	1712/1720 (99%)	-0.47	36 (2%) 63 61	18, 29, 55, 88	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	ALA	6.6
1	D	155	HIS	5.5
1	B	42	SER	5.3
1	B	43	THR	4.7
1	C	43	THR	4.3
1	C	253	ASP	3.6
1	B	155	HIS	3.5
1	C	42	SER	3.2
1	C	251	LYS	3.2
1	C	41	ALA	3.2
1	C	44	GLY	3.2
1	B	40	GLY	3.1
1	B	45	GLU	3.1
1	B	154	GLU	3.1
1	A	43	THR	3.0
1	B	252	GLU	3.0
1	B	44	GLY	3.0
1	B	253	ASP	3.0
1	C	46	TYR	3.0
1	B	262	GLY	3.0
1	B	46	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	154	GLU	2.6
1	C	263	VAL	2.5
1	C	40	GLY	2.5
1	B	263	VAL	2.4
1	A	44	GLY	2.4
1	B	251	LYS	2.4
1	A	45	GLU	2.3
1	C	157	ASP	2.3
1	B	254	GLY	2.2
1	D	157	ASP	2.2
1	C	56	LYS	2.2
1	B	260	GLY	2.1
1	B	255	LYS	2.1
1	B	307	LYS	2.0
1	C	156	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q < 0.9
3	NA	D	1431	1/1	0.87	0.10	41,41,41,41	0
2	CIT	D	1429	13/13	0.90	0.16	30,41,47,48	0
3	NA	D	1430	1/1	0.96	0.14	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.