



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:01 PM GMT

PDB ID : 1DQR
Title : CRYSTAL STRUCTURE OF RABBIT PHOSPHOGLUCOSE ISOMERASE,
A GLYCOLYTIC ENZYME THAT MOONLIGHTS AS NEUROLEUKIN,
AUTOCRINE MOTILITY FACTOR, AND DIFFERENTIATION MEDIA-
TOR
Authors : Bahnson, B.J.; Jeffery, C.J.; Ringe, D.; Petsko, G.A.
Deposited on : 2000-01-05
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

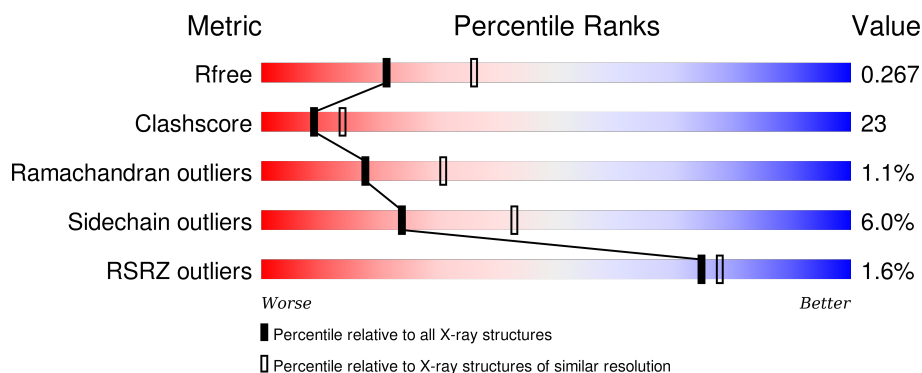
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	557	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 63%; height: 10px; background-color: green;"></div> <div style="width: 33%; height: 10px; background-color: yellow;"></div> • </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 63% 33% </div> </div>
1	B	557	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 2% <div style="width: 61%; height: 10px; background-color: green;"></div> <div style="width: 34%; height: 10px; background-color: yellow;"></div> • </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 61% 34% </div> </div>

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	6PG	A	600	-	-	-	X
2	6PG	B	601	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9194 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.

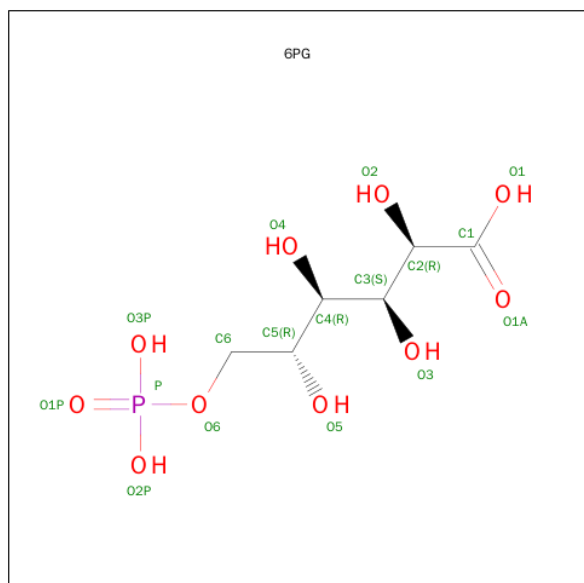
- Molecule 1 is a protein called PHOSPHOGLUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4395	2805	765	806	19			
1	B	555	Total	C	N	O	S	0	0	0
			4395	2805	765	806	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	PRO	LEU	see remark 999	UNP Q9N1E2
A	222	LYS	GLU	see remark 999	UNP Q9N1E2
A	283	ILE	VAL	see remark 999	UNP Q9N1E2
B	109	PRO	LEU	see remark 999	UNP Q9N1E2
B	222	LYS	GLU	see remark 999	UNP Q9N1E2
B	283	ILE	VAL	see remark 999	UNP Q9N1E2

- Molecule 2 is 6-PHOSPHOGLUCONATE (three-letter code: 6PG) (formula: $C_6H_{13}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			17	6	10	1		
2	B	1	Total	C	O	P	0	0
			17	6	10	1		

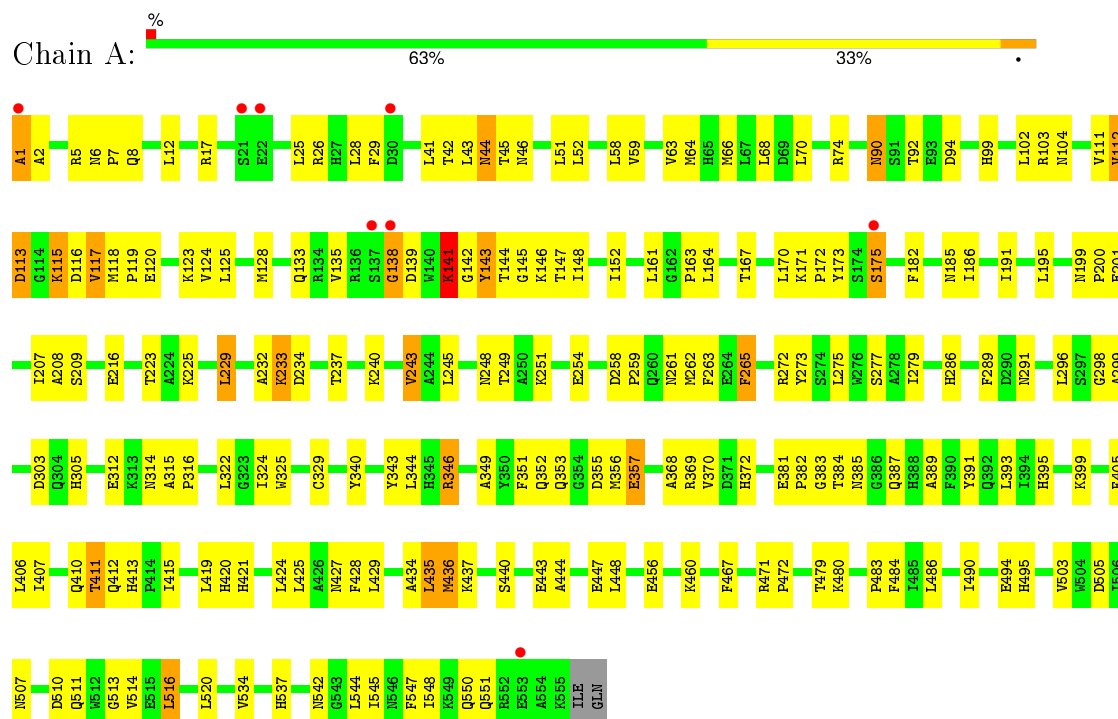
- Molecule 3 is water.

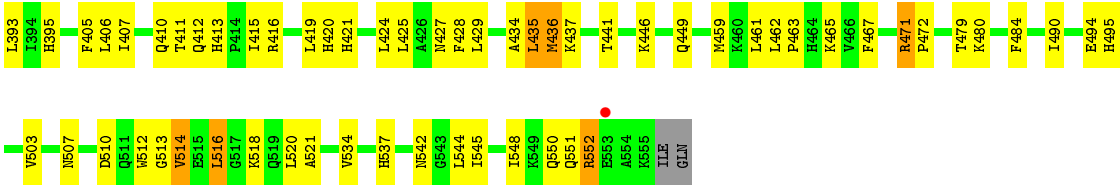
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	176	Total	O	0	0
			176	176		
3	B	194	Total	O	0	0
			194	194		

3 Residue-property plots

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

• Molecule 1: PHOSPHOGLUCOSE ISOMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	82.69Å 115.27Å 271.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.50 19.94 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.9 (35.00-2.50) 92.2 (19.94-2.51)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.48 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.265 0.213 , 0.267	Depositor DCC
R_{free} test set	4152 reflections (10.06%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 41256 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9194	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6PG

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	0.42	3/4504 (0.1%)	0.65	3/6101 (0.0%)
1	B	0.44	3/4504 (0.1%)	0.64	2/6101 (0.0%)
All	All	0.43	6/9008 (0.1%)	0.65	5/12202 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	514	VAL	CB-CG1	-8.29	1.35	1.52
1	B	514	VAL	CB-CG2	-6.59	1.39	1.52
1	A	514	VAL	CB-CG2	-6.17	1.39	1.52
1	A	1	ALA	CA-CB	-5.96	1.40	1.52
1	B	143	TYR	CD2-CE2	-5.91	1.30	1.39
1	A	514	VAL	CB-CG1	-5.60	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	VAL	CB-CA-C	-6.89	98.31	111.40
1	A	112	VAL	CB-CA-C	-6.76	98.56	111.40
1	A	141	LYS	N-CA-C	6.75	129.22	111.00
1	A	175	SER	N-CA-C	6.72	129.16	111.00
1	B	175	SER	N-CA-C	6.38	128.23	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4395	0	4352	219	0
1	B	4395	0	4352	216	0
2	A	17	0	10	1	0
2	B	17	0	10	1	0
3	A	176	0	0	12	0
3	B	194	0	0	15	0
All	All	9194	0	8724	408	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 23.

All (408) 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:B:143:TYR:CE2	3:B:787:HOH:O	1.87	1.24
1:A:1:ALA:CB	3:A:774:HOH:O	1.95	1.10
1:A:113:ASP:CG	3:A:724:HOH:O	1.89	1.10
1:B:112:VAL:O	1:B:112:VAL:HG23	1.48	1.10
1:A:112:VAL:O	1:A:112:VAL:HG23	1.38	1.08
1:B:112:VAL:O	1:B:113:ASP:HB2	1.61	1.00
1:A:142:GLY:O	1:A:145:GLY:N	1.95	0.98
1:A:141:LYS:HB2	1:A:240:LYS:HE2	1.50	0.93
1:B:550:GLN:HE21	1:B:551:GLN:HE21	1.09	0.92
1:B:143:TYR:CD2	3:B:787:HOH:O	2.13	0.91
1:A:112:VAL:CG2	1:A:112:VAL:O	2.13	0.91
1:A:1:ALA:HB1	3:A:774:HOH:O	1.61	0.91
1:B:6:ASN:HD21	1:B:8:GLN:HG2	1.37	0.89
1:B:240:LYS:HE3	3:B:787:HOH:O	1.76	0.86
1:B:90:ASN:ND2	1:B:507:ASN:HD21	1.78	0.81
1:A:59:VAL:HG23	1:A:63:VAL:HB	1.62	0.81
1:A:185:ASN:HD21	1:B:383:GLY:HA3	1.46	0.81
1:B:59:VAL:HG23	1:B:63:VAL:HB	1.61	0.81
1:A:5:ARG:HH11	1:A:5:ARG:HB2	1.48	0.79
1:A:233:LYS:HZ3	1:A:233:LYS:HB2	1.49	0.78
1:B:436:MET:HE2	1:B:437:LYS:HA	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:HH12	1:A:511:GLN:HE21	1.32	0.77
1:B:550:GLN:HE21	1:B:551:GLN:NE2	1.82	0.77
1:A:112:VAL:O	1:A:113:ASP:HB2	1.85	0.77
1:B:143:TYR:HE2	3:B:787:HOH:O	1.33	0.77
1:A:1:ALA:N	1:A:368:ALA:HB1	2.00	0.76
1:A:5:ARG:NH1	1:A:5:ARG:HB2	2.01	0.76
1:A:90:ASN:ND2	1:A:507:ASN:HD21	1.84	0.75
1:B:103:ARG:HD2	1:B:303:ASP:OD2	1.86	0.75
1:B:59:VAL:HG21	1:B:64:MET:SD	2.25	0.75
1:B:258:ASP:OD2	1:B:260:GLN:HG2	1.87	0.75
1:B:471:ARG:NH2	3:B:607:HOH:O	2.19	0.75
1:B:14:GLN:O	1:B:18:GLU:HB2	1.87	0.74
1:A:436:MET:HE2	1:A:437:LYS:HA	1.68	0.74
1:A:383:GLY:HA3	1:B:185:ASN:HD21	1.52	0.74
1:A:142:GLY:O	1:A:144:THR:N	2.21	0.73
1:A:139:ASP:O	1:A:139:ASP:OD2	2.04	0.73
1:A:209:SER:HA	2:A:600:6PG:O2P	1.87	0.73
1:A:44:ASN:ND2	1:A:46:ASN:H	1.87	0.73
1:A:1:ALA:H1	1:A:368:ALA:HB1	1.55	0.72
1:B:102:LEU:HD13	1:B:277:SER:HB3	1.72	0.72
1:A:185:ASN:ND2	1:B:383:GLY:HA3	2.03	0.72
1:B:6:ASN:HD22	1:B:9:PHE:H	1.38	0.71
1:B:550:GLN:NE2	1:B:551:GLN:HE21	1.87	0.71
1:B:315:ALA:HB3	1:B:316:PRO:HD3	1.71	0.71
1:B:248:ASN:ND2	1:B:251:LYS:HG3	2.05	0.71
1:A:353:GLN:O	1:A:357:GLU:HB2	1.91	0.71
1:B:324:ILE:HD13	1:B:503:VAL:HG11	1.73	0.70
1:A:315:ALA:HB3	1:A:316:PRO:HD3	1.73	0.70
1:A:172:PRO:HG2	1:A:412:GLN:HG3	1.72	0.70
1:A:550:GLN:HE21	1:A:551:GLN:HE21	1.39	0.70
1:B:240:LYS:HG3	3:B:787:HOH:O	1.92	0.70
1:B:253:LYS:HE2	1:B:253:LYS:HA	1.71	0.70
1:A:324:ILE:HD13	1:A:503:VAL:HG11	1.73	0.70
1:B:112:VAL:CG2	1:B:112:VAL:O	2.21	0.69
1:B:26:ARG:HA	1:B:436:MET:HE1	1.75	0.69
1:A:94:ASP:OD1	3:A:624:HOH:O	2.11	0.69
1:A:59:VAL:HG21	1:A:64:MET:SD	2.32	0.68
1:B:74:ARG:HD3	1:B:503:VAL:O	1.92	0.68
1:B:172:PRO:HG2	1:B:412:GLN:HG3	1.76	0.68
1:A:102:LEU:HD13	1:A:277:SER:HB3	1.75	0.68
1:A:383:GLY:HA3	1:B:185:ASN:ND2	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ALA:HA	1:A:352:GLN:HG3	1.76	0.67
1:A:26:ARG:HA	1:A:436:MET:HE1	1.76	0.67
1:A:125:LEU:HD23	1:A:128:MET:HE1	1.76	0.67
1:A:141:LYS:HG3	1:A:240:LYS:CE	2.24	0.67
1:A:407:ILE:HD13	1:A:425:LEU:HD23	1.76	0.67
1:A:340:TYR:HB3	1:A:424:LEU:HD11	1.76	0.67
3:A:765:HOH:O	1:B:49:HIS:HD2	1.77	0.66
1:A:8:GLN:NE2	1:A:8:GLN:H	1.94	0.66
1:B:254:GLU:HG3	3:B:671:HOH:O	1.93	0.66
1:A:537:HIS:H	1:A:542:ASN:HD21	1.43	0.65
1:B:59:VAL:HG23	1:B:63:VAL:CB	2.27	0.65
1:B:537:HIS:H	1:B:542:ASN:HD21	1.42	0.65
1:A:143:TYR:CZ	1:A:232:ALA:HB2	2.32	0.65
1:B:436:MET:HE2	1:B:437:LYS:CA	2.26	0.65
1:A:146:LYS:HD3	1:A:147:THR:H	1.63	0.64
1:B:17:ARG:NH1	1:B:17:ARG:HB2	2.12	0.64
1:B:441:THR:HG23	1:B:462:LEU:HD11	1.78	0.64
1:B:148:ILE:HD13	1:B:204:LEU:HB2	1.78	0.64
1:B:361:LYS:HZ3	1:B:510:ASP:HB2	1.62	0.64
1:A:243:VAL:HG22	1:A:261:ASN:O	1.99	0.63
1:B:387:GLN:HE22	1:B:427:ASN:HB3	1.63	0.63
1:A:59:VAL:HG23	1:A:63:VAL:CB	2.28	0.63
1:B:343:TYR:OH	1:B:413:HIS:HE1	1.82	0.63
1:A:436:MET:HE2	1:A:437:LYS:CA	2.28	0.62
1:A:141:LYS:N	1:A:141:LYS:HE3	2.13	0.62
1:B:357:GLU:OE2	2:B:601:6PG:O1	2.17	0.62
1:B:141:LYS:O	1:B:240:LYS:HD2	1.98	0.62
1:A:387:GLN:HE22	1:A:427:ASN:HB3	1.65	0.61
1:B:340:TYR:HB3	1:B:424:LEU:HD11	1.82	0.61
1:B:411:THR:HG23	1:B:421:HIS:CE1	2.34	0.61
1:A:314:ASN:OD1	1:A:316:PRO:HD2	2.01	0.61
1:A:385:ASN:H	1:A:385:ASN:HD22	1.48	0.61
1:B:103:ARG:HD3	1:B:299:ALA:CB	2.31	0.61
1:A:141:LYS:CB	1:A:240:LYS:HE2	2.27	0.61
1:B:125:LEU:HA	1:B:128:MET:HE3	1.83	0.61
1:A:411:THR:HG23	1:A:421:HIS:CE1	2.36	0.61
1:B:59:VAL:CG2	1:B:63:VAL:HB	2.32	0.60
1:A:144:THR:CG2	1:A:201:GLU:HB2	2.31	0.60
1:B:125:LEU:HD23	1:B:128:MET:HE1	1.83	0.60
1:B:44:ASN:ND2	1:B:46:ASN:H	1.99	0.60
1:B:59:VAL:HG23	1:B:63:VAL:CG1	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HA	1:A:128:MET:HE3	1.81	0.60
1:B:385:ASN:HD22	1:B:385:ASN:H	1.47	0.60
1:A:343:TYR:OH	1:A:413:HIS:HE1	1.85	0.59
1:B:395:HIS:HD2	3:B:660:HOH:O	1.84	0.59
1:A:58:LEU:CD2	1:A:472:PRO:HB3	2.32	0.59
1:A:103:ARG:NH2	1:A:494:GLU:OE1	2.35	0.59
1:A:59:VAL:HG23	1:A:63:VAL:CG1	2.33	0.59
1:A:59:VAL:CG2	1:A:63:VAL:HB	2.31	0.59
1:B:42:THR:HG23	3:B:632:HOH:O	2.02	0.59
1:A:233:LYS:NZ	1:A:233:LYS:HB2	2.18	0.59
1:B:407:ILE:HD13	1:B:425:LEU:HD23	1.83	0.59
1:A:113:ASP:OD1	3:A:724:HOH:O	2.11	0.58
1:A:141:LYS:N	1:A:141:LYS:CE	2.65	0.58
1:B:352:GLN:HG3	1:B:378:VAL:O	2.03	0.58
1:B:544:LEU:O	1:B:548:ILE:HG13	2.03	0.58
1:A:381:GLU:HG3	1:A:382:PRO:HD2	1.84	0.58
1:A:104:ASN:HB3	1:A:118:MET:HE1	1.85	0.58
1:B:143:TYR:CD1	1:B:237:THR:HG22	2.38	0.58
1:A:249:THR:HA	1:A:262:MET:SD	2.44	0.57
1:B:58:LEU:CD2	1:B:472:PRO:HB3	2.35	0.57
1:B:146:LYS:NZ	1:B:201:GLU:OE1	2.36	0.57
1:B:361:LYS:NZ	1:B:510:ASP:HB2	2.19	0.56
1:A:410:GLN:HG3	1:A:480:LYS:HD2	1.87	0.56
1:B:234:ASP:HB3	1:B:237:THR:HG23	1.85	0.56
1:B:257:ILE:HG22	1:B:258:ASP:N	2.21	0.56
1:A:234:ASP:HB3	1:A:237:THR:HG23	1.86	0.56
1:A:141:LYS:O	1:A:240:LYS:HB3	2.04	0.56
1:B:117:VAL:O	1:B:120:GLU:HG2	2.06	0.56
1:A:117:VAL:O	1:A:120:GLU:HG2	2.06	0.56
1:B:253:LYS:HE2	1:B:253:LYS:CA	2.34	0.56
1:B:6:ASN:ND2	1:B:8:GLN:HG2	2.13	0.56
1:A:124:VAL:HG12	1:A:128:MET:HE2	1.88	0.56
1:B:56:LYS:HB2	3:B:621:HOH:O	2.06	0.55
1:B:20:GLY:C	1:B:22:GLU:H	2.10	0.55
1:A:443:GLU:O	1:A:447:GLU:HG3	2.07	0.55
1:B:490:ILE:O	1:B:494:GLU:HG3	2.06	0.55
1:A:420:HIS:HD2	1:B:186:ILE:O	1.90	0.55
1:A:103:ARG:HD3	1:A:299:ALA:CB	2.37	0.55
1:B:100:VAL:HG22	3:B:617:HOH:O	2.06	0.55
1:A:103:ARG:HD2	1:A:303:ASP:OD2	2.07	0.55
1:A:353:GLN:HA	1:B:389:ALA:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HD13	1:A:216:GLU:HA	1.88	0.55
1:A:223:THR:OG1	1:B:420:HIS:HE1	1.90	0.54
1:B:393:LEU:HD23	1:B:393:LEU:O	2.07	0.54
1:B:167:THR:HG23	1:B:286:HIS:ND1	2.23	0.54
1:A:370:VAL:HG12	1:A:372:HIS:H	1.71	0.54
1:A:141:LYS:H	1:A:141:LYS:CD	2.19	0.54
1:A:490:ILE:O	1:A:494:GLU:HG3	2.08	0.54
1:A:185:ASN:HD21	1:B:383:GLY:CA	2.19	0.54
1:A:135:VAL:HG13	1:A:148:ILE:CG1	2.38	0.54
1:B:446:LYS:HE3	1:B:449:GLN:HE22	1.73	0.53
1:A:545:ILE:HG12	1:B:429:LEU:HD13	1.89	0.53
1:A:142:GLY:C	1:A:144:THR:N	2.60	0.53
1:B:199:ASN:OD1	1:B:201:GLU:HG2	2.09	0.53
1:A:186:ILE:CG2	1:B:424:LEU:HD23	2.39	0.53
1:B:275:LEU:C	1:B:275:LEU:HD12	2.29	0.53
1:A:393:LEU:O	1:A:393:LEU:HD23	2.09	0.53
1:B:152:ILE:N	1:B:152:ILE:HD12	2.24	0.53
1:A:113:ASP:HB2	3:A:724:HOH:O	2.08	0.52
1:A:8:GLN:HE21	1:A:8:GLN:H	1.56	0.52
1:B:45:THR:O	1:B:46:ASN:HB2	2.09	0.52
1:A:135:VAL:HG13	1:A:148:ILE:HG12	1.90	0.52
1:B:381:GLU:HG3	1:B:382:PRO:HD2	1.90	0.52
1:A:207:ILE:N	1:A:207:ILE:HD12	2.25	0.52
1:A:312:GLU:CD	1:A:312:GLU:H	2.12	0.52
1:A:124:VAL:HG12	1:A:128:MET:CE	2.40	0.52
1:A:167:THR:HG23	1:A:286:HIS:ND1	2.24	0.52
1:B:370:VAL:HG12	1:B:372:HIS:H	1.75	0.52
1:A:164:LEU:HD22	1:A:346:ARG:HG2	1.91	0.52
1:B:163:PRO:HB2	1:B:182:PHE:HE2	1.75	0.52
1:B:143:TYR:HD1	1:B:237:THR:HG22	1.75	0.52
1:B:20:GLY:C	1:B:22:GLU:N	2.63	0.52
1:A:199:ASN:OD1	1:A:201:GLU:HG2	2.10	0.51
1:A:90:ASN:HD22	1:A:90:ASN:C	2.12	0.51
1:A:415:ILE:HD11	1:A:420:HIS:CG	2.45	0.51
1:B:99:HIS:HE1	3:B:604:HOH:O	1.91	0.51
1:A:410:GLN:HG2	1:A:479:THR:O	2.10	0.51
1:A:44:ASN:HD22	1:A:45:THR:N	2.09	0.51
1:B:186:ILE:HD13	1:B:216:GLU:HA	1.91	0.51
1:B:141:LYS:HD2	1:B:141:LYS:O	2.10	0.51
1:A:303:ASP:OD1	1:A:495:HIS:CE1	2.63	0.51
1:B:207:ILE:HD12	1:B:207:ILE:N	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:C	1:B:164:LEU:HD23	2.31	0.51
1:A:1:ALA:H2	1:A:368:ALA:HB1	1.76	0.51
1:B:80:ARG:HG3	1:B:306:PHE:CE2	2.46	0.51
1:B:104:ASN:HB3	1:B:118:MET:HE1	1.92	0.51
1:B:243:VAL:HG22	1:B:261:ASN:O	2.11	0.51
1:A:223:THR:OG1	1:B:416:ARG:NH1	2.43	0.51
1:A:275:LEU:HD12	1:A:275:LEU:C	2.31	0.51
1:A:116:ASP:OD2	1:A:119:PRO:HD3	2.11	0.51
1:B:245:LEU:HA	1:B:263:PHE:O	2.11	0.51
1:B:305:HIS:HE1	1:B:315:ALA:H	1.58	0.50
1:A:152:ILE:N	1:A:152:ILE:HD12	2.26	0.50
1:A:395:HIS:NE2	1:A:435:LEU:HD13	2.27	0.50
1:B:314:ASN:OD1	1:B:316:PRO:HD2	2.11	0.50
1:B:471:ARG:HB3	3:B:744:HOH:O	2.12	0.50
1:B:124:VAL:HG12	1:B:128:MET:HE2	1.93	0.50
1:B:99:HIS:CE1	3:B:604:HOH:O	2.64	0.50
1:B:41:LEU:HD12	1:B:41:LEU:O	2.11	0.50
1:B:248:ASN:HD21	1:B:251:LYS:HG3	1.77	0.50
1:A:186:ILE:HG23	1:B:424:LEU:HD23	1.94	0.50
1:A:113:ASP:CB	3:A:724:HOH:O	2.42	0.50
1:A:249:THR:HG22	1:A:262:MET:SD	2.51	0.50
1:A:272:ARG:HH12	1:A:511:GLN:NE2	2.05	0.49
1:B:462:LEU:C	1:B:462:LEU:HD13	2.32	0.49
1:A:2:ALA:HA	1:A:5:ARG:HD3	1.94	0.49
1:A:141:LYS:HG3	1:A:240:LYS:HD2	1.94	0.49
1:A:440:SER:OG	1:A:443:GLU:HG3	2.12	0.49
1:A:429:LEU:HD13	1:B:545:ILE:HG12	1.94	0.49
1:B:303:ASP:OD1	1:B:495:HIS:HE1	1.96	0.49
1:A:163:PRO:HB2	1:A:182:PHE:HE2	1.77	0.49
1:B:410:GLN:HE21	1:B:480:LYS:HD2	1.76	0.49
1:B:14:GLN:O	1:B:18:GLU:N	2.43	0.49
1:B:6:ASN:HD22	1:B:9:PHE:N	2.08	0.49
1:B:90:ASN:HD22	1:B:90:ASN:C	2.15	0.48
1:A:45:THR:O	1:A:46:ASN:HB2	2.13	0.48
1:B:248:ASN:O	1:B:252:VAL:HG23	2.12	0.48
1:B:461:LEU:HG	1:B:465:LYS:HD2	1.94	0.48
1:B:292:PHE:O	1:B:295:LEU:HB3	2.12	0.48
1:A:208:ALA:HB2	1:A:245:LEU:HD12	1.94	0.48
1:B:411:THR:HG23	1:B:421:HIS:ND1	2.29	0.48
1:A:41:LEU:HD12	1:A:41:LEU:O	2.13	0.48
1:A:138:GLY:HA2	1:A:147:THR:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:VAL:HG21	1:B:545:ILE:HG21	1.94	0.48
1:A:513:GLY:HA2	1:B:467:PHE:CZ	2.49	0.48
1:A:143:TYR:CE2	1:A:232:ALA:HB2	2.48	0.48
1:A:413:HIS:ND1	1:B:189:THR:HG22	2.29	0.48
1:A:424:LEU:HD23	1:B:186:ILE:CG2	2.44	0.48
1:B:312:GLU:H	1:B:312:GLU:CD	2.16	0.48
1:B:289:PHE:O	1:B:293:GLU:HG3	2.14	0.47
1:A:186:ILE:HB	1:A:216:GLU:HG3	1.95	0.47
1:A:467:PHE:CZ	1:B:513:GLY:HA2	2.50	0.47
1:B:518:LYS:O	1:B:521:ALA:HB3	2.14	0.47
1:B:242:PHE:HB3	1:B:257:ILE:CD1	2.45	0.47
1:B:103:ARG:HD3	1:B:299:ALA:HB3	1.94	0.47
1:B:510:ASP:HB3	3:B:784:HOH:O	2.14	0.47
1:A:510:ASP:HB3	3:A:767:HOH:O	2.15	0.47
1:B:132:CYS:O	1:B:136:ARG:HG3	2.14	0.47
1:A:434:ALA:HB2	1:B:520:LEU:HD12	1.97	0.47
1:A:12:LEU:HD23	1:A:66:MET:CB	2.45	0.47
1:B:103:ARG:HD3	1:B:299:ALA:HB1	1.96	0.47
1:B:462:LEU:HD13	1:B:463:PRO:N	2.28	0.47
1:A:104:ASN:HD22	1:A:118:MET:CE	2.28	0.47
1:B:410:GLN:HG2	1:B:479:THR:O	2.13	0.47
1:A:272:ARG:NH1	1:A:511:GLN:HE21	2.07	0.47
1:B:303:ASP:OD1	1:B:495:HIS:CE1	2.68	0.47
1:B:92:THR:HG1	1:B:510:ASP:CG	2.16	0.47
1:A:411:THR:HG23	1:A:421:HIS:ND1	2.30	0.47
1:A:164:LEU:HD23	1:A:164:LEU:C	2.35	0.47
1:A:142:GLY:O	1:A:143:TYR:C	2.53	0.47
1:B:294:GLN:O	1:B:484:PHE:HA	2.14	0.47
1:B:103:ARG:O	1:B:300:HIS:HB2	2.14	0.47
1:B:361:LYS:NZ	1:B:510:ASP:CB	2.78	0.47
1:B:395:HIS:NE2	1:B:435:LEU:HD13	2.30	0.47
1:B:142:GLY:O	1:B:144:THR:N	2.39	0.46
1:A:144:THR:HB	1:A:201:GLU:HB2	1.97	0.46
1:B:42:THR:HG22	1:B:51:LEU:HD13	1.96	0.46
1:B:17:ARG:HG2	1:B:17:ARG:O	2.14	0.46
1:B:124:VAL:HG12	1:B:128:MET:CE	2.44	0.46
1:B:128:MET:SD	1:B:278:ALA:HA	2.55	0.46
1:B:243:VAL:HG23	1:B:261:ASN:HB3	1.97	0.46
1:A:92:THR:HG1	1:A:510:ASP:CG	2.18	0.46
1:A:355:ASP:HB2	3:A:746:HOH:O	2.14	0.46
1:A:544:LEU:O	1:A:548:ILE:HG13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HG13	1:A:115:LYS:N	2.31	0.46
1:B:14:GLN:O	1:B:18:GLU:CB	2.61	0.46
1:A:387:GLN:HA	1:A:391:TYR:CG	2.51	0.46
1:A:385:ASN:H	1:A:385:ASN:ND2	2.14	0.46
1:B:21:SER:O	1:B:22:GLU:C	2.53	0.46
1:B:112:VAL:O	1:B:113:ASP:CB	2.39	0.46
1:A:141:LYS:HG3	1:A:240:LYS:HE3	1.98	0.46
1:A:12:LEU:HD23	1:A:66:MET:HB3	1.97	0.46
1:A:298:GLY:HA3	1:A:484:PHE:O	2.16	0.46
1:A:112:VAL:O	1:A:113:ASP:CB	2.57	0.46
1:B:436:MET:HE2	1:B:437:LYS:N	2.31	0.46
1:A:537:HIS:HB2	1:A:542:ASN:ND2	2.31	0.46
1:B:387:GLN:HA	1:B:391:TYR:CG	2.50	0.46
1:A:303:ASP:OD1	1:A:495:HIS:HE1	1.97	0.46
1:B:334:THR:HG22	1:B:377:ILE:HB	1.97	0.46
1:A:424:LEU:HD23	1:B:186:ILE:HG23	1.98	0.45
1:B:537:HIS:HB2	1:B:542:ASN:ND2	2.31	0.45
1:A:534:VAL:HG21	1:A:545:ILE:HG21	1.97	0.45
1:A:144:THR:HG21	1:A:201:GLU:HB2	1.98	0.45
1:A:6:ASN:HA	1:A:7:PRO:HD3	1.72	0.45
1:A:170:LEU:HD11	1:A:486:LEU:HD23	1.98	0.45
1:A:138:GLY:O	1:A:139:ASP:HB3	2.16	0.45
1:B:141:LYS:HD2	1:B:141:LYS:C	2.37	0.45
1:B:393:LEU:HD23	1:B:393:LEU:C	2.37	0.45
1:A:471:ARG:HA	1:A:472:PRO:HD2	1.85	0.45
1:B:369:ARG:HD3	1:B:369:ARG:O	2.16	0.45
1:A:8:GLN:NE2	1:A:8:GLN:N	2.62	0.45
1:A:420:HIS:CD2	1:B:186:ILE:O	2.70	0.45
1:A:142:GLY:C	1:A:144:THR:H	2.20	0.45
1:A:58:LEU:HD22	1:A:58:LEU:N	2.31	0.45
1:A:303:ASP:HA	1:A:495:HIS:HE1	1.81	0.45
1:B:186:ILE:HB	1:B:216:GLU:HG3	1.99	0.45
1:B:58:LEU:HD23	1:B:472:PRO:HB3	1.99	0.44
1:B:462:LEU:HB3	1:B:463:PRO:HD3	1.99	0.44
1:B:385:ASN:H	1:B:385:ASN:ND2	2.15	0.44
1:B:335:GLN:HB3	1:B:378:VAL:HG22	1.99	0.44
1:B:415:ILE:HD11	1:B:420:HIS:CG	2.51	0.44
1:A:103:ARG:HD3	1:A:299:ALA:HB3	1.99	0.44
1:A:141:LYS:HG3	1:A:240:LYS:CD	2.48	0.44
1:B:415:ILE:HD12	1:B:415:ILE:C	2.37	0.44
1:B:415:ILE:HD12	1:B:415:ILE:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ALA:HB1	1:B:516:LEU:HD13	2.00	0.44
1:B:17:ARG:HH11	1:B:17:ARG:CB	2.31	0.44
1:A:103:ARG:HD3	1:A:299:ALA:HB1	1.99	0.44
1:B:117:VAL:HG22	1:B:120:GLU:OE1	2.18	0.44
1:A:144:THR:HB	1:A:201:GLU:CB	2.48	0.44
1:A:265:PHE:CZ	1:A:279:ILE:HD11	2.53	0.44
1:A:516:LEU:HD13	1:B:434:ALA:HB1	2.00	0.44
1:A:405:PHE:HB3	1:A:428:PHE:CE1	2.53	0.44
1:B:5:ARG:HB3	1:B:5:ARG:HH11	1.82	0.44
1:A:393:LEU:C	1:A:393:LEU:HD23	2.38	0.43
1:B:116:ASP:OD2	1:B:119:PRO:HD3	2.18	0.43
1:B:92:THR:OG1	1:B:510:ASP:OD1	2.37	0.43
1:A:384:THR:O	1:A:387:GLN:HB2	2.18	0.43
1:A:171:LYS:HD2	1:A:286:HIS:HE1	1.83	0.43
1:A:325:TRP:O	1:A:329:CYS:HB2	2.19	0.43
1:B:102:LEU:CD1	1:B:277:SER:HB3	2.46	0.43
1:A:99:HIS:ND1	1:A:103:ARG:NH2	2.64	0.43
1:B:111:VAL:HG13	1:B:115:LYS:N	2.33	0.43
1:A:26:ARG:HA	1:A:436:MET:CE	2.47	0.43
1:B:17:ARG:C	1:B:19:HIS:N	2.72	0.43
1:A:415:ILE:C	1:A:415:ILE:HD12	2.39	0.43
1:A:480:LYS:HG3	3:A:601:HOH:O	2.19	0.43
1:B:23:LEU:HD22	1:B:23:LEU:H	1.83	0.43
1:B:106:SER:O	1:B:107:ASN:HB2	2.18	0.43
1:A:383:GLY:CA	1:B:185:ASN:HD21	2.26	0.43
1:A:389:ALA:O	1:B:357:GLU:HB2	2.19	0.43
1:B:461:LEU:O	1:B:465:LYS:HG3	2.19	0.43
1:A:42:THR:HG22	1:A:51:LEU:HD13	2.01	0.43
1:B:405:PHE:HB3	1:B:428:PHE:CE1	2.54	0.43
1:B:471:ARG:HA	1:B:472:PRO:HD2	1.85	0.43
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.84	0.43
1:A:12:LEU:CD1	1:A:329:CYS:SG	3.07	0.43
1:A:173:TYR:CZ	1:A:483:PRO:HD3	2.54	0.42
1:B:44:ASN:HD22	1:B:45:THR:N	2.18	0.42
1:B:29:PHE:CE1	1:B:35:ARG:HD3	2.55	0.42
1:B:552:ARG:HH11	1:B:552:ARG:CB	2.32	0.42
1:B:358:SER:C	1:B:359:ASN:HD22	2.22	0.42
1:B:41:LEU:HD12	1:B:41:LEU:C	2.40	0.42
1:A:248:ASN:CB	1:A:251:LYS:HG3	2.49	0.42
1:A:435:LEU:HD12	1:A:435:LEU:HA	1.92	0.42
1:A:460:LYS:HG3	1:A:460:LYS:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:O	1:A:325:TRP:HB3	2.20	0.42
1:A:272:ARG:HG3	1:A:273:TYR:CE1	2.54	0.42
1:B:257:ILE:CG2	1:B:258:ASP:N	2.83	0.42
1:A:44:ASN:HD22	1:A:46:ASN:H	1.65	0.42
1:A:68:LEU:HD13	1:A:312:GLU:HG3	2.00	0.42
1:A:415:ILE:O	1:A:415:ILE:HD12	2.19	0.42
1:B:446:LYS:CE	1:B:449:GLN:HE22	2.32	0.42
1:A:263:PHE:CD1	1:A:263:PHE:N	2.88	0.42
1:A:41:LEU:HD12	1:A:41:LEU:C	2.39	0.42
1:A:191:ILE:HG12	1:A:195:LEU:HD13	2.01	0.42
1:A:406:LEU:HD12	1:A:406:LEU:N	2.34	0.42
1:B:406:LEU:N	1:B:406:LEU:HD12	2.35	0.42
1:A:12:LEU:HD11	1:A:325:TRP:CE3	2.55	0.42
1:A:103:ARG:NH1	1:A:303:ASP:OD1	2.53	0.42
1:A:370:VAL:HG13	1:A:372:HIS:CE1	2.54	0.42
1:B:52:LEU:CD2	1:B:52:LEU:C	2.88	0.42
1:A:258:ASP:HA	1:A:259:PRO:HD3	1.87	0.42
1:A:352:GLN:O	1:A:356:MET:HB2	2.20	0.42
1:A:245:LEU:HA	1:A:263:PHE:O	2.20	0.42
1:A:399:LYS:HD3	1:B:373:GLN:OE1	2.19	0.42
1:B:104:ASN:HD22	1:B:118:MET:CE	2.32	0.41
1:A:420:HIS:HE1	1:B:223:THR:OG1	2.03	0.41
1:B:352:GLN:O	1:B:356:MET:HB2	2.20	0.41
1:A:444:ALA:O	1:A:448:LEU:HD23	2.20	0.41
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.92	0.41
1:A:41:LEU:CD1	1:A:43:LEU:HG	2.50	0.41
1:A:125:LEU:HD23	1:A:128:MET:CE	2.49	0.41
1:A:407:ILE:HD11	1:A:424:LEU:HD12	2.03	0.41
1:B:104:ASN:HB3	1:B:118:MET:CE	2.50	0.41
1:B:249:THR:HG22	1:B:262:MET:SD	2.61	0.41
1:B:361:LYS:HZ3	1:B:510:ASP:CB	2.29	0.41
1:B:512:TRP:C	1:B:514:VAL:H	2.24	0.41
1:A:104:ASN:HB3	1:A:118:MET:CE	2.50	0.41
1:A:225:LYS:O	1:A:229:LEU:HB2	2.20	0.41
1:A:436:MET:HE2	1:A:437:LYS:N	2.36	0.41
1:B:194:THR:O	1:B:198:LEU:HG	2.21	0.41
1:B:317:VAL:O	1:B:321:MET:HG2	2.21	0.41
1:B:322:LEU:O	1:B:325:TRP:HB3	2.20	0.41
1:B:234:ASP:HA	1:B:235:PRO:HD2	1.96	0.41
1:B:186:ILE:HB	1:B:216:GLU:CG	2.51	0.41
1:A:186:ILE:HB	1:A:216:GLU:CG	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:VAL:HG13	1:B:372:HIS:CE1	2.55	0.41
1:A:520:LEU:HD12	1:B:434:ALA:HB2	2.02	0.41
1:A:173:TYR:HB3	1:A:291:ASN:ND2	2.35	0.41
1:B:514:VAL:O	1:B:514:VAL:HG12	2.19	0.41
1:B:242:PHE:HB3	1:B:257:ILE:HD11	2.02	0.41
1:A:547:PHE:CZ	1:A:551:GLN:HG3	2.56	0.41
1:A:415:ILE:HD11	1:A:420:HIS:ND1	2.36	0.41
1:B:4:THR:HG23	1:B:372:HIS:HD2	1.86	0.41
1:A:25:LEU:O	1:A:29:PHE:HD1	2.04	0.41
1:B:90:ASN:HD22	1:B:507:ASN:HD21	1.59	0.40
1:B:276:TRP:CZ3	1:B:299:ALA:HB2	2.56	0.40
1:A:351:PHE:HB3	3:A:746:HOH:O	2.21	0.40
1:A:44:ASN:HD22	1:A:44:ASN:C	2.25	0.40
1:A:248:ASN:HB3	1:A:251:LYS:CG	2.52	0.40
1:A:74:ARG:NH2	1:A:505:ASP:HB2	2.37	0.40
1:B:225:LYS:O	1:B:229:LEU:HB2	2.22	0.40
1:A:63:VAL:HA	1:A:66:MET:HE2	2.03	0.40
1:A:305:HIS:HE1	1:A:315:ALA:H	1.68	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	553/557 (99%)	514 (93%)	34 (6%)	5 (1%)	21	37
1	B	553/557 (99%)	511 (92%)	35 (6%)	7 (1%)	15	26
All	All	1106/1114 (99%)	1025 (93%)	69 (6%)	12 (1%)	17	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	TYR
1	A	138	GLY
1	B	113	ASP
1	A	113	ASP
1	A	175	SER
1	B	16	HIS
1	B	22	GLU
1	B	2	ALA
1	B	3	LEU
1	B	383	GLY
1	A	200	PRO
1	B	200	PRO

5.3.2 Protein sidechains ⓘ

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	475/478 (99%)	446 (94%)	29 (6%)	23	42
1	B	475/478 (99%)	447 (94%)	28 (6%)	24	44
All	All	950/956 (99%)	893 (94%)	57 (6%)	24	43

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	28	LEU
1	A	44	ASN
1	A	52	LEU
1	A	70	LEU
1	A	90	ASN
1	A	115	LYS
1	A	117	VAL
1	A	123	LYS
1	A	133	GLN
1	A	141	LYS
1	A	161	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	229	LEU
1	A	233	LYS
1	A	243	VAL
1	A	254	GLU
1	A	265	PHE
1	A	289	PHE
1	A	296	LEU
1	A	344	LEU
1	A	346	ARG
1	A	357	GLU
1	A	369	ARG
1	A	411	THR
1	A	419	LEU
1	A	435	LEU
1	A	436	MET
1	A	456	GLU
1	A	516	LEU
1	B	8	GLN
1	B	44	ASN
1	B	52	LEU
1	B	56	LYS
1	B	70	LEU
1	B	74	ARG
1	B	90	ASN
1	B	105	ARG
1	B	115	LYS
1	B	141	LYS
1	B	143	TYR
1	B	144	THR
1	B	161	LEU
1	B	229	LEU
1	B	243	VAL
1	B	253	LYS
1	B	265	PHE
1	B	289	PHE
1	B	344	LEU
1	B	346	ARG
1	B	369	ARG
1	B	419	LEU
1	B	435	LEU
1	B	436	MET
1	B	459	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	471	ARG
1	B	516	LEU
1	B	552	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	37	ASN
1	A	44	ASN
1	A	49	HIS
1	A	90	ASN
1	A	104	ASN
1	A	215	GLN
1	A	261	ASN
1	A	286	HIS
1	A	352	GLN
1	A	385	ASN
1	A	387	GLN
1	A	395	HIS
1	A	410	GLN
1	A	413	HIS
1	A	420	HIS
1	A	431	GLN
1	A	495	HIS
1	A	511	GLN
1	A	542	ASN
1	A	550	GLN
1	B	6	ASN
1	B	10	GLN
1	B	16	HIS
1	B	44	ASN
1	B	49	HIS
1	B	90	ASN
1	B	99	HIS
1	B	104	ASN
1	B	153	ASN
1	B	215	GLN
1	B	359	ASN
1	B	385	ASN
1	B	387	GLN
1	B	395	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	410	GLN
1	B	413	HIS
1	B	420	HIS
1	B	449	GLN
1	B	495	HIS
1	B	542	ASN
1	B	550	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	6PG	A	600	-	12,16,16	1.06	1 (8%)	14,23,23	0.81	1 (7%)
2	6PG	B	601	-	12,16,16	0.96	0	14,23,23	0.70	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
2	6PG	A	600	-	-	0/18/22/22	0/0/0/0
2	6PG	B	601	-	-	0/18/22/22	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	6PG	P-O6	-2.19	1.52	1.60

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	6PG	O5-C5-C6	-2.11	105.59	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	6PG	1	0
2	B	601	6PG	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	555/557 (99%)	-0.20	8 (1%) 78 80	10, 27, 61, 87	0
1	B	555/557 (99%)	-0.29	10 (1%) 71 75	9, 25, 52, 86	0
All	All	1110/1114 (99%)	-0.25	18 (1%) 74 78	9, 26, 57, 87	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	GLY	5.5
1	B	21	SER	5.3
1	B	18	GLU	5.1
1	A	1	ALA	4.4
1	B	175	SER	4.1
1	B	143	TYR	4.0
1	B	19	HIS	3.2
1	A	137	SER	3.1
1	A	175	SER	3.1
1	B	369	ARG	2.9
1	A	138	GLY	2.8
1	A	22	GLU	2.7
1	B	17	ARG	2.5
1	A	30	ASP	2.5
1	A	21	SER	2.5
1	B	553	GLU	2.2
1	B	260	GLN	2.1
1	A	553	GLU	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	6PG	B	601	17/17	0.93	0.17	3.74	31,41,49,54	0
2	6PG	A	600	17/17	0.94	0.20	3.05	42,57,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.