



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:49 pm GMT

PDB ID : 1KI1  
Title : Guanine Nucleotide Exchange Region of Intersectin in Complex with Cdc42  
Authors : Snyder, J.T.; Pruitt, W.M.; Der, C.J.; Sondek, J.  
Deposited on : 2001-12-02  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

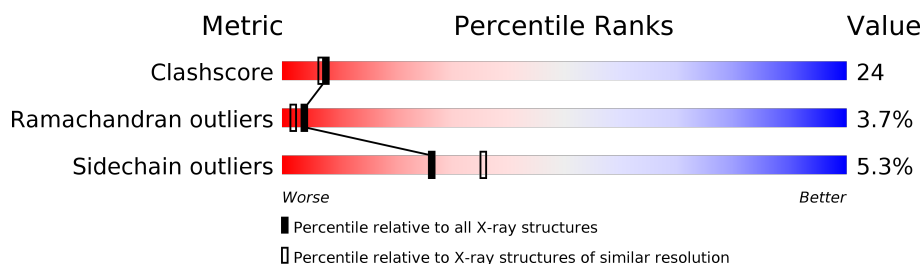
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	188	
1	C	188	
2	B	352	
2	D	352	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8565 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 G25K GTP-binding protein, placental isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1388	893	221	267	7			
1	C	178	Total	C	N	O	S	0	0	0
			1388	893	221	267	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	SER	CYS	ENGINEERED	UNP P60953
C	188	SER	CYS	ENGINEERED	UNP P60953

- Molecule 2 is a protein called intersectin long form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	342	Total	C	N	O	S	0	0	0
			2799	1790	484	507	18			
2	D	342	Total	C	N	O	S	0	0	0
			2799	1790	484	507	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	DELETION	UNP Q15811
D	?	-	LYS	DELETION	UNP Q15811

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

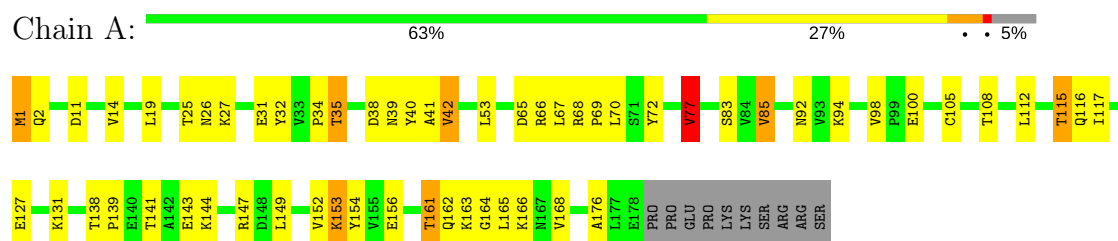
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	45	Total	O	0	0
			45	45		
4	C	39	Total	O	0	0
			39	39		
4	D	53	Total	O	0	0
			53	53		

### 3 Residue-property plots

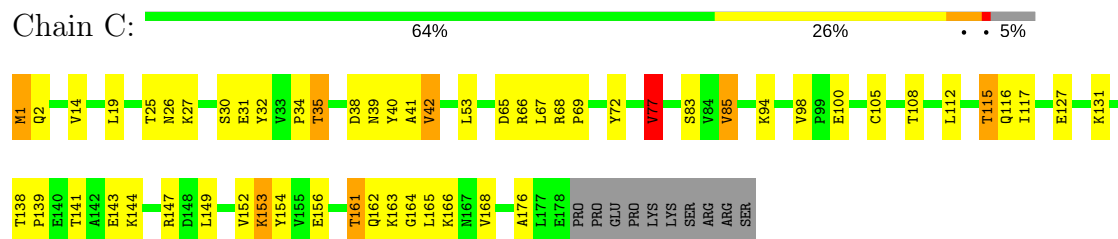
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

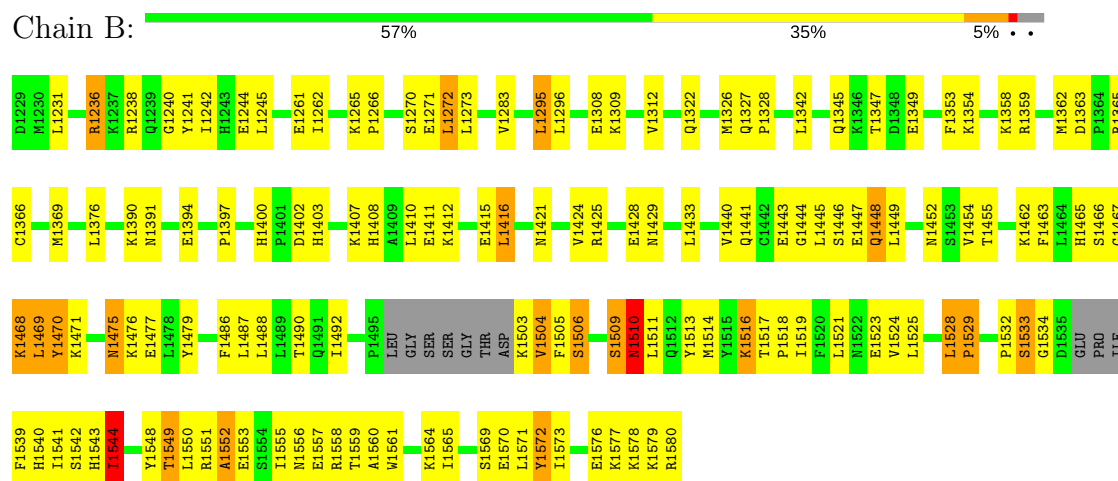
- Molecule 1: G25K GTP-binding protein, placental isoform



- Molecule 1: G25K GTP-binding protein, placental isoform



- Molecule 2: intersectin long form



- Molecule 2: intersectin long form



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.37Å 79.23Å 116.41Å 90.00° 111.51° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.3 (15.00-2.30)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.231 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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	0.43	0/1418	0.70	1/1930 (0.1%)
1	C	0.43	0/1418	0.70	1/1930 (0.1%)
2	B	0.46	0/2854	0.65	2/3840 (0.1%)
2	D	0.45	0/2854	0.66	2/3840 (0.1%)
All	All	0.45	0/8544	0.67	6/11540 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1544	ILE	CA-CB-CG2	6.58	124.05	110.90
2	D	1544	ILE	CA-CB-CG2	6.58	124.05	110.90
1	C	77	VAL	CB-CA-C	-5.10	101.71	111.40
2	B	1549	THR	N-CA-C	-5.03	97.43	111.00
2	D	1549	THR	N-CA-C	-5.01	97.46	111.00
1	A	77	VAL	CB-CA-C	-5.01	101.89	111.40

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	1388	0	1405	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1388	0	1405	60	0
2	B	2799	0	2869	165	0
2	D	2799	0	2869	166	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	44	0	0	2	0
4	B	45	0	0	1	0
4	C	39	0	0	2	0
4	D	53	0	0	2	0
All	All	8565	0	8548	410	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 24.

All (410) 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)
2:B:1468:LYS:NZ	2:B:1492:ILE:CD1	1.71	1.50
2:D:1468:LYS:NZ	2:D:1492:ILE:CD1	1.71	1.50
2:B:1468:LYS:NZ	2:B:1492:ILE:HD11	1.32	1.24
2:D:1468:LYS:NZ	2:D:1492:ILE:HD11	1.32	1.24
2:D:1468:LYS:HD3	2:D:1479:TYR:HD1	1.08	1.11
2:B:1468:LYS:HD3	2:B:1479:TYR:HD1	1.08	1.11
2:D:1468:LYS:NZ	2:D:1492:ILE:HD13	1.54	1.09
2:B:1468:LYS:NZ	2:B:1492:ILE:HD13	1.54	1.09
2:B:1468:LYS:HD3	2:B:1479:TYR:CD1	1.91	1.06
2:D:1468:LYS:HD3	2:D:1479:TYR:CD1	1.91	1.05
1:C:161:THR:HG22	1:C:163:LYS:H	1.21	1.05
1:A:161:THR:HG22	1:A:163:LYS:H	1.21	1.05
1:C:115:THR:HG23	1:C:116:GLN:HG3	1.41	1.03
1:A:115:THR:HG23	1:A:116:GLN:HG3	1.41	1.03
2:D:1468:LYS:O	2:D:1469:LEU:HB3	1.55	1.01
2:B:1468:LYS:O	2:B:1469:LEU:HB3	1.55	1.01
2:B:1468:LYS:CD	2:B:1479:TYR:HD1	1.78	0.97
2:D:1468:LYS:CD	2:D:1479:TYR:HD1	1.78	0.97
1:A:14:VAL:O	1:A:115:THR:HG21	1.64	0.97
1:C:14:VAL:O	1:C:115:THR:HG21	1.64	0.97
2:B:1468:LYS:O	2:B:1469:LEU:CB	2.11	0.95
2:D:1468:LYS:O	2:D:1469:LEU:CB	2.11	0.95
2:D:1242:ILE:HG21	2:D:1312:VAL:HG11	1.48	0.94
2:B:1242:ILE:HG21	2:B:1312:VAL:HG11	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1468:LYS:HZ1	2:D:1492:ILE:HD13	1.33	0.89
1:C:115:THR:CG2	1:C:116:GLN:HG3	2.04	0.87
1:A:115:THR:CG2	1:A:116:GLN:HG3	2.04	0.87
2:B:1519:ILE:HG13	2:B:1543:HIS:ND1	1.90	0.86
2:D:1519:ILE:HG13	2:D:1543:HIS:ND1	1.90	0.86
2:B:1468:LYS:CD	2:B:1479:TYR:CD1	2.57	0.86
2:B:1469:LEU:HD12	2:B:1551:ARG:O	1.76	0.85
2:D:1469:LEU:HD12	2:D:1551:ARG:O	1.76	0.85
2:D:1468:LYS:CD	2:D:1479:TYR:CD1	2.57	0.83
1:C:77:VAL:HG22	1:C:176:ALA:HB2	1.59	0.83
1:A:77:VAL:HG22	1:A:176:ALA:HB2	1.59	0.82
2:D:1236:ARG:HH11	2:D:1236:ARG:HB2	1.43	0.82
2:B:1236:ARG:HB2	2:B:1236:ARG:HH11	1.43	0.82
2:B:1468:LYS:HZ1	2:B:1492:ILE:HD13	1.41	0.82
2:B:1523:GLU:OE1	2:B:1544:ILE:HD11	1.80	0.81
2:D:1523:GLU:OE1	2:D:1544:ILE:HD11	1.80	0.81
2:B:1403:HIS:NE2	2:B:1407:LYS:HE3	1.98	0.79
2:B:1528:LEU:H	2:B:1528:LEU:HD12	1.47	0.79
2:D:1403:HIS:NE2	2:D:1407:LYS:HE3	1.98	0.79
2:D:1528:LEU:H	2:D:1528:LEU:HD12	1.47	0.79
2:B:1468:LYS:CE	2:B:1492:ILE:HD11	2.13	0.77
2:D:1468:LYS:CE	2:D:1492:ILE:HD11	2.13	0.77
2:D:1429:ASN:HD21	2:D:1463:PHE:H	1.33	0.77
2:B:1429:ASN:HD21	2:B:1463:PHE:H	1.33	0.77
2:D:1487:LEU:HB3	2:D:1519:ILE:HG23	1.67	0.76
2:B:1487:LEU:HB3	2:B:1519:ILE:HG23	1.67	0.76
1:C:83:SER:HA	1:C:115:THR:HG22	1.66	0.76
1:A:83:SER:HA	1:A:115:THR:HG22	1.67	0.75
2:B:1504:VAL:HG12	2:B:1505:PHE:CD1	2.20	0.75
2:D:1504:VAL:HG12	2:D:1505:PHE:CD1	2.20	0.75
2:B:1503:LYS:O	2:B:1505:PHE:N	2.20	0.75
2:D:1503:LYS:O	2:D:1505:PHE:N	2.20	0.75
2:D:1400:HIS:HD2	2:D:1402:ASP:H	1.32	0.75
2:B:1400:HIS:HD2	2:B:1402:ASP:H	1.32	0.74
1:A:138:THR:HG23	1:A:141:THR:H	1.52	0.74
1:C:138:THR:HG23	1:C:141:THR:H	1.52	0.74
2:D:1441:GLN:HE21	2:D:1443:GLU:CG	2.01	0.73
2:B:1390:LYS:O	2:B:1394:GLU:HG3	1.88	0.73
2:B:1441:GLN:HE21	2:B:1443:GLU:CG	2.01	0.73
2:D:1390:LYS:O	2:D:1394:GLU:HG3	1.89	0.73
1:A:166:LYS:HG2	4:A:4040:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:H	2:B:1421:ASN:HD21	1.36	0.71
1:C:40:TYR:CE2	1:C:42:VAL:HG13	2.25	0.71
1:A:40:TYR:CE2	1:A:42:VAL:HG13	2.25	0.71
2:B:1231:LEU:HB2	2:B:1236:ARG:HH12	1.55	0.71
1:C:66:ARG:H	2:D:1421:ASN:HD21	1.36	0.71
2:D:1231:LEU:HB2	2:D:1236:ARG:HH12	1.55	0.71
2:B:1504:VAL:HG12	2:B:1505:PHE:CE1	2.25	0.71
2:D:1504:VAL:HG12	2:D:1505:PHE:CE1	2.25	0.71
2:B:1429:ASN:ND2	2:B:1463:PHE:H	1.89	0.71
2:D:1429:ASN:ND2	2:D:1463:PHE:H	1.89	0.71
2:B:1529:PRO:HB3	2:B:1534:GLY:HA3	1.72	0.70
2:D:1529:PRO:HB3	2:D:1534:GLY:HA3	1.72	0.70
2:B:1236:ARG:HB2	2:B:1236:ARG:NH1	2.07	0.70
2:D:1236:ARG:NH1	2:D:1236:ARG:HB2	2.06	0.70
1:C:166:LYS:HG2	4:C:4039:HOH:O	1.93	0.69
2:B:1510:ASN:HD22	2:B:1511:LEU:N	1.90	0.68
2:D:1470:TYR:HB3	2:D:1476:LYS:HA	1.77	0.68
2:D:1510:ASN:HD22	2:D:1511:LEU:N	1.90	0.68
2:B:1470:TYR:HB3	2:B:1476:LYS:HA	1.77	0.67
2:B:1471:LYS:HG2	2:B:1550:LEU:HD23	1.74	0.67
1:A:32:TYR:HD1	2:B:1241:TYR:CZ	2.12	0.67
1:C:32:TYR:HD1	2:D:1241:TYR:CZ	2.12	0.67
2:D:1471:LYS:HG2	2:D:1550:LEU:HD23	1.74	0.67
2:D:1543:HIS:O	2:D:1544:ILE:C	2.33	0.67
2:B:1543:HIS:O	2:B:1544:ILE:C	2.33	0.67
1:C:32:TYR:OH	2:D:1240:GLY:O	2.13	0.66
1:A:32:TYR:OH	2:B:1240:GLY:O	2.13	0.66
2:D:1441:GLN:HE21	2:D:1443:GLU:HG3	1.61	0.66
2:B:1441:GLN:HE21	2:B:1443:GLU:HG3	1.61	0.65
2:B:1261:GLU:CD	2:B:1365:ARG:HH22	1.99	0.65
2:D:1261:GLU:CD	2:D:1365:ARG:HH22	1.99	0.65
2:D:1468:LYS:HA	2:D:1479:TYR:HA	1.78	0.65
2:B:1468:LYS:HA	2:B:1479:TYR:HA	1.78	0.64
2:B:1516:LYS:HD2	2:B:1548:TYR:OH	1.96	0.64
2:D:1516:LYS:HD2	2:D:1548:TYR:OH	1.96	0.64
2:B:1529:PRO:HB3	2:B:1540:HIS:NE2	2.13	0.63
2:B:1529:PRO:CB	2:B:1534:GLY:HA3	2.27	0.63
2:D:1529:PRO:HB3	2:D:1540:HIS:NE2	2.13	0.63
2:D:1529:PRO:CB	2:D:1534:GLY:HA3	2.27	0.63
1:A:161:THR:HG22	1:A:163:LYS:N	2.04	0.63
2:B:1555:ILE:HG23	2:B:1558:ARG:HH21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1363:ASP:OD1	2:D:1365:ARG:HD3	1.99	0.62
2:B:1363:ASP:OD1	2:B:1365:ARG:HD3	1.99	0.62
2:D:1555:ILE:HG23	2:D:1558:ARG:HH21	1.65	0.62
1:C:161:THR:HG22	1:C:163:LYS:N	2.04	0.62
2:B:1469:LEU:CD1	2:B:1552:ALA:HA	2.30	0.62
1:C:32:TYR:CE2	2:D:1240:GLY:HA3	2.35	0.62
2:D:1469:LEU:CD1	2:D:1552:ALA:HA	2.30	0.62
1:A:32:TYR:CE2	2:B:1240:GLY:HA3	2.35	0.62
2:B:1441:GLN:HG2	2:B:1443:GLU:HG2	1.80	0.62
2:B:1529:PRO:HB3	2:B:1540:HIS:CD2	2.35	0.62
2:D:1441:GLN:HG2	2:D:1443:GLU:HG2	1.80	0.62
2:D:1469:LEU:HD12	2:D:1552:ALA:HA	1.81	0.62
2:B:1469:LEU:HD12	2:B:1552:ALA:HA	1.81	0.62
2:D:1529:PRO:HB3	2:D:1540:HIS:CD2	2.35	0.62
2:B:1475:ASN:ND2	2:B:1476:LYS:H	1.97	0.61
2:D:1475:ASN:ND2	2:D:1476:LYS:H	1.97	0.61
2:D:1400:HIS:CD2	2:D:1402:ASP:H	2.16	0.61
2:B:1486:PHE:HA	2:B:1521:LEU:HD13	1.82	0.61
2:B:1400:HIS:CD2	2:B:1402:ASP:H	2.16	0.61
1:C:35:THR:HG23	2:D:1391:ASN:HD21	1.65	0.61
2:B:1570:GLU:HA	2:B:1573:ILE:HD12	1.82	0.61
2:D:1468:LYS:NZ	2:D:1492:ILE:CG1	2.60	0.61
2:D:1570:GLU:HA	2:D:1573:ILE:HD12	1.82	0.61
1:A:35:THR:HG23	2:B:1391:ASN:HD21	1.65	0.60
2:B:1468:LYS:NZ	2:B:1492:ILE:CG1	2.60	0.60
2:D:1486:PHE:HA	2:D:1521:LEU:HD13	1.83	0.60
1:A:152:VAL:O	1:A:153:LYS:HB3	2.01	0.60
2:B:1345:GLN:O	2:B:1349:GLU:HG2	2.01	0.60
2:D:1345:GLN:O	2:D:1349:GLU:HG2	2.01	0.60
1:C:152:VAL:O	1:C:153:LYS:HB3	2.01	0.60
2:B:1465:HIS:ND1	2:B:1466:SER:N	2.48	0.60
2:D:1465:HIS:ND1	2:D:1466:SER:N	2.48	0.60
2:B:1490:THR:HG22	2:B:1514:MET:HA	1.83	0.60
2:D:1490:THR:HG22	2:D:1514:MET:HA	1.83	0.60
2:B:1440:VAL:HG11	2:B:1488:LEU:HD21	1.84	0.59
2:D:1440:VAL:HG11	2:D:1488:LEU:HD21	1.84	0.59
2:B:1470:TYR:CD2	2:B:1476:LYS:HB3	2.37	0.59
2:D:1470:TYR:CD2	2:D:1476:LYS:HB3	2.37	0.59
2:B:1231:LEU:HB2	2:B:1236:ARG:NH1	2.17	0.59
2:B:1541:ILE:HG23	2:B:1548:TYR:HB2	1.85	0.59
2:D:1541:ILE:HG23	2:D:1548:TYR:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:THR:HG22	1:C:141:THR:OG1	2.03	0.59
1:C:25:THR:O	1:C:26:ASN:HB2	2.02	0.59
1:A:138:THR:HG22	1:A:141:THR:OG1	2.03	0.59
2:D:1231:LEU:HB2	2:D:1236:ARG:NH1	2.17	0.59
2:D:1408:HIS:O	2:D:1412:LYS:HG2	2.03	0.59
1:A:25:THR:O	1:A:26:ASN:HB2	2.02	0.59
2:D:1468:LYS:CD	2:D:1492:ILE:HD11	2.32	0.59
2:B:1468:LYS:CD	2:B:1492:ILE:HD11	2.32	0.59
2:D:1528:LEU:N	2:D:1528:LEU:HD12	2.17	0.59
2:B:1528:LEU:N	2:B:1528:LEU:HD12	2.17	0.58
2:B:1408:HIS:O	2:B:1412:LYS:HG2	2.03	0.58
1:C:32:TYR:CD1	2:D:1241:TYR:CZ	2.91	0.58
1:A:32:TYR:CD1	2:B:1241:TYR:CZ	2.91	0.58
2:B:1270:SER:O	2:B:1271:GLU:HB2	2.05	0.57
2:D:1270:SER:O	2:D:1271:GLU:HB2	2.05	0.56
1:A:65:ASP:OD2	2:B:1425:ARG:NH2	2.38	0.56
1:C:65:ASP:OD2	2:D:1425:ARG:NH2	2.38	0.56
2:B:1505:PHE:O	2:B:1506:SER:HB3	2.06	0.56
2:D:1505:PHE:O	2:D:1506:SER:HB3	2.06	0.56
2:B:1424:VAL:O	2:B:1428:GLU:HG3	2.05	0.56
2:D:1265:LYS:HB2	2:D:1266:PRO:HD3	1.87	0.56
2:B:1265:LYS:HB2	2:B:1266:PRO:HD3	1.87	0.56
2:B:1517:THR:HG23	2:B:1518:PRO:HD2	1.88	0.56
2:D:1424:VAL:O	2:D:1428:GLU:HG3	2.05	0.56
1:A:98:VAL:HG21	1:A:149:LEU:HD13	1.88	0.56
2:D:1347:THR:HG23	2:D:1354:LYS:HD3	1.88	0.56
2:D:1517:THR:HG23	2:D:1518:PRO:HD2	1.88	0.56
1:A:32:TYR:OH	2:B:1240:GLY:C	2.45	0.55
2:B:1347:THR:HG23	2:B:1354:LYS:HD3	1.88	0.55
1:C:98:VAL:HG21	1:C:149:LEU:HD13	1.88	0.55
1:C:32:TYR:OH	2:D:1240:GLY:C	2.45	0.55
2:B:1555:ILE:HA	2:B:1558:ARG:NE	2.22	0.55
2:D:1555:ILE:HA	2:D:1558:ARG:NE	2.22	0.55
2:B:1262:ILE:HD11	2:B:1366:CYS:SG	2.48	0.54
1:A:154:TYR:CZ	1:A:156:GLU:HG2	2.43	0.54
1:C:154:TYR:CZ	1:C:156:GLU:HG2	2.43	0.54
2:B:1441:GLN:HB3	2:B:1513:TYR:HD1	1.72	0.54
2:D:1262:ILE:HD11	2:D:1366:CYS:SG	2.48	0.54
2:D:1441:GLN:HB3	2:D:1513:TYR:HD1	1.72	0.54
2:B:1569:SER:O	2:B:1573:ILE:HG13	2.07	0.54
2:D:1569:SER:O	2:D:1573:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1469:LEU:HD12	2:D:1551:ARG:C	2.29	0.53
2:B:1469:LEU:HD12	2:B:1551:ARG:C	2.29	0.53
1:A:117:ILE:HG21	1:A:156:GLU:HB3	1.90	0.53
1:A:35:THR:HG23	2:B:1391:ASN:ND2	2.23	0.53
1:C:35:THR:HG23	2:D:1391:ASN:ND2	2.23	0.53
1:A:166:LYS:HE3	4:A:4012:HOH:O	2.09	0.53
2:B:1468:LYS:HG2	2:B:1479:TYR:CE1	2.44	0.53
1:C:117:ILE:HG21	1:C:156:GLU:HB3	1.90	0.53
1:A:32:TYR:O	1:A:32:TYR:CD1	2.62	0.53
2:D:1468:LYS:HG2	2:D:1479:TYR:CE1	2.44	0.53
1:C:32:TYR:O	1:C:32:TYR:CD1	2.62	0.52
2:B:1525:LEU:HB2	2:B:1542:SER:HB3	1.90	0.52
2:D:1525:LEU:HB2	2:D:1542:SER:HB3	1.90	0.52
2:B:1510:ASN:HD22	2:B:1511:LEU:H	1.57	0.52
2:D:1510:ASN:HD22	2:D:1511:LEU:H	1.57	0.52
2:D:1558:ARG:HG3	2:D:1559:THR:N	2.24	0.52
2:B:1558:ARG:HG3	2:B:1559:THR:N	2.24	0.51
1:A:164:GLY:O	1:A:168:VAL:HG23	2.09	0.51
2:D:1295:LEU:HG	2:D:1322:GLN:HG2	1.92	0.51
2:B:1295:LEU:HG	2:B:1322:GLN:HG2	1.92	0.51
1:A:154:TYR:OH	1:A:156:GLU:HG2	2.10	0.51
2:B:1509:SER:O	2:B:1510:ASN:HB2	2.11	0.51
2:B:1523:GLU:HB2	2:B:1544:ILE:HD11	1.93	0.51
1:C:164:GLY:O	1:C:168:VAL:HG23	2.10	0.51
2:D:1509:SER:O	2:D:1510:ASN:HB2	2.11	0.51
2:D:1523:GLU:HB2	2:D:1544:ILE:HD11	1.93	0.51
1:C:154:TYR:OH	1:C:156:GLU:HG2	2.10	0.51
2:D:1238:ARG:NH1	4:D:2:HOH:O	2.43	0.51
1:A:35:THR:CG2	2:B:1391:ASN:ND2	2.74	0.51
2:D:1400:HIS:HD2	2:D:1402:ASP:N	2.06	0.51
2:B:1400:HIS:HD2	2:B:1402:ASP:N	2.06	0.50
1:C:35:THR:CG2	2:D:1391:ASN:ND2	2.74	0.50
2:B:1555:ILE:HG12	2:B:1558:ARG:CZ	2.42	0.50
2:D:1555:ILE:HG12	2:D:1558:ARG:CZ	2.42	0.50
2:B:1555:ILE:HG23	2:B:1558:ARG:NH2	2.25	0.50
2:D:1555:ILE:HG23	2:D:1558:ARG:NH2	2.25	0.50
2:B:1541:ILE:CG2	2:B:1548:TYR:HB2	2.42	0.50
1:C:77:VAL:CG2	1:C:176:ALA:HB2	2.34	0.50
1:A:77:VAL:CG2	1:A:176:ALA:HB2	2.34	0.50
2:B:1576:GLU:C	2:B:1578:LYS:H	2.15	0.50
2:D:1541:ILE:CG2	2:D:1548:TYR:HB2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1475:ASN:CG	2:B:1476:LYS:H	2.15	0.50
2:D:1475:ASN:CG	2:D:1476:LYS:H	2.15	0.50
1:A:35:THR:CG2	2:B:1391:ASN:HD21	2.25	0.49
2:D:1576:GLU:C	2:D:1578:LYS:H	2.16	0.49
1:C:139:PRO:O	1:C:143:GLU:HG3	2.13	0.49
1:C:35:THR:CG2	2:D:1391:ASN:HD21	2.25	0.49
2:B:1445:LEU:HD11	2:B:1514:MET:HE3	1.93	0.49
1:A:139:PRO:O	1:A:143:GLU:HG3	2.13	0.49
2:D:1335:ARG:NH1	4:D:172:HOH:O	2.45	0.49
2:B:1468:LYS:CE	2:B:1479:TYR:CD1	2.95	0.49
2:D:1468:LYS:CE	2:D:1479:TYR:CD1	2.95	0.49
2:D:1557:GLU:O	2:D:1560:ALA:HB3	2.13	0.49
1:A:32:TYR:HH	2:B:1240:GLY:C	2.15	0.48
2:B:1476:LYS:HD3	2:B:1476:LYS:N	2.28	0.48
2:D:1441:GLN:HB3	2:D:1513:TYR:HA	1.94	0.48
2:B:1557:GLU:O	2:B:1560:ALA:HB3	2.13	0.48
1:C:68:ARG:NH1	1:C:100:GLU:OE2	2.45	0.48
2:D:1429:ASN:HD21	2:D:1463:PHE:N	2.08	0.48
2:D:1470:TYR:HB3	2:D:1476:LYS:CA	2.41	0.48
2:B:1429:ASN:HD21	2:B:1463:PHE:N	2.08	0.48
2:B:1441:GLN:HB3	2:B:1513:TYR:HA	1.94	0.48
2:B:1470:TYR:HB3	2:B:1476:LYS:CA	2.41	0.48
2:D:1476:LYS:HD3	2:D:1476:LYS:N	2.29	0.48
1:C:32:TYR:HH	2:D:1240:GLY:C	2.15	0.48
1:A:68:ARG:NH1	1:A:100:GLU:OE2	2.46	0.48
2:B:1429:ASN:HD21	2:B:1462:LYS:HA	1.79	0.48
1:C:166:LYS:HE3	4:C:4018:HOH:O	2.13	0.48
1:A:85:VAL:HG13	1:A:85:VAL:O	2.14	0.48
1:C:127:GLU:HG2	1:C:131:LYS:HE3	1.96	0.48
2:D:1445:LEU:HD11	2:D:1514:MET:HE3	1.94	0.48
1:A:127:GLU:HG2	1:A:131:LYS:HE3	1.96	0.48
2:B:1242:ILE:HG21	2:B:1312:VAL:CG1	2.33	0.48
2:B:1446:SER:C	2:B:1447:GLU:HG3	2.35	0.47
2:D:1242:ILE:HG21	2:D:1312:VAL:CG1	2.33	0.47
2:D:1446:SER:C	2:D:1447:GLU:HG3	2.35	0.47
2:D:1429:ASN:HD21	2:D:1462:LYS:HA	1.79	0.47
2:B:1523:GLU:CD	2:B:1544:ILE:HD11	2.34	0.47
1:C:34:PRO:HB3	2:D:1244:GLU:OE2	2.14	0.47
2:D:1523:GLU:CD	2:D:1544:ILE:HD11	2.34	0.47
1:A:34:PRO:HB3	2:B:1244:GLU:OE2	2.14	0.47
1:C:85:VAL:O	1:C:85:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1468:LYS:CG	2:B:1479:TYR:HD1	2.25	0.47
2:D:1561:TRP:O	2:D:1565:ILE:HG13	2.15	0.47
2:B:1470:TYR:CD1	2:B:1470:TYR:N	2.83	0.47
2:B:1561:TRP:O	2:B:1565:ILE:HG13	2.15	0.47
1:A:161:THR:O	1:A:162:GLN:HB2	2.15	0.47
2:D:1470:TYR:N	2:D:1470:TYR:CD1	2.83	0.47
2:D:1468:LYS:CG	2:D:1479:TYR:HD1	2.25	0.47
1:A:138:THR:CG2	1:A:141:THR:H	2.23	0.47
1:C:161:THR:O	1:C:162:GLN:HB2	2.15	0.47
2:B:1468:LYS:CG	2:B:1479:TYR:CD1	2.97	0.47
2:D:1468:LYS:CG	2:D:1479:TYR:CD1	2.97	0.47
2:D:1519:ILE:HG13	2:D:1543:HIS:CE1	2.49	0.46
2:D:1524:VAL:HG22	2:D:1525:LEU:N	2.30	0.46
2:B:1519:ILE:HG13	2:B:1543:HIS:CE1	2.49	0.46
2:B:1524:VAL:HG22	2:B:1525:LEU:N	2.30	0.46
1:C:138:THR:CG2	1:C:141:THR:H	2.23	0.46
2:D:1327:GLN:N	2:D:1328:PRO:CD	2.79	0.46
2:B:1271:GLU:OE1	2:B:1271:GLU:HA	2.15	0.46
2:D:1271:GLU:OE1	2:D:1271:GLU:HA	2.15	0.46
2:B:1265:LYS:NZ	1:C:30:SER:HB3	2.31	0.46
2:B:1327:GLN:N	2:B:1328:PRO:CD	2.79	0.46
2:B:1454:VAL:HG12	2:B:1455:THR:O	2.16	0.46
2:D:1342:LEU:HD13	2:D:1342:LEU:C	2.36	0.46
2:B:1342:LEU:HD13	2:B:1342:LEU:C	2.36	0.46
2:D:1359:ARG:HA	2:D:1362:MET:HE2	1.98	0.46
2:B:1465:HIS:HD2	2:B:1564:LYS:NZ	2.14	0.46
2:D:1454:VAL:HG12	2:D:1455:THR:O	2.16	0.46
2:D:1465:HIS:HD2	2:D:1564:LYS:NZ	2.14	0.46
2:B:1359:ARG:HA	2:B:1362:MET:HE2	1.98	0.45
1:A:144:LYS:HA	1:A:147:ARG:NH1	2.32	0.45
1:A:32:TYR:HE1	2:B:1241:TYR:CD2	2.34	0.45
2:D:1558:ARG:HG3	2:D:1559:THR:H	1.80	0.45
2:B:1397:PRO:HG2	2:B:1400:HIS:HB2	1.99	0.45
1:C:144:LYS:HA	1:C:147:ARG:NH1	2.32	0.45
1:C:32:TYR:HE1	2:D:1241:TYR:CD2	2.34	0.45
2:B:1262:ILE:CD1	2:B:1366:CYS:SG	3.05	0.45
2:B:1468:LYS:HZ3	2:B:1492:ILE:CD1	2.08	0.45
2:B:1558:ARG:HG3	2:B:1559:THR:H	1.80	0.45
2:B:1579:LYS:O	2:B:1580:ARG:HB2	2.16	0.45
2:D:1397:PRO:HG2	2:D:1400:HIS:HB2	1.99	0.45
2:D:1411:GLU:O	2:D:1415:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1579:LYS:O	2:D:1580:ARG:HB2	2.16	0.45
2:B:1411:GLU:O	2:B:1415:GLU:HG3	2.17	0.45
2:D:1272:LEU:HB3	2:D:1273:LEU:HD22	1.99	0.45
2:B:1272:LEU:HB3	2:B:1273:LEU:HD22	1.99	0.44
2:D:1262:ILE:CD1	2:D:1366:CYS:SG	3.05	0.44
2:B:1347:THR:CG2	2:B:1354:LYS:HD3	2.47	0.44
1:A:41:ALA:HB2	2:B:1369:MET:SD	2.58	0.44
1:C:41:ALA:HB2	2:D:1369:MET:SD	2.58	0.44
2:D:1347:THR:CG2	2:D:1354:LYS:HD3	2.47	0.44
2:B:1556:ASN:O	2:B:1560:ALA:HB2	2.18	0.44
2:D:1354:LYS:O	2:D:1358:LYS:HG3	2.17	0.44
2:D:1556:ASN:O	2:D:1560:ALA:HB2	2.18	0.44
1:A:32:TYR:CE1	2:B:1241:TYR:CD2	3.06	0.44
1:C:32:TYR:CE1	2:D:1241:TYR:CD2	3.06	0.44
1:A:105:CYS:HB3	1:A:108:THR:OG1	2.18	0.44
2:B:1354:LYS:O	2:B:1358:LYS:HG3	2.17	0.44
1:C:105:CYS:HB3	1:C:108:THR:OG1	2.18	0.44
2:D:1505:PHE:O	2:D:1506:SER:CB	2.65	0.44
2:B:1505:PHE:O	2:B:1506:SER:CB	2.65	0.43
1:C:38:ASP:O	1:C:39:ASN:C	2.56	0.43
2:B:1532:PRO:O	2:B:1533:SER:HB2	2.19	0.43
2:D:1532:PRO:O	2:D:1533:SER:HB2	2.19	0.43
2:B:1555:ILE:HG12	2:B:1558:ARG:NH2	2.34	0.43
1:A:38:ASP:O	1:A:39:ASN:C	2.57	0.43
2:D:1468:LYS:HG2	2:D:1479:TYR:HE1	1.83	0.43
2:D:1555:ILE:HG12	2:D:1558:ARG:NH2	2.34	0.43
2:D:1521:LEU:HA	2:D:1524:VAL:CG1	2.47	0.43
2:B:1468:LYS:HG2	2:B:1479:TYR:HE1	1.83	0.43
2:B:1447:GLU:O	2:B:1448:GLN:HB2	2.19	0.43
2:B:1521:LEU:HA	2:B:1524:VAL:CG1	2.47	0.43
2:D:1447:GLU:O	2:D:1448:GLN:HB2	2.19	0.42
2:B:1238:ARG:NH1	4:B:6:HOH:O	2.52	0.42
2:D:1572:TYR:O	2:D:1572:TYR:HD2	2.02	0.42
2:B:1470:TYR:HD2	2:B:1477:GLU:H	1.66	0.42
2:B:1523:GLU:CB	2:B:1544:ILE:HD11	2.49	0.42
2:D:1539:PHE:HB3	2:D:1550:LEU:O	2.20	0.42
2:B:1539:PHE:HB3	2:B:1550:LEU:O	2.20	0.42
1:C:69:PRO:HA	1:C:72:TYR:CD1	2.54	0.42
2:D:1470:TYR:HD2	2:D:1477:GLU:H	1.66	0.42
2:B:1553:GLU:HB2	2:B:1557:GLU:OE1	2.20	0.42
2:B:1572:TYR:O	2:B:1572:TYR:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1510:ASN:ND2	2:D:1511:LEU:N	2.65	0.42
2:D:1523:GLU:CB	2:D:1544:ILE:HD11	2.49	0.42
2:D:1553:GLU:HB2	2:D:1557:GLU:OE1	2.20	0.42
1:A:138:THR:OG1	1:A:139:PRO:HD2	2.20	0.42
1:A:69:PRO:HA	1:A:72:TYR:CD1	2.54	0.42
1:A:32:TYR:O	1:A:32:TYR:CG	2.72	0.41
1:C:138:THR:OG1	1:C:139:PRO:HD2	2.20	0.41
1:A:41:ALA:HA	1:A:53:LEU:O	2.20	0.41
1:C:32:TYR:O	1:C:32:TYR:CG	2.72	0.41
2:D:1238:ARG:NH2	2:D:1402:ASP:OD2	2.53	0.41
2:B:1571:LEU:HD23	2:B:1571:LEU:O	2.21	0.41
2:D:1571:LEU:HD23	2:D:1571:LEU:O	2.21	0.41
1:A:161:THR:CG2	1:A:163:LYS:HB2	2.50	0.41
1:A:19:LEU:HD12	1:A:19:LEU:C	2.40	0.41
1:A:67:LEU:HG	2:B:1421:ASN:HD22	1.85	0.41
2:B:1446:SER:O	2:B:1447:GLU:HG3	2.19	0.41
2:D:1446:SER:O	2:D:1447:GLU:HG3	2.19	0.41
2:D:1471:LYS:HG2	2:D:1549:THR:O	2.20	0.41
2:D:1558:ARG:CG	2:D:1559:THR:N	2.83	0.41
1:A:1:MET:HB2	1:A:2:GLN:H	1.54	0.41
1:A:94:LYS:HB3	1:A:149:LEU:HD11	2.03	0.41
2:B:1471:LYS:HG2	2:B:1549:THR:O	2.20	0.41
2:B:1558:ARG:CG	2:B:1559:THR:N	2.83	0.41
1:C:161:THR:CG2	1:C:163:LYS:HB2	2.50	0.41
1:C:19:LEU:HD12	1:C:19:LEU:C	2.40	0.41
2:B:1238:ARG:NH2	2:B:1402:ASP:OD2	2.53	0.41
1:C:94:LYS:HB3	1:C:149:LEU:HD11	2.03	0.41
1:C:32:TYR:CD1	2:D:1241:TYR:CE2	3.08	0.41
2:D:1555:ILE:HG23	2:D:1558:ARG:HE	1.86	0.41
1:A:32:TYR:CD1	2:B:1241:TYR:CE2	3.09	0.41
2:B:1555:ILE:HG23	2:B:1558:ARG:HE	1.86	0.41
2:D:1309:LYS:HE3	2:D:1309:LYS:HB2	1.85	0.41
2:D:1523:GLU:HB2	2:D:1544:ILE:CG1	2.50	0.41
2:B:1273:LEU:HD21	2:B:1353:PHE:HE1	1.86	0.41
2:B:1523:GLU:HB2	2:B:1544:ILE:CG1	2.50	0.41
1:C:32:TYR:CE1	2:D:1241:TYR:CE2	3.09	0.41
1:C:67:LEU:HG	2:D:1421:ASN:HD22	1.86	0.41
2:D:1273:LEU:HD21	2:D:1353:PHE:HE1	1.86	0.41
1:A:32:TYR:CE1	2:B:1241:TYR:CE2	3.09	0.41
2:B:1309:LYS:HE3	2:B:1309:LYS:HB2	1.85	0.41
1:C:41:ALA:HA	1:C:53:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TYR:CZ	2:B:1240:GLY:C	2.94	0.40
2:B:1326:MET:HB2	2:B:1416:LEU:HD11	2.03	0.40
1:C:1:MET:HB2	1:C:2:GLN:H	1.54	0.40
1:C:32:TYR:CZ	2:D:1240:GLY:C	2.94	0.40
2:D:1551:ARG:HG3	2:D:1551:ARG:HH11	1.86	0.40
1:A:85:VAL:CG1	1:A:85:VAL:O	2.69	0.40
2:B:1551:ARG:HG3	2:B:1551:ARG:HH11	1.86	0.40
1:A:11:ASP:OD2	1:A:92:ASN:ND2	2.50	0.40
1:A:70:LEU:O	2:B:1376:LEU:HD21	2.22	0.40
1:C:85:VAL:O	1:C:85:VAL:CG1	2.69	0.40
2:D:1326:MET:HB2	2:D:1416:LEU:HD11	2.03	0.40
2:B:1529:PRO:CD	2:B:1539:PHE:N	2.84	0.40
2:D:1468:LYS:HE2	2:D:1479:TYR:CD1	2.56	0.40
2:D:1534:GLY:O	2:D:1535:ASP:HB2	2.21	0.40
2:D:1558:ARG:CG	2:D:1559:THR:H	2.35	0.40
2:B:1558:ARG:CG	2:B:1559:THR:H	2.35	0.40
2:D:1529:PRO:CD	2:D:1539:PHE:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	176/188 (94%)	167 (95%)	7 (4%)	2 (1%)	17	18
1	C	176/188 (94%)	167 (95%)	7 (4%)	2 (1%)	17	18
2	B	336/352 (96%)	302 (90%)	17 (5%)	17 (5%)	2	1
2	D	336/352 (96%)	303 (90%)	16 (5%)	17 (5%)	2	1
All	All	1024/1080 (95%)	939 (92%)	47 (5%)	38 (4%)	4	2

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1504	VAL
2	B	1506	SER
2	B	1509	SER
2	B	1533	SER
2	B	1544	ILE
2	D	1504	VAL
2	D	1506	SER
2	D	1509	SER
2	D	1533	SER
2	D	1544	ILE
1	A	31	GLU
2	B	1444	GLY
2	B	1510	ASN
1	C	31	GLU
2	D	1444	GLY
2	D	1510	ASN
2	B	1516	LYS
2	B	1552	ALA
2	D	1283	VAL
2	D	1516	LYS
2	D	1552	ALA
2	B	1283	VAL
2	B	1469	LEU
2	B	1529	PRO
2	B	1577	LYS
2	D	1469	LEU
2	D	1529	PRO
2	D	1577	LYS
1	A	153	LYS
2	B	1308	GLU
1	C	153	LYS
2	D	1308	GLU
2	B	1448	GLN
2	B	1467	GLY
2	B	1468	LYS
2	D	1448	GLN
2	D	1467	GLY
2	D	1468	LYS

### 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	158/168 (94%)	148 (94%)	10 (6%)	21	28
1	C	158/168 (94%)	148 (94%)	10 (6%)	21	28
2	B	316/325 (97%)	301 (95%)	15 (5%)	30	41
2	D	316/325 (97%)	301 (95%)	15 (5%)	30	41
All	All	948/986 (96%)	898 (95%)	50 (5%)	26	35

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	27	LYS
1	A	35	THR
1	A	42	VAL
1	A	77	VAL
1	A	85	VAL
1	A	112	LEU
1	A	115	THR
1	A	161	THR
1	A	165	LEU
2	B	1236	ARG
2	B	1245	LEU
2	B	1272	LEU
2	B	1295	LEU
2	B	1296	LEU
2	B	1410	LEU
2	B	1416	LEU
2	B	1433	LEU
2	B	1449	LEU
2	B	1452	ASN
2	B	1470	TYR
2	B	1475	ASN
2	B	1510	ASN
2	B	1528	LEU
2	B	1572	TYR
1	C	1	MET
1	C	27	LYS
1	C	35	THR

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Mol	Chain	Res	Type
1	C	42	VAL
1	C	77	VAL
1	C	85	VAL
1	C	112	LEU
1	C	115	THR
1	C	161	THR
1	C	165	LEU
2	D	1236	ARG
2	D	1245	LEU
2	D	1272	LEU
2	D	1295	LEU
2	D	1296	LEU
2	D	1410	LEU
2	D	1416	LEU
2	D	1433	LEU
2	D	1449	LEU
2	D	1452	ASN
2	D	1470	TYR
2	D	1475	ASN
2	D	1510	ASN
2	D	1528	LEU
2	D	1572	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
2	B	1264	GLN
2	B	1292	ASN
2	B	1322	GLN
2	B	1391	ASN
2	B	1400	HIS
2	B	1421	ASN
2	B	1429	ASN
2	B	1441	GLN
2	B	1452	ASN
2	B	1465	HIS
2	B	1475	ASN
2	B	1510	ASN
1	C	2	GLN
2	D	1264	GLN
2	D	1292	ASN

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Mol	Chain	Res	Type
2	D	1322	GLN
2	D	1338	ASN
2	D	1391	ASN
2	D	1400	HIS
2	D	1421	ASN
2	D	1429	ASN
2	D	1441	GLN
2	D	1452	ASN
2	D	1465	HIS
2	D	1475	ASN
2	D	1510	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	SO4	A	4001	-	4,4,4	0.42	0	6,6,6	0.25	0
3	SO4	C	4002	-	4,4,4	0.39	0	6,6,6	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	4001	-	-	0/0/0/0	0/0/0/0
3	SO4	C	4002	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.