Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 08:31 AM EDT

PDB ID	:	1NXE
Title	:	A Novel NADH Allosteric Regulator Site is Found on the Surface of the Hexameric Type II Phe383Ala Variant of Citrate Synthase
Authors	:	Maurus, R.; Nguyen, N.T.; Stokell, D.J.; Ayed, A.; Hultin, P.G.; Duckworth, H.W.; Brayer, G.D.
Deposited on	:	2003-02-10
Resolution	:	2.30 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
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:

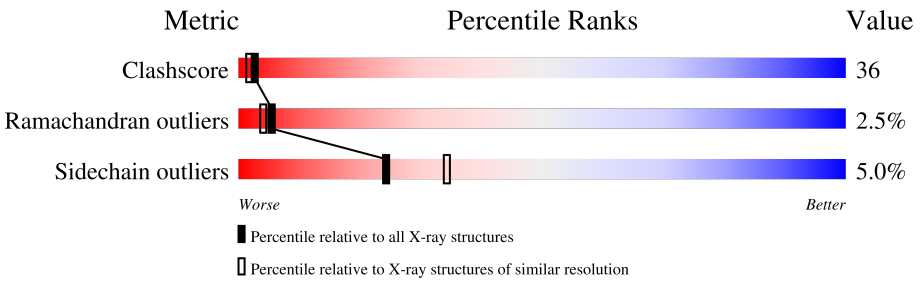
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	427	57% 37% 5%
1	B	427	50% 45% 5%

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
2	SO4	B	2001	-	X	X	-
2	SO4	B	2003	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7475 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.

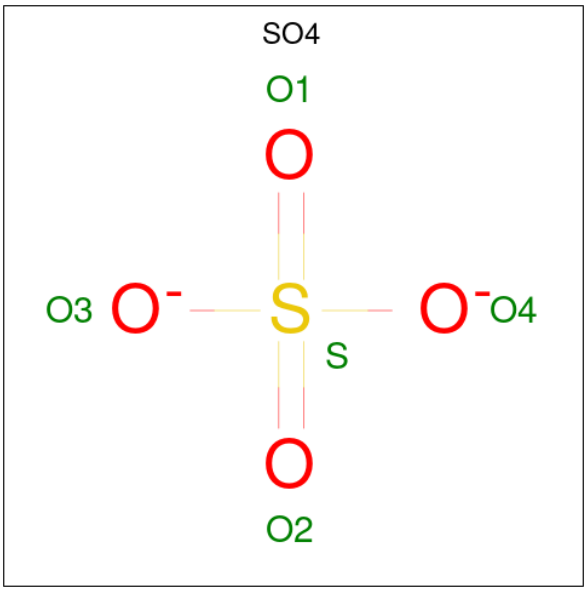
- Molecule 1 is a protein called Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	3359	2129	579	626	25	0	0	0
1	B	426	3360	2129	579	627	25	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ALA	PHE	engineered mutation	UNP P0ABH7
B	1383	ALA	PHE	engineered mutation	UNP P0ABH7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	378	378	378	0	0
			Total	O		
3	B	348	348	348	0	0

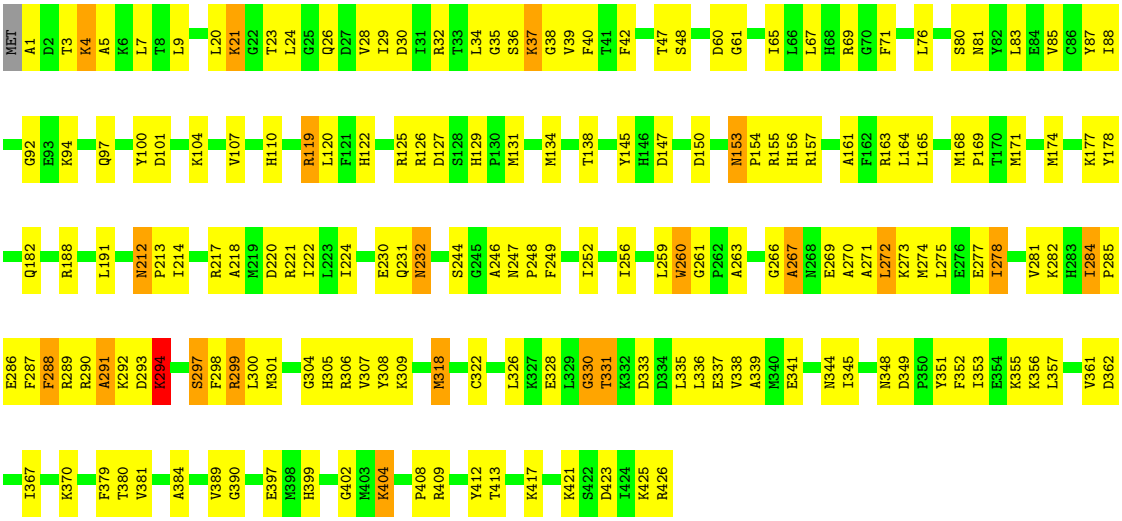
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

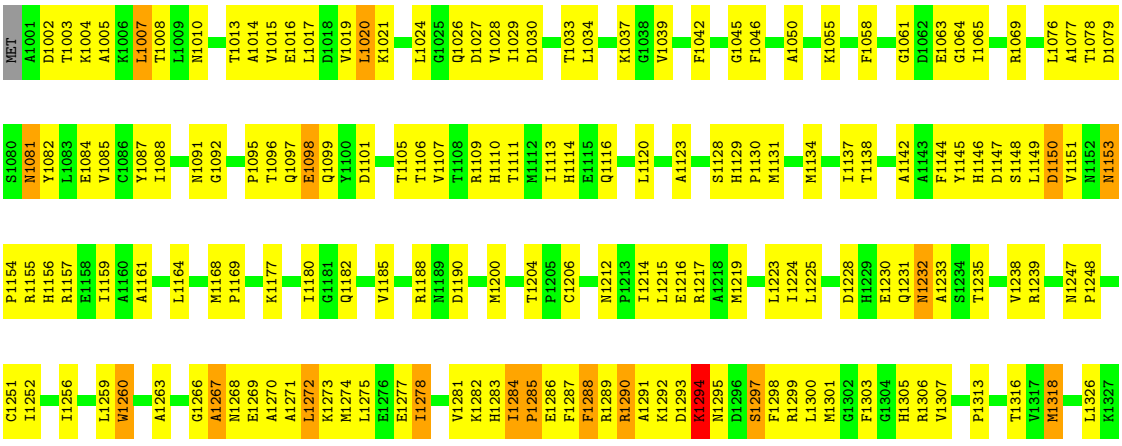
• Molecule 1: Citrate synthase

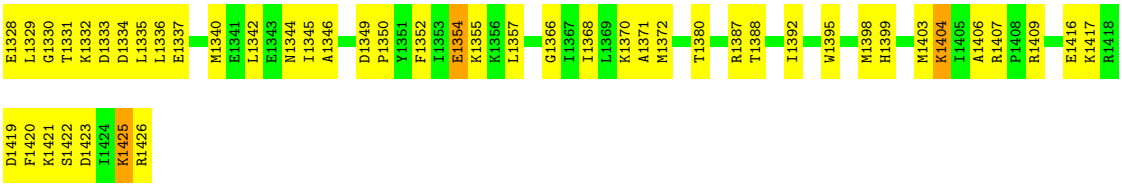
Chain A: 57% 37% 5%



• Molecule 1: Citrate synthase

Chain B: 50% 45% 5%




E1328
L1329
G1330
T1331
K1332
D1333
D1334
L1335
L1336
E1337
M1340
E1341
L1342
E1343
N1344
I1345
A1346
D1349
P1350
Y1351
F1352
I1353
E1354
K1355
K1356
L1357
G1366
I1367
I1368
L1369
K1370
A1371
M1372
T1380
R1387
T1388
I1392
W1395
M1398
H1399
M1403
K1404
I1405
A1406
R1407
P1408
R1409
E1416
K1417
R1418
D1419
F1420
K1421
S1422
D1423
I1424
K1425
R1426

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	165.24Å 165.24Å 157.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	77.0 (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7475	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

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: SO4

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	0.36	0/3436	0.64	0/4645
1	B	0.36	0/3437	0.61	0/4645
All	All	0.36	0/6873	0.62	0/9290

There are no bond length outliers.

There are no bond angle outliers.

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	3359	0	3309	243	0
1	B	3360	0	3306	273	0
2	A	15	0	0	0	0
2	B	15	0	0	2	0
3	A	378	0	0	31	0
3	B	348	0	0	37	0
All	All	7475	0	6615	485	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 36.

All (485) 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:21:LYS:HE2	1:A:21:LYS:H	1.05	1.13
1:B:1295:ASN:HB3	3:B:443:HOH:O	1.51	1.08
1:A:269:GLU:HA	1:A:272:LEU:HB2	1.38	1.05
1:B:1287:PHE:HA	1:B:1291:ALA:HB3	1.41	1.03
1:B:1020:LEU:HD21	1:B:1030:ASP:HB2	1.39	1.00
1:B:1269:GLU:HA	1:B:1272:LEU:HB2	1.41	1.00
1:B:1081:ASN:ND2	1:B:1084:GLU:H	1.58	0.99
1:A:287:PHE:HA	1:A:291:ALA:HB3	1.47	0.97
1:B:1081:ASN:HD21	1:B:1084:GLU:H	0.96	0.96
1:B:1129:HIS:HD2	1:B:1131:MET:H	1.07	0.94
1:A:288:PHE:HD1	1:A:289:ARG:H	0.96	0.94
1:B:1081:ASN:C	1:B:1081:ASN:HD22	1.71	0.93
1:A:150:ASP:OD2	1:A:153:ASN:HB2	1.72	0.88
1:B:1274:MET:HG3	1:B:1293:ASP:HA	1.53	0.88
1:A:217:ARG:HH21	1:A:221:ARG:NH1	1.70	0.87
1:A:294:LYS:HZ1	1:A:298:PHE:H	1.23	0.87
1:A:274:MET:HG3	1:A:293:ASP:HA	1.54	0.87
1:B:1288:PHE:HD1	1:B:1289:ARG:H	1.22	0.86
1:A:21:LYS:HE2	1:A:21:LYS:N	1.90	0.86
1:B:1275:LEU:HD22	1:B:1289:ARG:HE	1.40	0.85
1:B:1252:ILE:HG22	3:B:496:HOH:O	1.77	0.85
1:B:1138:THR:HG21	3:B:496:HOH:O	1.77	0.84
1:A:305:HIS:HD2	1:A:307:VAL:H	1.26	0.83
1:A:288:PHE:HD1	1:A:289:ARG:N	1.76	0.83
1:A:244:SER:HB3	1:B:1233:ALA:HB1	1.61	0.83
1:A:21:LYS:H	1:A:21:LYS:CE	1.94	0.79
1:B:1007:LEU:HD13	1:B:1029:ILE:HD13	1.64	0.79
1:B:1153:ASN:ND2	1:B:1155:ARG:H	1.81	0.79
1:B:1275:LEU:CD2	1:B:1289:ARG:HE	1.94	0.79
1:A:404:LYS:H	1:A:404:LYS:HD3	1.48	0.78
1:B:1294:LYS:HZ1	1:B:1298:PHE:H	1.30	0.78
1:A:294:LYS:NZ	1:A:298:PHE:H	1.82	0.77
1:B:1388:THR:O	1:B:1392:ILE:HG13	1.84	0.77
1:A:275:LEU:HD11	3:A:2131:HOH:O	1.83	0.77
1:B:1335:LEU:H	1:B:1335:LEU:HD23	1.50	0.77
1:B:1020:LEU:HD22	1:B:1020:LEU:H	1.50	0.76
1:B:1294:LYS:HE2	1:B:1357:LEU:HD13	1.68	0.76
1:A:309:LYS:HZ3	1:A:356:LYS:HE3	1.52	0.73
1:B:1081:ASN:HD21	1:B:1084:GLU:N	1.80	0.73
1:B:1098:GLU:HG3	1:B:1099:GLN:N	2.04	0.73
1:B:1288:PHE:HD1	1:B:1289:ARG:N	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:LEU:HB3	1:B:1039:VAL:HG13	1.71	0.73
1:B:1151:VAL:HB	1:B:1399:HIS:NE2	2.05	0.72
1:A:413:THR:HB	1:B:1055:LYS:HZ3	1.55	0.72
1:B:1069:ARG:HD2	1:B:1092:GLY:HA2	1.70	0.71
1:B:1149:LEU:HD22	1:B:1247:ASN:HB2	1.71	0.71
1:B:1129:HIS:CD2	1:B:1131:MET:H	1.99	0.71
1:B:1020:LEU:CD2	1:B:1030:ASP:HB2	2.19	0.71
1:B:1284:ILE:HD12	1:B:1287:PHE:H	1.55	0.71
1:B:1287:PHE:HA	1:B:1291:ALA:CB	2.17	0.71
1:B:1294:LYS:NZ	1:B:1298:PHE:H	1.88	0.71
1:A:284:ILE:HD12	1:A:287:PHE:H	1.56	0.71
1:B:1081:ASN:ND2	1:B:1081:ASN:C	2.42	0.71
1:A:326:LEU:HG	1:A:333:ASP:OD1	1.89	0.70
1:A:352:PHE:HA	1:A:357:LEU:HD23	1.73	0.70
1:A:272:LEU:HA	1:A:275:LEU:HG	1.73	0.70
1:B:1272:LEU:HA	1:B:1275:LEU:HG	1.74	0.70
1:A:339:ALA:HB1	1:A:367:ILE:HD13	1.74	0.70
1:A:261:GLY:HA3	3:A:2165:HOH:O	1.92	0.70
1:B:1305:HIS:HD2	1:B:1307:VAL:H	1.39	0.69
1:A:48:SER:HA	3:A:2246:HOH:O	1.92	0.69
1:A:217:ARG:HH21	1:A:221:ARG:HH11	1.35	0.69
1:A:294:LYS:HA	3:A:2171:HOH:O	1.92	0.69
1:B:1164:LEU:HD13	1:B:1252:ILE:HG13	1.76	0.68
1:A:278:ILE:HD13	1:A:278:ILE:O	1.93	0.68
1:A:425:LYS:H	1:B:1097:GLN:HE22	1.41	0.68
1:B:1270:ALA:HB3	3:B:204:HOH:O	1.92	0.68
1:A:413:THR:HG21	3:B:457:HOH:O	1.94	0.68
1:B:1113:ILE:HD12	1:B:1113:ILE:O	1.94	0.68
1:A:131:MET:HE2	1:A:260:TRP:HB3	1.76	0.67
3:A:2087:HOH:O	1:B:1128:SER:HA	1.94	0.67
1:B:1278:ILE:HD13	1:B:1278:ILE:O	1.94	0.67
1:B:1004:LYS:HB3	1:B:1021:LYS:HD3	1.74	0.67
1:B:1275:LEU:HD22	1:B:1289:ARG:NE	2.09	0.66
1:A:294:LYS:NZ	1:A:301:MET:HE1	2.11	0.66
1:A:275:LEU:HD22	1:A:289:ARG:HH11	1.60	0.66
1:B:1013:THR:HG21	3:B:413:HOH:O	1.96	0.66
1:A:404:LYS:HE3	3:A:2010:HOH:O	1.94	0.66
3:A:2246:HOH:O	1:B:1409:ARG:HG3	1.96	0.66
1:B:1272:LEU:HD12	1:B:1272:LEU:N	2.11	0.66
1:B:1305:HIS:CD2	1:B:1307:VAL:H	2.13	0.66
1:B:1155:ARG:HD3	3:B:596:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:PHE:HA	1:A:291:ALA:CB	2.23	0.65
1:B:1069:ARG:HA	3:B:61:HOH:O	1.96	0.65
1:B:1129:HIS:HD2	1:B:1131:MET:N	1.89	0.65
1:A:272:LEU:HD11	3:A:2255:HOH:O	1.97	0.64
1:A:217:ARG:O	1:A:221:ARG:HG3	1.98	0.64
1:A:270:ALA:HB1	3:A:2279:HOH:O	1.95	0.64
1:A:404:LYS:HD3	1:A:404:LYS:N	2.12	0.64
1:A:7:LEU:HD21	1:A:29:ILE:HG12	1.78	0.64
1:B:1096:THR:HG22	1:B:1097:GLN:H	1.63	0.64
1:A:145:TYR:HB3	1:A:163:ARG:NH2	2.13	0.64
1:B:1021:LYS:HG2	1:B:1027:ASP:OD1	1.98	0.64
1:A:153:ASN:HD22	1:A:154:PRO:N	1.96	0.63
1:B:1333:ASP:OD1	1:B:1336:LEU:HB3	1.97	0.63
1:A:230:GLU:CG	1:A:231:GLN:H	2.12	0.63
1:A:272:LEU:HD12	1:A:272:LEU:N	2.13	0.63
1:A:274:MET:HB2	1:A:293:ASP:OD2	1.97	0.63
1:A:413:THR:HG23	3:B:577:HOH:O	1.99	0.63
1:B:1266:GLY:O	1:B:1267:ALA:HB2	1.98	0.63
1:A:101:ASP:HA	1:B:1426:ARG:HH21	1.63	0.63
1:A:212:ASN:HD22	1:A:213:PRO:N	1.95	0.63
1:A:230:GLU:HG2	1:A:231:GLN:H	1.63	0.63
1:A:88:ILE:HG12	1:A:94:LYS:HA	1.80	0.63
1:A:120:LEU:HD23	1:B:1123:ALA:HB3	1.81	0.63
1:A:397:GLU:HG2	3:A:2021:HOH:O	1.98	0.63
1:A:161:ALA:O	1:A:165:LEU:HB2	1.99	0.62
1:A:275:LEU:CD2	1:A:289:ARG:HE	2.12	0.62
1:A:273:LYS:NZ	1:A:273:LYS:HB3	2.14	0.62
1:B:1164:LEU:O	1:B:1168:MET:HG2	1.99	0.62
1:B:1232:ASN:ND2	1:B:1235:THR:H	1.98	0.62
1:A:1:ALA:H1	1:A:4:LYS:HZ3	1.47	0.62
1:B:1274:MET:CG	1:B:1293:ASP:HA	2.29	0.62
1:A:413:THR:HB	1:B:1055:LYS:NZ	2.15	0.62
1:B:1153:ASN:C	1:B:1153:ASN:HD22	2.01	0.62
1:B:1425:LYS:HE3	1:B:1425:LYS:C	2.20	0.62
1:A:294:LYS:HZ3	1:A:301:MET:HE1	1.64	0.61
1:B:1096:THR:HG21	3:B:398:HOH:O	1.99	0.61
1:A:138:THR:HG21	1:A:252:ILE:HG22	1.81	0.61
1:A:299:ARG:HB2	1:A:304:GLY:O	2.00	0.61
1:B:1131:MET:HE2	1:B:1260:TRP:HB3	1.83	0.61
1:A:153:ASN:HD22	1:A:154:PRO:CD	2.13	0.61
1:A:288:PHE:CD1	1:A:289:ARG:N	2.57	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:LEU:HD22	1:B:1085:VAL:HG22	1.83	0.60
1:A:306:ARG:CZ	1:B:1407:ARG:HD3	2.31	0.60
1:A:370:LYS:HE3	1:A:379:PHE:HE1	1.67	0.60
1:A:294:LYS:HB2	1:A:297:SER:HA	1.84	0.60
1:A:94:LYS:HG2	3:A:2100:HOH:O	2.01	0.60
1:B:1131:MET:HE2	1:B:1380:THR:CG2	2.32	0.60
1:A:252:ILE:O	1:A:256:ILE:HG13	2.02	0.59
1:B:1096:THR:HG22	1:B:1097:GLN:N	2.17	0.59
1:B:1420:PHE:CZ	1:B:1422:SER:HB2	2.37	0.59
1:B:1275:LEU:HD22	1:B:1289:ARG:HH11	1.66	0.59
1:B:1274:MET:HB2	1:B:1293:ASP:OD2	2.01	0.59
1:A:212:ASN:HD22	1:A:213:PRO:CD	2.16	0.59
1:A:266:GLY:C	1:A:270:ALA:HB2	2.23	0.59
1:B:1269:GLU:HB2	1:B:1273:LYS:CA	2.33	0.59
1:B:1232:ASN:HB2	2:B:2001:SO4:O2	2.03	0.58
1:A:1:ALA:N	1:A:4:LYS:HZ3	2.01	0.58
1:A:119:ARG:HD2	3:A:2258:HOH:O	2.02	0.58
1:A:129:HIS:CD2	1:A:131:MET:H	2.20	0.58
1:A:30:ASP:OD1	1:A:32:ARG:HD3	2.02	0.58
1:B:1003:THR:O	1:B:1019:VAL:HG11	2.04	0.58
1:A:120:LEU:HD23	1:B:1123:ALA:CB	2.34	0.58
1:A:263:ALA:HA	1:A:300:LEU:HD11	1.85	0.58
1:B:1333:ASP:HB2	3:B:313:HOH:O	2.04	0.58
1:A:294:LYS:HZ2	1:A:297:SER:HA	1.69	0.57
1:A:47:THR:HG23	3:B:529:HOH:O	2.04	0.57
1:A:404:LYS:HG2	1:A:404:LYS:O	2.04	0.57
1:B:1303:PHE:HB3	1:B:1357:LEU:HB3	1.85	0.57
1:A:153:ASN:HD22	1:A:153:ASN:C	2.07	0.57
1:B:1114:HIS:HD2	1:B:1116:GLN:HB3	1.70	0.57
1:A:119:ARG:O	1:A:119:ARG:HG3	2.04	0.57
1:A:272:LEU:HA	1:A:275:LEU:CG	2.35	0.57
1:A:322:CYS:O	1:A:326:LEU:HD13	2.05	0.57
1:B:1155:ARG:HH11	1:B:1156:HIS:HE1	1.53	0.57
1:A:60:ASP:HB3	1:A:65:ILE:HB	1.86	0.57
1:A:107:VAL:HA	3:A:2152:HOH:O	2.04	0.57
1:A:47:THR:HG22	1:B:1409:ARG:HH11	1.70	0.57
1:B:1404:LYS:HD3	1:B:1404:LYS:N	2.19	0.57
1:A:402:GLY:HA3	3:A:2172:HOH:O	2.03	0.57
1:A:266:GLY:O	1:A:267:ALA:HB2	2.05	0.56
1:B:1149:LEU:HD22	1:B:1247:ASN:CB	2.35	0.56
1:B:1288:PHE:CD1	1:B:1289:ARG:N	2.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1329:LEU:HD12	1:B:1371:ALA:HB1	1.87	0.56
1:A:425:LYS:HG3	3:A:2326:HOH:O	2.06	0.56
1:A:244:SER:CB	1:B:1233:ALA:HB1	2.33	0.56
1:B:1069:ARG:CD	1:B:1092:GLY:HA2	2.34	0.56
1:A:20:LEU:HB2	1:A:28:VAL:CG2	2.35	0.56
1:B:1077:ALA:HA	1:B:1224:ILE:HG21	1.88	0.56
1:B:1188:ARG:HB3	1:B:1190:ASP:OD1	2.05	0.55
1:A:134:MET:SD	1:A:381:VAL:HG13	2.46	0.55
1:A:272:LEU:HA	1:A:275:LEU:CD1	2.35	0.55
1:B:1423:ASP:HA	3:B:708:HOH:O	2.05	0.55
1:B:1168:MET:HB2	1:B:1169:PRO:HD3	1.88	0.55
1:B:1007:LEU:HD11	1:B:1017:LEU:HD12	1.87	0.55
1:B:1332:LYS:HG2	3:B:672:HOH:O	2.07	0.55
1:A:71:PHE:CD2	1:B:1420:PHE:HB2	2.42	0.55
1:A:122:HIS:HB2	3:A:2169:HOH:O	2.06	0.55
1:B:1231:GLN:HB3	3:B:206:HOH:O	2.05	0.55
1:B:1231:GLN:HE22	1:B:1239:ARG:NE	2.04	0.55
1:B:1274:MET:HB2	1:B:1293:ASP:CG	2.27	0.55
1:B:1333:ASP:OD2	1:B:1336:LEU:HD23	2.06	0.55
1:B:1148:SER:HA	1:B:1156:HIS:CD2	2.42	0.55
1:A:298:PHE:HZ	3:A:2279:HOH:O	1.89	0.54
1:B:1098:GLU:HG3	1:B:1099:GLN:H	1.72	0.54
1:B:1114:HIS:HD2	1:B:1116:GLN:CB	2.20	0.54
1:A:164:LEU:HG	1:A:249:PHE:CE2	2.42	0.54
1:A:294:LYS:HB3	1:A:301:MET:HE1	1.89	0.54
1:B:1318:MET:CE	1:B:1318:MET:HA	2.37	0.54
1:A:275:LEU:HA	1:A:289:ARG:NE	2.23	0.54
1:A:426:ARG:HD2	3:A:2283:HOH:O	2.08	0.54
1:B:1007:LEU:HD21	1:B:1029:ILE:HG23	1.90	0.54
1:B:1259:LEU:HD12	3:B:229:HOH:O	2.07	0.54
1:A:37:LYS:HD2	3:A:2299:HOH:O	2.07	0.54
1:A:275:LEU:HD22	1:A:289:ARG:HE	1.72	0.54
1:A:284:ILE:C	1:A:284:ILE:HD13	2.28	0.54
1:A:294:LYS:NZ	1:A:301:MET:CE	2.70	0.54
1:A:150:ASP:HB3	1:A:156:HIS:CD2	2.43	0.54
3:A:2217:HOH:O	1:B:1150:ASP:HB3	2.08	0.54
1:B:1277:GLU:O	1:B:1277:GLU:HG2	2.08	0.54
1:A:150:ASP:H	1:A:156:HIS:HD2	1.56	0.53
1:A:284:ILE:HD12	1:A:287:PHE:N	2.24	0.53
1:B:1037:LYS:HB2	1:B:1039:VAL:HG12	1.89	0.53
1:B:1342:LEU:HA	3:B:586:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HD3	1:A:221:ARG:HH11	1.74	0.53
1:A:269:GLU:HB2	1:A:273:LYS:CA	2.38	0.53
1:B:1144:PHE:O	1:B:1146:HIS:N	2.41	0.53
1:B:1153:ASN:ND2	1:B:1153:ASN:C	2.61	0.53
1:B:1284:ILE:HD13	1:B:1284:ILE:C	2.28	0.53
1:A:7:LEU:HD21	1:A:29:ILE:CD1	2.38	0.53
1:A:3:THR:C	1:A:5:ALA:H	2.12	0.53
1:A:100:TYR:CE1	1:B:1426:ARG:HB3	2.43	0.53
1:B:1010:ASN:HA	1:B:1013:THR:O	2.08	0.53
1:B:1063:GLU:HB3	1:B:1065:ILE:HG12	1.90	0.53
1:B:1283:HIS:HA	3:B:695:HOH:O	2.09	0.53
1:A:217:ARG:CD	1:A:221:ARG:HH11	2.22	0.53
1:A:230:GLU:HG2	1:A:231:GLN:N	2.24	0.53
1:A:294:LYS:HZ3	1:A:301:MET:CE	2.21	0.53
1:A:326:LEU:HG	1:A:333:ASP:CG	2.29	0.53
1:A:7:LEU:C	1:A:7:LEU:HD12	2.29	0.53
1:B:1153:ASN:HD22	1:B:1154:PRO:N	2.08	0.52
1:B:1275:LEU:HD13	1:B:1289:ARG:HH11	1.74	0.52
1:A:277:GLU:O	1:A:277:GLU:HG2	2.09	0.52
3:A:2099:HOH:O	1:B:1079:ASP:HB3	2.09	0.52
1:B:1316:THR:HG23	3:B:605:HOH:O	2.09	0.52
1:A:339:ALA:HB1	1:A:367:ILE:CD1	2.38	0.52
1:B:1331:THR:HA	1:B:1334:ASP:OD2	2.09	0.52
1:A:1:ALA:N	1:A:4:LYS:NZ	2.57	0.52
1:B:1008:THR:HA	1:B:1015:VAL:O	2.10	0.52
1:B:1284:ILE:CD1	1:B:1287:PHE:H	2.22	0.52
1:B:1272:LEU:HA	1:B:1275:LEU:CG	2.39	0.52
1:A:97:GLN:OE1	1:B:1425:LYS:N	2.43	0.52
1:A:129:HIS:HD2	1:A:131:MET:H	1.58	0.52
1:A:328:GLU:C	1:A:330:GLY:H	2.14	0.52
1:A:341:GLU:O	1:A:345:ILE:HG13	2.10	0.52
1:A:177:LYS:NZ	1:A:182:GLN:NE2	2.58	0.52
1:B:1271:ALA:H	1:B:1272:LEU:HD12	1.75	0.52
1:B:1274:MET:O	1:B:1289:ARG:HG3	2.08	0.52
1:B:1355:LYS:HD2	1:B:1355:LYS:N	2.25	0.52
1:A:305:HIS:CD2	1:A:307:VAL:HB	2.45	0.51
1:B:1045:GLY:HA3	3:B:485:HOH:O	2.10	0.51
1:B:1272:LEU:HD21	3:B:408:HOH:O	2.10	0.51
1:B:1335:LEU:H	1:B:1335:LEU:CD2	2.20	0.51
1:A:101:ASP:HA	1:B:1426:ARG:NH2	2.25	0.51
1:A:274:MET:HB2	1:A:293:ASP:CG	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:HE3	1:A:297:SER:OG	2.11	0.51
1:A:284:ILE:CD1	1:A:287:PHE:H	2.21	0.51
1:B:1131:MET:CE	1:B:1380:THR:HG22	2.41	0.51
1:A:309:LYS:NZ	1:A:356:LYS:HE3	2.24	0.51
1:A:348:ASN:HA	1:A:353:ILE:HD11	1.92	0.51
1:B:1294:LYS:HB2	1:B:1297:SER:HA	1.93	0.51
1:A:36:SER:C	1:A:38:GLY:H	2.13	0.51
1:B:1368:ILE:O	1:B:1372:MET:HG3	2.11	0.51
1:A:174:MET:HG3	3:A:2022:HOH:O	2.11	0.50
1:B:1010:ASN:OD1	1:B:1014:ALA:HA	2.10	0.50
1:B:1034:LEU:HD22	1:B:1039:VAL:HG11	1.93	0.50
1:B:1337:GLU:HA	3:B:13:HOH:O	2.11	0.50
1:B:1404:LYS:HB3	3:B:219:HOH:O	2.10	0.50
1:B:1131:MET:HG2	1:B:1260:TRP:CD2	2.47	0.50
1:B:1177:LYS:HE2	1:B:1200:MET:O	2.12	0.50
1:B:1273:LYS:NZ	1:B:1273:LYS:HB3	2.26	0.50
1:B:1404:LYS:HD3	1:B:1404:LYS:H	1.76	0.50
1:A:274:MET:CG	1:A:293:ASP:HA	2.33	0.50
1:B:1272:LEU:HD11	3:B:408:HOH:O	2.11	0.50
1:B:1277:GLU:O	1:B:1281:VAL:HG22	2.11	0.50
1:B:1335:LEU:HD23	1:B:1335:LEU:N	2.23	0.50
1:A:76:LEU:O	1:A:80:SER:HB3	2.12	0.50
1:A:212:ASN:HD22	1:A:212:ASN:C	2.15	0.50
1:A:409:ARG:HB2	1:B:1050:ALA:HA	1.93	0.50
1:B:1130:PRO:O	1:B:1134:MET:HB2	2.11	0.50
1:A:153:ASN:HD22	1:A:154:PRO:HD2	1.77	0.50
1:B:1180:ILE:HG13	1:B:1182:GLN:HG3	1.94	0.50
1:B:1284:ILE:HG23	1:B:1284:ILE:O	2.12	0.50
1:A:277:GLU:O	1:A:281:VAL:HG22	2.12	0.50
1:A:247:ASN:HB2	1:A:248:PRO:HD2	1.94	0.49
1:B:1109:ARG:HD3	3:B:610:HOH:O	2.11	0.49
1:B:1204:THR:HG22	1:B:1206:CYS:H	1.76	0.49
1:A:287:PHE:O	1:A:292:LYS:HB2	2.12	0.49
1:A:298:PHE:HB2	1:A:301:MET:HE3	1.94	0.49
1:B:1219:MET:O	1:B:1223:LEU:HD13	2.12	0.49
1:A:7:LEU:HD21	1:A:29:ILE:CG1	2.42	0.49
1:A:274:MET:O	1:A:289:ARG:HG3	2.11	0.49
1:B:1155:ARG:O	1:B:1159:ILE:HG13	2.13	0.49
1:B:1275:LEU:HD22	1:B:1289:ARG:NH1	2.26	0.49
1:B:1366:GLY:O	1:B:1370:LYS:HG3	2.12	0.49
1:B:1154:PRO:HG3	1:B:1157:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1266:GLY:O	1:B:1267:ALA:CB	2.60	0.49
1:A:9:LEU:HD11	1:B:1007:LEU:CD1	2.43	0.49
1:A:259:LEU:HD23	1:A:384:ALA:HB2	1.95	0.49
1:A:275:LEU:HD22	1:A:289:ARG:NH1	2.25	0.49
1:B:1069:ARG:HG3	1:B:1088:ILE:HG22	1.95	0.49
1:A:110:HIS:CE1	3:A:2106:HOH:O	2.66	0.49
1:B:1269:GLU:HB2	1:B:1273:LYS:HA	1.95	0.49
1:B:1269:GLU:O	1:B:1273:LYS:HB2	2.12	0.48
1:B:1425:LYS:HE3	1:B:1425:LYS:CA	2.43	0.48
1:A:284:ILE:HG23	1:A:284:ILE:O	2.13	0.48
1:A:34:LEU:HB3	1:A:39:VAL:HB	1.96	0.48
1:B:1212:ASN:HB3	1:B:1215:LEU:CG	2.43	0.48
1:A:35:GLY:HA2	1:A:40:PHE:CE2	2.47	0.48
1:A:271:ALA:HB2	1:A:298:PHE:CD2	2.49	0.48
1:B:1144:PHE:HB3	3:B:520:HOH:O	2.13	0.48
1:B:1024:LEU:HB3	1:B:1058:PHE:CE2	2.49	0.48
1:A:370:LYS:HG3	1:A:379:PHE:HZ	1.79	0.48
1:B:1147:ASP:OD2	1:B:1147:ASP:N	2.44	0.48
1:A:412:TYR:CD1	1:B:1024:LEU:HB2	2.49	0.48
1:B:1081:ASN:ND2	1:B:1084:GLU:N	2.43	0.48
1:B:1326:LEU:HG	1:B:1333:ASP:CG	2.34	0.48
1:A:42:PHE:HB2	1:B:1028:VAL:CG2	2.44	0.48
1:A:47:THR:O	1:B:1409:ARG:NE	2.36	0.48
1:A:212:ASN:HD22	1:A:213:PRO:HD2	1.79	0.48
1:B:1003:THR:C	1:B:1005:ALA:H	2.17	0.48
1:B:1021:LYS:HA	1:B:1027:ASP:CG	2.34	0.48
1:B:1346:ALA:HA	1:B:1352:PHE:CG	2.49	0.48
1:B:1069:ARG:HG3	1:B:1088:ILE:O	2.13	0.48
1:B:1131:MET:HE2	1:B:1380:THR:HG22	1.94	0.47
1:A:306:ARG:HD3	1:B:1407:ARG:NH1	2.29	0.47
1:B:1107:VAL:O	1:B:1111:THR:HG23	2.14	0.47
1:A:370:LYS:HG3	1:A:379:PHE:CZ	2.50	0.47
1:B:1082:TYR:CD1	1:B:1223:LEU:HB3	2.50	0.47
1:B:1114:HIS:CD2	1:B:1116:GLN:HB3	2.50	0.47
1:A:337:GLU:O	1:A:337:GLU:HG2	2.15	0.47
1:A:413:THR:CB	1:B:1055:LYS:HZ3	2.27	0.47
1:B:1061:GLY:HA3	3:B:622:HOH:O	2.13	0.47
1:B:1150:ASP:OD2	1:B:1150:ASP:N	2.48	0.47
1:B:1214:ILE:HD12	1:B:1328:GLU:OE2	2.15	0.47
1:B:1294:LYS:HZ2	1:B:1297:SER:HA	1.79	0.47
1:B:1331:THR:O	1:B:1331:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1340:MET:O	1:B:1344:ASN:HB2	2.13	0.47
1:B:1212:ASN:HB3	1:B:1215:LEU:HG	1.96	0.47
1:A:294:LYS:HZ1	1:A:298:PHE:N	2.03	0.47
1:B:1232:ASN:HB2	2:B:2001:SO4:S	2.55	0.47
1:B:1284:ILE:HD12	1:B:1287:PHE:N	2.26	0.47
1:A:404:LYS:H	1:A:404:LYS:CD	2.25	0.46
1:A:104:LYS:HD3	1:B:1426:ARG:NE	2.31	0.46
1:A:294:LYS:NZ	1:A:297:SER:HA	2.29	0.46
1:A:157:ARG:HE	1:A:399:HIS:CG	2.33	0.46
1:B:1087:TYR:CE1	1:B:1095:PRO:HB3	2.51	0.46
1:B:1154:PRO:HG3	1:B:1157:ARG:HH11	1.80	0.46
1:A:81:ASN:HA	1:A:220:ASP:OD1	2.14	0.46
1:A:157:ARG:HE	1:A:399:HIS:CD2	2.34	0.46
1:A:260:TRP:HB3	1:A:380:THR:HG21	1.98	0.46
1:A:305:HIS:CD2	1:A:307:VAL:H	2.17	0.46
1:B:1008:THR:HG22	1:B:1016:GLU:HG2	1.96	0.46
1:B:1131:MET:O	1:B:1134:MET:HB3	2.16	0.46
1:B:1426:ARG:NH1	3:B:268:HOH:O	2.48	0.46
1:A:126:ARG:HD2	1:A:178:TYR:CZ	2.51	0.46
1:A:47:THR:HA	3:B:529:HOH:O	2.16	0.46
1:B:1019:VAL:HG13	1:B:1019:VAL:O	2.15	0.46
1:A:20:LEU:HB2	1:A:28:VAL:HG23	1.97	0.46
1:A:83:LEU:HB2	3:A:2064:HOH:O	2.15	0.46
1:A:1:ALA:H2	1:A:4:LYS:NZ	2.14	0.46
1:B:1013:THR:HG22	1:B:1014:ALA:N	2.31	0.46
1:B:1298:PHE:HB2	1:B:1301:MET:HE2	1.98	0.46
1:B:1345:ILE:HD12	3:B:586:HOH:O	2.16	0.46
1:B:1238:VAL:HG22	1:B:1251:CYS:O	2.16	0.45
1:B:1278:ILE:HD11	1:B:1288:PHE:CE2	2.51	0.45
1:B:1157:ARG:HG2	1:B:1395:TRP:HH2	1.81	0.45
1:B:1289:ARG:HG2	1:B:1290:ARG:N	2.31	0.45
1:A:61:GLY:HA2	1:A:308:TYR:HD1	1.81	0.45
1:B:1120:LEU:HD23	1:B:1137:ILE:HD13	1.98	0.45
1:A:5:ALA:HB3	3:A:2353:HOH:O	2.16	0.45
1:A:24:LEU:HD11	1:B:1416:GLU:HA	1.99	0.45
1:A:37:LYS:O	1:A:39:VAL:HG23	2.16	0.45
1:A:278:ILE:O	1:A:278:ILE:CD1	2.62	0.45
1:A:344:ASN:OD1	1:A:348:ASN:ND2	2.50	0.45
1:B:1026:GLN:NE2	3:B:181:HOH:O	2.49	0.45
1:A:177:LYS:HZ3	1:A:182:GLN:NE2	2.15	0.45
1:B:1105:THR:O	1:B:1109:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1248:PRO:HG3	1:B:1395:TRP:CZ2	2.52	0.45
1:B:1346:ALA:HA	1:B:1352:PHE:CD2	2.51	0.45
1:B:1275:LEU:HA	1:B:1289:ARG:NE	2.31	0.45
1:A:423:ASP:HB3	3:B:52:HOH:O	2.16	0.45
1:B:1005:ALA:HA	3:B:675:HOH:O	2.16	0.45
1:A:188:ARG:HB2	1:A:191:LEU:HD12	1.99	0.45
1:A:351:TYR:CE1	1:A:355:LYS:HD2	2.52	0.45
1:A:408:PRO:HA	1:B:1046:PHE:O	2.17	0.45
1:A:417:LYS:HD3	1:A:417:LYS:C	2.36	0.45
3:A:2037:HOH:O	1:B:1142:ALA:HB3	2.15	0.45
1:B:1278:ILE:O	1:B:1278:ILE:CD1	2.62	0.45
1:B:1230:GLU:CG	1:B:1231:GLN:H	2.30	0.44
1:B:1298:PHE:HB2	1:B:1301:MET:CE	2.47	0.44
1:A:9:LEU:HD11	1:B:1007:LEU:HD12	1.98	0.44
1:A:34:LEU:O	1:A:35:GLY:C	2.56	0.44
1:A:85:VAL:HG21	1:A:224:ILE:HG23	1.99	0.44
1:B:1272:LEU:N	1:B:1272:LEU:CD1	2.79	0.44
1:A:230:GLU:CG	1:A:231:GLN:N	2.79	0.44
1:B:1225:LEU:HD12	1:B:1318:MET:SD	2.58	0.44
1:B:1272:LEU:HA	1:B:1275:LEU:CD1	2.47	0.44
1:A:413:THR:HG22	1:A:413:THR:O	2.18	0.44
1:B:1033:THR:HA	3:B:130:HOH:O	2.17	0.44
1:A:212:ASN:ND2	1:A:213:PRO:HD2	2.33	0.44
1:A:269:GLU:HB2	1:A:273:LYS:HA	2.00	0.44
1:A:335:LEU:HD23	1:A:335:LEU:H	1.82	0.44
1:B:1287:PHE:CA	1:B:1291:ALA:HB3	2.30	0.44
1:B:1326:LEU:HG	1:B:1333:ASP:OD1	2.18	0.44
1:B:1020:LEU:HB3	3:B:200:HOH:O	2.17	0.44
1:B:1232:ASN:C	1:B:1232:ASN:HD22	2.19	0.44
1:A:164:LEU:HG	1:A:249:PHE:HE2	1.81	0.43
1:A:335:LEU:HD23	1:A:335:LEU:N	2.33	0.43
1:A:269:GLU:O	1:A:273:LYS:HB2	2.18	0.43
1:A:267:ALA:N	1:A:270:ALA:HB2	2.33	0.43
1:A:290:ARG:HH22	1:A:370:LYS:HZ3	1.66	0.43
1:A:168:MET:HA	1:A:171:MET:HE3	2.00	0.43
1:B:1228:ASP:HA	1:B:1387:ARG:CD	2.49	0.43
1:B:1350:PRO:O	1:B:1354:GLU:HB2	2.18	0.43
1:A:168:MET:N	1:A:169:PRO:HD2	2.33	0.43
1:B:1337:GLU:O	1:B:1337:GLU:HG2	2.18	0.43
1:A:125:ARG:HB3	1:A:127:ASP:OD1	2.18	0.43
1:B:1256:ILE:CD1	3:B:496:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1263:ALA:HA	1:B:1300:LEU:HD11	2.00	0.43
1:B:1298:PHE:HD2	1:B:1301:MET:HE1	1.82	0.43
1:A:266:GLY:O	1:A:267:ALA:CB	2.67	0.43
1:A:389:VAL:HG13	1:A:390:GLY:N	2.34	0.43
1:B:1285:PRO:HA	1:B:1288:PHE:CE2	2.54	0.43
1:B:1114:HIS:CD2	1:B:1116:GLN:H	2.37	0.43
1:B:1282:LYS:HD2	1:B:1282:LYS:O	2.18	0.42
1:B:1153:ASN:OD1	1:B:1156:HIS:ND1	2.52	0.42
1:B:1294:LYS:HE3	1:B:1297:SER:OG	2.19	0.42
1:B:1398:MET:SD	1:B:1403:MET:HG3	2.59	0.42
1:A:28:VAL:HB	1:B:1042:PHE:HB2	2.01	0.42
1:B:1305:HIS:HD2	1:B:1306:ARG:N	2.17	0.42
1:A:336:LEU:HG	3:A:2084:HOH:O	2.19	0.42
1:A:232:ASN:C	1:A:232:ASN:HD22	2.23	0.42
1:A:290:ARG:HG2	1:A:290:ARG:O	2.20	0.42
1:A:338:VAL:HG22	3:A:2084:HOH:O	2.19	0.42
1:A:426:ARG:HD3	1:B:1101:ASP:OD1	2.19	0.42
1:B:1064:GLY:O	1:B:1313:PRO:HB3	2.20	0.42
1:A:104:LYS:HZ2	1:B:1426:ARG:HG2	1.85	0.42
1:B:1267:ALA:C	1:B:1269:GLU:H	2.22	0.42
1:A:100:TYR:HE1	1:B:1426:ARG:HB3	1.84	0.42
1:A:275:LEU:HD22	1:A:289:ARG:NE	2.35	0.42
1:A:298:PHE:HB2	1:A:301:MET:CE	2.49	0.42
1:B:1185:VAL:HB	1:B:1200:MET:HA	2.02	0.42
1:B:1294:LYS:O	1:B:1294:LYS:HG3	2.20	0.42
1:A:267:ALA:C	1:A:269:GLU:N	2.73	0.42
1:A:349:ASP:O	1:A:353:ILE:HG13	2.20	0.42
1:B:1275:LEU:HD22	1:B:1289:ARG:CZ	2.50	0.41
1:A:267:ALA:C	1:A:269:GLU:H	2.22	0.41
1:A:423:ASP:HB3	1:B:1095:PRO:O	2.20	0.41
1:A:331:THR:HG22	1:A:331:THR:O	2.19	0.41
1:B:1002:ASP:OD1	1:B:1003:THR:N	2.52	0.41
1:B:1087:TYR:O	1:B:1091:ASN:HB2	2.20	0.41
1:B:1421:LYS:C	1:B:1421:LYS:HD2	2.40	0.41
1:A:119:ARG:NE	3:A:2121:HOH:O	2.53	0.41
1:B:1078:THR:HG21	3:B:488:HOH:O	2.21	0.41
1:A:47:THR:CG2	1:B:1409:ARG:HH11	2.31	0.41
1:A:147:ASP:HA	3:A:2277:HOH:O	2.19	0.41
1:A:212:ASN:ND2	1:A:214:ILE:H	2.18	0.41
1:A:230:GLU:HG2	1:A:231:GLN:HG2	2.03	0.41
1:A:421:LYS:HA	3:A:2146:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:N	1:A:272:LEU:CD1	2.82	0.41
1:A:273:LYS:HB3	1:A:273:LYS:HZ2	1.85	0.41
1:A:355:LYS:HB2	1:A:357:LEU:HD21	2.02	0.41
1:B:1425:LYS:HE3	1:B:1426:ARG:N	2.36	0.41
1:A:282:LYS:HD2	1:A:282:LYS:O	2.20	0.41
1:A:294:LYS:NZ	1:A:298:PHE:N	2.61	0.41
1:B:1287:PHE:O	1:B:1292:LYS:HB2	2.20	0.41
1:B:1305:HIS:CD2	1:B:1306:ARG:N	2.88	0.41
1:B:1345:ILE:O	1:B:1349:ASP:HB3	2.21	0.41
1:A:23:THR:O	1:A:24:LEU:HD23	2.20	0.41
1:A:69:ARG:NE	1:A:92:GLY:HA2	2.36	0.41
1:A:361:VAL:HG13	1:A:362:ASP:N	2.35	0.41
1:A:370:LYS:HE3	1:A:379:PHE:CE1	2.52	0.41
1:B:1106:THR:O	1:B:1110:HIS:HD2	2.04	0.41
1:B:1161:ALA:HB1	1:B:1392:ILE:HG21	2.03	0.41
1:B:1177:LYS:HD2	1:B:1182:GLN:HB2	2.03	0.41
1:B:1231:GLN:HE22	1:B:1239:ARG:HE	1.68	0.41
1:B:1277:GLU:HG2	1:B:1281:VAL:HG22	2.02	0.41
1:B:1287:PHE:CD1	1:B:1291:ALA:HB1	2.55	0.41
1:A:87:TYR:CD1	1:A:87:TYR:C	2.94	0.41
1:A:278:ILE:CG1	1:A:289:ARG:HB2	2.51	0.41
1:A:305:HIS:HD2	1:A:307:VAL:N	2.06	0.41
1:B:1007:LEU:HD13	1:B:1029:ILE:CD1	2.45	0.41
1:B:1271:ALA:N	1:B:1272:LEU:HD12	2.36	0.41
1:A:218:ALA:O	1:A:222:ILE:HG13	2.20	0.40
1:A:271:ALA:H	1:A:272:LEU:HD12	1.87	0.40
1:A:318:MET:CE	1:A:318:MET:HA	2.51	0.40
1:B:1417:LYS:NZ	1:B:1419:ASP:OD2	2.45	0.40
1:B:1421:LYS:HD2	1:B:1422:SER:N	2.36	0.40
1:A:275:LEU:HA	1:A:289:ARG:HE	1.84	0.40
1:B:1007:LEU:HD11	1:B:1029:ILE:CG2	2.52	0.40
1:A:67:LEU:HA	1:A:71:PHE:O	2.22	0.40
1:B:1267:ALA:C	1:B:1269:GLU:N	2.75	0.40
1:B:1335:LEU:C	1:B:1337:GLU:H	2.24	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	424/427 (99%)	369 (87%)	44 (10%)	11 (3%)	5 4
1	B	424/427 (99%)	374 (88%)	40 (9%)	10 (2%)	6 4
All	All	848/854 (99%)	743 (88%)	84 (10%)	21 (2%)	5 4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	B	1297	SER
1	A	246	ALA
1	A	267	ALA
1	A	294	LYS
1	A	330	GLY
1	B	1267	ALA
1	B	1294	LYS
1	B	1330	GLY
1	A	4	LYS
1	B	1145	TYR
1	B	1268	ASN
1	B	1290	ARG
1	B	1406	ALA
1	A	285	PRO
1	A	286	GLU
1	B	1285	PRO
1	B	1286	GLU
1	A	37	LYS
1	A	331	THR
1	A	291	ALA

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	360/361 (100%)	344 (96%)	16 (4%)	28	39
1	B	360/361 (100%)	340 (94%)	20 (6%)	21	29
All	All	720/722 (100%)	684 (95%)	36 (5%)	24	34

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	26	GLN
1	A	119	ARG
1	A	153	ASN
1	A	155	ARG
1	A	212	ASN
1	A	232	ASN
1	A	260	TRP
1	A	272	LEU
1	A	278	ILE
1	A	284	ILE
1	A	288	PHE
1	A	294	LYS
1	A	299	ARG
1	A	318	MET
1	A	404	LYS
1	B	1007	LEU
1	B	1020	LEU
1	B	1081	ASN
1	B	1098	GLU
1	B	1150	ASP
1	B	1153	ASN
1	B	1216	GLU
1	B	1217	ARG
1	B	1232	ASN
1	B	1260	TRP
1	B	1272	LEU

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Mol	Chain	Res	Type
1	B	1278	ILE
1	B	1284	ILE
1	B	1288	PHE
1	B	1294	LYS
1	B	1299	ARG
1	B	1318	MET
1	B	1354	GLU
1	B	1404	LYS
1	B	1425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	129	HIS
1	A	153	ASN
1	A	156	HIS
1	A	182	GLN
1	A	212	ASN
1	A	231	GLN
1	A	232	ASN
1	A	305	HIS
1	B	1026	GLN
1	B	1081	ASN
1	B	1097	GLN
1	B	1110	HIS
1	B	1114	HIS
1	B	1129	HIS
1	B	1153	ASN
1	B	1231	GLN
1	B	1232	ASN
1	B	1305	HIS

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)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	2001	-	4,4,4	0.60	0	6,6,6	3.85	4 (66%)
2	SO4	B	2003	-	4,4,4	0.61	0	6,6,6	3.86	4 (66%)
2	SO4	A	2005	-	4,4,4	0.69	0	6,6,6	0.39	0
2	SO4	B	2002	-	4,4,4	0.73	0	6,6,6	0.26	0
2	SO4	A	2006	-	4,4,4	0.67	0	6,6,6	0.46	0
2	SO4	A	2004	-	4,4,4	0.68	0	6,6,6	0.32	0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2003	SO4	O4-S-O1	-5.81	79.01	109.31
2	B	2001	SO4	O4-S-O1	-5.73	79.40	109.31
2	B	2003	SO4	O4-S-O3	-5.24	86.68	109.06
2	B	2001	SO4	O4-S-O3	-5.09	87.32	109.06
2	B	2001	SO4	O4-S-O2	-4.71	84.72	109.31
2	B	2003	SO4	O4-S-O2	-4.55	85.54	109.31
2	B	2001	SO4	O2-S-O1	2.42	127.27	109.43
2	B	2003	SO4	O2-S-O1	2.32	126.53	109.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	SO4	2	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.