



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2017 – 04:33 PM EDT

PDB ID : 2POP
Title : The Crystal Structure of TAB1 and BIR1 complex
Authors : Lin, S.C.
Deposited on : 2007-04-27
Resolution : 3.10 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

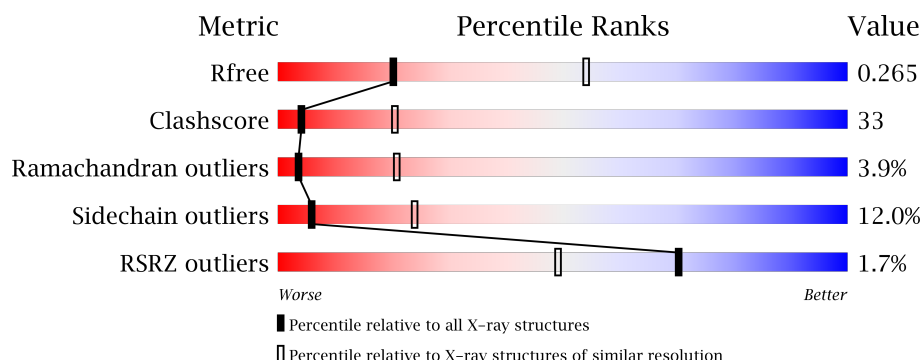
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	353	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 43%, green 41%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 1% 43% 41% 7% 8% </div> </div>
1	C	353	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 43%, green 42%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 43% 42% 7% 8% </div> </div>
2	B	95	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 41%, green 36%, orange 5%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 41% 36% 5% 17% </div> </div>
2	D	95	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 49%, yellow 28%, orange 5%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 49% 28% 5% 16% </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6264 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 Mitogen-activated protein kinase kinase kinase 7-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2503	1561	442	491	9			
1	C	325	Total	C	N	O	S	0	0	0
			2498	1558	441	490	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q15750
A	0	SER	-	expression tag	UNP Q15750
C	1999	GLY	-	expression tag	UNP Q15750
C	2000	SER	-	expression tag	UNP Q15750

- Molecule 2 is a protein called Baculoviral IAP repeat-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			626	394	113	116	3			
2	D	80	Total	C	N	O	S	0	0	0
			635	401	114	117	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1006	GLY	-	expression tag	UNP P98170
B	1007	SER	-	expression tag	UNP P98170
B	1008	HIS	-	expression tag	UNP P98170
B	1009	MET	-	expression tag	UNP P98170
D	3006	GLY	-	expression tag	UNP P98170
D	3007	SER	-	expression tag	UNP P98170
D	3008	HIS	-	expression tag	UNP P98170

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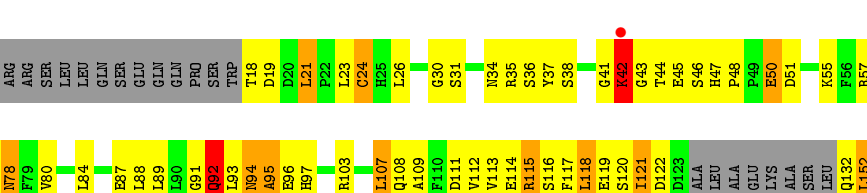
Chain	Residue	Modelled	Actual	Comment	Reference
D	3009	MET	-	expression tag	UNP P98170


- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

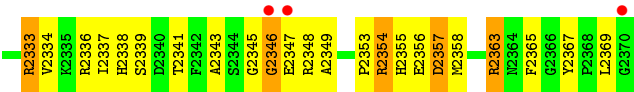
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

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 ($\text{RSRZ} > 2$). 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.

- Chain A: 



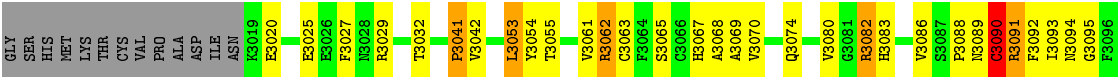
- Chain C: 
- | Label | Value |
|-------|-------|
| GLY | 2068 |
| SER | N2069 |
| MET | G2070 |
| ALA | R2075 |
| ALA | V2076 |
| GLN | T2077 |
| ARG | V2080 |
| SER | R2083 |
| LEU | L2084 |
| LEU | L2088 |
| GLN | L2089 |
| GLN | V2183 |
| PRO | G2091 |
| SER | Q2092 |
| TRP | L2093 |
| T2018 | N2094 |
| D2019 | A2095 |
| D2020 | E2096 |
| L2021 | H2097 |
| P2022 | A2100 |
| L2023 | V2101 |
| L2026 | V2102 |
| S2027 | R2103 |
| N2034 | F2104 |
| R2035 | V2105 |
| S2036 | L2106 |
| Y2037 | L2107 |
| S2038 | V2113 |
| A2039 | F2114 |
| D2040 | R2115 |
| G2041 | S2116 |
| K2042 | F2117 |
| G2043 | L2118 |
| T2044 | E2119 |
| E2045 | S2120 |
| S2046 | L2121 |
| H2047 | L2122 |
| E2050 | ALA |
| D2051 | LEU |
| L2054 | ALA |
| K2055 | GLU |
| R2056 | LVS |
| R2057 | ALA |
| S2058 | SER |
| E2059 | LEU |
| N2060 | GLN |
| N2061 | L2152 |
| C2062 | E2153 |
| F2063 | K2156 |
| L2064 | D2245 |
| Y2065 | Y2246 |
| | L2158 |
| | E2159 |



● Molecule 2: Baculoviral IAP repeat-containing protein 4



● Molecule 2: Baculoviral IAP repeat-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.99Å 108.71Å 175.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 34.16 – 3.11	Depositor EDS
% Data completeness (in resolution range)	77.2 (30.00-3.10) 78.1 (34.16-3.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.12Å)	Xtriage
Refinement program	CNS1.2	Depositor
R, R_{free}	0.209 , 0.254 0.215 , 0.265	Depositor DCC
R_{free} test set	1326 reflections (7.84%)	DCC
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/2541	0.60	1/3434 (0.0%)
1	C	0.36	0/2536	0.58	0/3427
2	B	0.43	0/643	0.62	0/867
2	D	0.47	0/652	0.66	1/879 (0.1%)
All	All	0.39	0/6372	0.60	2/8607 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	LEU	CA-CB-CG	5.70	128.41	115.30
2	D	3090	CYS	CA-CB-SG	5.07	123.12	114.00

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	2503	0	2465	172	0
1	C	2498	0	2463	168	0
2	B	626	0	580	39	0
2	D	635	0	593	28	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
All	All	6264	0	6101	403	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 33.

All (403) 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:194:THR:HG22	1:A:196:ASP:H	1.11	1.14
1:C:2211:ASN:ND2	1:C:2214:GLU:H	1.56	1.02
1:C:2184:GLY:H	1:C:2207:HIS:HD2	1.07	1.00
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.29	0.96
1:A:194:THR:HG22	1:A:196:ASP:N	1.81	0.94
1:C:2211:ASN:HD22	1:C:2214:GLU:N	1.69	0.90
1:C:2189:LEU:HD12	1:C:2286:VAL:HB	1.52	0.89
1:C:2022:PRO:HG2	1:C:2057:ARG:O	1.75	0.86
1:A:266:ILE:H	1:A:266:ILE:HD12	1.39	0.86
1:C:2211:ASN:HD22	1:C:2214:GLU:H	0.88	0.85
1:C:2080:VAL:HG13	1:C:2113:VAL:HG11	1.59	0.85
1:C:2184:GLY:H	1:C:2207:HIS:CD2	1.95	0.83
1:C:2292:LEU:HD13	1:C:2358:MET:HB3	1.60	0.83
1:A:211:ASN:HB3	1:A:214:GLU:HB2	1.59	0.83
1:C:2021:LEU:HB2	1:C:2022:PRO:HD2	1.61	0.82
1:A:169:VAL:HG23	1:A:186:ASN:HB2	1.61	0.81
1:C:2211:ASN:HD21	1:C:2213:ASP:HB2	1.44	0.80
2:D:3063:CYS:HB2	2:D:3083:HIS:CE1	2.17	0.79
1:C:2021:LEU:HD23	1:C:2021:LEU:H	1.47	0.78
1:A:153:GLU:HA	1:A:156:LYS:HD3	1.64	0.78
1:A:18:THR:HG23	1:A:19:ASP:H	1.47	0.77
1:A:262:LYS:NZ	2:B:1098:LEU:HD23	1.99	0.77
1:C:2036:SER:HB3	1:C:2045:GLU:HG2	1.66	0.77
1:A:169:VAL:CG2	1:A:186:ASN:HB2	2.15	0.77
1:A:21:LEU:H	1:A:21:LEU:HD12	1.49	0.76
2:B:1072:ARG:NH1	2:D:3074:GLN:HG3	2.01	0.76
1:A:42:LYS:NZ	1:A:42:LYS:HA	2.00	0.76
1:A:47:HIS:HB3	1:A:48:PRO:HD2	1.68	0.76
2:B:1084:ARG:HG3	2:B:1093:ILE:HG21	1.68	0.75
2:D:3082:ARG:HG3	2:D:3082:ARG:HH11	1.51	0.75
1:A:115:ARG:O	1:A:119:GLU:HG2	1.87	0.74
1:C:2267:ILE:HG13	1:C:2269:GLU:H	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:H	1:A:204:ASN:HD21	1.34	0.73
1:A:111:ASP:OD1	1:A:115:ARG:HD3	1.89	0.72
1:A:31:SER:H	1:A:328:GLN:HE22	1.35	0.72
1:A:76:VAL:HG22	1:A:117:PHE:CZ	2.26	0.71
1:C:2153:GLU:HA	1:C:2156:LYS:HG3	1.71	0.70
1:C:2303:GLY:O	1:C:2304:GLN:HG2	1.90	0.70
2:D:3082:ARG:O	2:D:3086:VAL:HG23	1.90	0.69
1:A:353:PRO:HG2	1:A:354:ARG:HD3	1.75	0.69
1:C:2169:VAL:HG22	1:C:2186:ASN:HB2	1.75	0.69
2:D:3029:ARG:HG2	2:D:3053:LEU:HD23	1.75	0.68
2:B:1053:LEU:HD12	2:B:1053:LEU:O	1.93	0.68
1:C:2356:GLU:HG2	1:C:2357:ASP:H	1.58	0.68
1:A:188:ALA:H	1:A:204:ASN:ND2	1.91	0.68
2:D:3025:GLU:OE1	2:D:3027:PHE:HB3	1.92	0.68
2:D:3063:CYS:SG	2:D:3065:SER:HB3	2.34	0.68
1:A:80:VAL:HG13	1:A:113:VAL:HG11	1.76	0.67
1:A:153:GLU:HA	1:A:156:LYS:CD	2.24	0.67
2:B:1028:ASN:N	2:B:1028:ASN:HD22	1.91	0.67
1:C:2330:VAL:O	1:C:2334:VAL:HG23	1.94	0.67
1:A:91:GLY:H	1:A:94:ASN:ND2	1.93	0.67
1:C:2347:GLU:HG2	1:C:2348:ARG:N	2.11	0.66
1:C:2103:ARG:HG3	1:C:2272:ILE:HG21	1.77	0.66
1:C:2021:LEU:HD11	1:C:2089:LEU:HD13	1.78	0.65
1:A:347:GLU:H	1:A:347:GLU:CD	1.99	0.65
2:D:3097:TYR:O	2:D:3098:LEU:HD22	1.97	0.65
1:C:2088:LEU:HD21	1:C:2106:LEU:HD23	1.79	0.64
1:C:2317:PHE:CD1	1:C:2326:VAL:HG11	2.32	0.64
2:B:1030:LEU:O	2:B:1030:LEU:HD23	1.97	0.64
2:D:3089:ASN:HA	2:D:3094:ASN:HD21	1.62	0.64
1:C:2189:LEU:HD12	1:C:2286:VAL:CB	2.27	0.64
1:C:2101:ASP:O	1:C:2105:VAL:HG23	1.97	0.64
1:A:152:LEU:C	1:A:154:ARG:H	2.01	0.63
1:A:91:GLY:H	1:A:94:ASN:HD21	1.45	0.63
1:C:2347:GLU:HG2	1:C:2348:ARG:H	1.63	0.63
2:B:1091:ARG:HG2	2:B:1091:ARG:HH11	1.63	0.63
2:B:1089:ASN:O	2:B:1091:ARG:N	2.31	0.62
2:D:3090:CYS:O	2:D:3092:PHE:N	2.32	0.62
1:C:2333:ARG:O	1:C:2337:ILE:HG13	1.99	0.62
2:B:1090:CYS:O	2:B:1092:PHE:N	2.32	0.62
1:C:2076:VAL:O	1:C:2080:VAL:HG23	1.99	0.62
1:A:262:LYS:HZ1	2:B:1098:LEU:HD23	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2169:VAL:HG22	1:C:2186:ASN:CB	2.29	0.61
1:A:58:SER:HB2	1:A:89:LEU:HD22	1.82	0.61
1:A:278:LEU:HD22	1:A:281:VAL:HG21	1.81	0.61
1:C:2021:LEU:HD11	1:C:2056:PHE:HB3	1.81	0.61
1:C:2095:ALA:HB3	1:C:2097:HIS:CD2	2.35	0.61
1:C:2299:ALA:HB1	1:C:2341:THR:HG21	1.82	0.61
1:C:2060:ASN:HB3	1:C:2094:ASN:OD1	2.02	0.60
2:B:1080:VAL:HG12	2:B:1084:ARG:HH12	1.66	0.60
2:D:3089:ASN:O	2:D:3091:ARG:N	2.33	0.60
2:B:1097:TYR:O	2:B:1098:LEU:HD12	2.01	0.60
1:A:333:ARG:NH1	1:A:333:ARG:HG2	2.05	0.60
1:C:2027:SER:OG	1:C:2055:LYS:HE3	2.02	0.59
1:C:2092:GLN:HE21	1:C:2092:GLN:N	2.01	0.59
1:A:169:VAL:CG2	1:A:186:ASN:CB	2.80	0.59
1:C:2021:LEU:HD21	1:C:2056:PHE:CD1	2.38	0.59
1:C:2100:ALA:HA	1:C:2103:ARG:NH1	2.16	0.59
1:A:63:PHE:HB2	1:A:173:LEU:HB2	1.85	0.59
1:A:41:GLY:O	1:A:43:GLY:N	2.35	0.59
1:A:258:LEU:HD13	1:A:265:PRO:HG3	1.84	0.59
1:A:262:LYS:HZ2	2:B:1098:LEU:HD23	1.67	0.59
1:A:155:LEU:HD13	1:A:155:LEU:O	2.03	0.58
1:C:2075:ARG:NH2	1:C:2117:PHE:CE1	2.71	0.58
1:C:2211:ASN:ND2	1:C:2214:GLU:N	2.36	0.58
1:A:68:PHE:CD1	1:A:68:PHE:N	2.71	0.58
1:A:42:LYS:HZ3	1:A:42:LYS:HA	1.67	0.58
1:A:278:LEU:O	1:A:281:VAL:HG22	2.04	0.58
1:A:238:GLU:CD	1:A:238:GLU:N	2.56	0.58
1:A:266:ILE:H	1:A:266:ILE:CD1	2.12	0.58
1:A:21:LEU:HD12	1:A:21:LEU:N	2.17	0.57
1:A:91:GLY:O	1:A:93:LEU:N	2.38	0.57
1:C:2267:ILE:HG13	1:C:2268:ALA:N	2.19	0.57
1:A:57:ARG:HD2	1:A:57:ARG:O	2.05	0.57
1:C:2157:THR:O	1:C:2160:ARG:HB3	2.04	0.57
2:B:1062:ARG:HD3	2:B:1067:HIS:O	2.04	0.57
1:C:2036:SER:HB3	1:C:2045:GLU:CG	2.34	0.57
2:D:3082:ARG:CG	2:D:3082:ARG:HH11	2.17	0.57
1:C:2035:ARG:O	1:C:2354:ARG:HB2	2.05	0.57
1:A:153:GLU:CA	1:A:156:LYS:HD3	2.34	0.57
1:A:36:SER:HA	1:A:354:ARG:HB2	1.87	0.57
1:C:2214:GLU:OE1	1:C:2214:GLU:HA	2.03	0.57
1:A:296:LEU:HD23	1:A:309:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2095:ALA:HB3	1:C:2097:HIS:NE2	2.20	0.56
1:A:238:GLU:H	1:A:238:GLU:CD	2.09	0.56
1:C:2091:GLY:O	1:C:2093:LEU:N	2.38	0.56
1:A:214:GLU:OE1	1:A:214:GLU:HA	2.05	0.56
1:C:2211:ASN:HB3	1:C:2214:GLU:HB2	1.87	0.56
1:C:2169:VAL:CG2	1:C:2186:ASN:HB3	2.36	0.56
2:D:3062:ARG:HD3	2:D:3067:HIS:O	2.06	0.56
1:A:18:THR:HG23	1:A:19:ASP:N	2.18	0.55
1:A:84:LEU:O	1:A:88:LEU:HD23	2.06	0.55
1:C:2038:SER:C	1:C:2040:ASP:H	2.08	0.55
1:A:36:SER:HA	1:A:354:ARG:CB	2.36	0.55
1:C:2115:ARG:O	1:C:2119:GLU:HG2	2.07	0.55
2:D:3080:VAL:HG23	2:D:3093:ILE:CD1	2.37	0.55
1:A:179:TYR:CZ	1:A:275:ALA:HB2	2.42	0.54
2:B:1024:VAL:HG13	2:B:1097:TYR:OH	2.06	0.54
1:A:76:VAL:HG22	1:A:117:PHE:CE1	2.43	0.54
1:C:2092:GLN:NE2	1:C:2092:GLN:N	2.56	0.54
1:C:2254:ASP:C	1:C:2255:ILE:HD12	2.28	0.54
1:C:2217:ARG:NH2	1:C:2267:ILE:HG22	2.23	0.54
1:C:2223:LEU:N	1:C:2223:LEU:HD12	2.23	0.54
1:A:333:ARG:O	1:A:337:ILE:HG13	2.07	0.54
1:A:112:VAL:O	1:A:116:SER:HB3	2.08	0.54
1:A:157:THR:O	1:A:160:ARG:HB3	2.07	0.54
1:C:2117:PHE:O	1:C:2120:SER:HB3	2.08	0.54
1:C:2153:GLU:HA	1:C:2156:LYS:CG	2.38	0.54
1:A:103:ARG:NH2	1:A:274:GLY:HA2	2.23	0.54
1:A:235:CYS:C	1:A:237:GLN:H	2.12	0.54
1:C:2102:VAL:HB	1:C:2179:TYR:CE2	2.43	0.53
2:D:3029:ARG:HA	2:D:3053:LEU:CD2	2.38	0.53
1:A:299:ALA:O	1:A:348:ARG:NH1	2.42	0.53
2:D:3041:PRO:HG2	2:D:3042:VAL:H	1.73	0.53
1:A:108:GLN:O	1:A:112:VAL:HG23	2.09	0.53
1:A:94:ASN:O	1:A:95:ALA:HB2	2.08	0.53
1:A:153:GLU:HA	1:A:156:LYS:CE	2.39	0.53
1:A:114:GLU:OE2	1:A:243:ILE:HG23	2.07	0.53
1:A:266:ILE:N	1:A:266:ILE:HD12	2.14	0.53
1:C:2094:ASN:O	1:C:2095:ALA:HB2	2.08	0.53
1:C:2285:LEU:HD22	1:C:2286:VAL:N	2.23	0.53
2:B:1022:GLU:C	2:B:1024:VAL:H	2.12	0.53
2:B:1084:ARG:HG3	2:B:1093:ILE:CG2	2.36	0.52
1:C:2169:VAL:HG21	1:C:2186:ASN:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2183:VAL:HG22	1:C:2270:PRO:HA	1.91	0.52
1:A:184:GLY:H	1:A:207:HIS:HD2	1.57	0.52
1:C:2278:LEU:HA	1:C:2281:VAL:CG2	2.39	0.52
1:A:347:GLU:O	1:A:350:ARG:HD3	2.09	0.52
1:C:2347:GLU:HG2	1:C:2348:ARG:HG2	1.92	0.52
2:B:1036:PHE:CD1	2:B:1037:PRO:HD2	2.45	0.52
1:A:46:SER:C	1:A:47:HIS:ND1	2.63	0.52
1:A:114:GLU:O	1:A:118:LEU:HD23	2.10	0.52
1:C:2023:LEU:HD23	1:C:2023:LEU:H	1.75	0.52
1:C:2070:GLY:HA3	1:C:2077:THR:CG2	2.40	0.52
1:C:2300:HIS:HE1	1:C:2337:ILE:HG21	1.74	0.52
1:C:2292:LEU:HD12	1:C:2358:MET:CE	2.40	0.52
1:A:217:ARG:HG2	1:A:217:ARG:HH11	1.75	0.52
1:C:2278:LEU:HA	1:C:2281:VAL:HG21	1.91	0.52
1:A:194:THR:HB	1:A:197:GLY:O	2.10	0.52
1:A:26:LEU:O	1:A:363:ARG:HD3	2.10	0.52
2:B:1070:VAL:HG22	2:B:1086:VAL:HG21	1.92	0.51
1:C:2021:LEU:HD23	1:C:2021:LEU:N	2.21	0.51
1:C:2346:GLY:H	1:C:2349:ALA:HB2	1.75	0.51
1:C:2034:ASN:HD22	1:C:2034:ASN:N	2.06	0.51
2:D:3062:ARG:HG3	2:D:3069:ALA:HB2	1.93	0.51
1:A:114:GLU:OE2	1:A:114:GLU:HA	2.10	0.51
1:A:36:SER:O	1:A:44:THR:HA	2.11	0.51
1:A:120:SER:O	1:A:122:ASP:N	2.42	0.51
1:A:278:LEU:CD2	1:A:281:VAL:HG21	2.40	0.51
1:A:346:GLY:H	1:A:349:ALA:HB2	1.75	0.51
1:A:347:GLU:N	1:A:347:GLU:CD	2.63	0.51
1:C:2235:CYS:C	1:C:2237:GLN:H	2.14	0.51
2:B:1022:GLU:OE1	2:B:1022:GLU:N	2.44	0.51
1:C:2169:VAL:CG2	1:C:2186:ASN:CB	2.89	0.51
1:C:2211:ASN:ND2	1:C:2213:ASP:HB2	2.21	0.51
1:A:26:LEU:HD23	1:A:363:ARG:NH1	2.26	0.51
1:C:2036:SER:HA	1:C:2354:ARG:CB	2.41	0.51
1:A:117:PHE:O	1:A:120:SER:HB3	2.11	0.51
1:C:2063:PHE:CD1	1:C:2173:LEU:HB3	2.46	0.51
1:C:2248:VAL:HG21	1:C:2266:ILE:HG13	1.93	0.51
1:A:91:GLY:N	1:A:94:ASN:ND2	2.57	0.50
1:C:2120:SER:O	1:C:2122:ASP:N	2.45	0.50
1:C:2248:VAL:O	1:C:2252:TYR:HB3	2.12	0.50
1:C:2283:GLY:O	1:C:2365:PHE:HB2	2.10	0.50
1:A:87:GLU:O	1:A:92:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1024:VAL:HG13	2:B:1097:TYR:CE2	2.47	0.50
1:C:2036:SER:O	1:C:2045:GLU:HG2	2.10	0.50
1:C:2319:LYS:NZ	1:C:2319:LYS:CB	2.75	0.50
1:C:2353:PRO:HG2	1:C:2354:ARG:HD3	1.92	0.50
2:D:3032:THR:O	2:D:3054:TYR:HB3	2.11	0.50
2:D:3063:CYS:HB2	2:D:3083:HIS:HE1	1.72	0.50
1:A:283:GLY:O	1:A:365:PHE:HB2	2.12	0.50
2:B:1091:ARG:O	2:B:1094:ASN:N	2.42	0.50
2:B:1032:THR:O	2:B:1054:TYR:HB3	2.12	0.50
1:C:2100:ALA:HA	1:C:2103:ARG:HH11	1.75	0.50
1:A:267:ILE:HD13	1:A:269:GLU:HB2	1.94	0.50
1:A:248:VAL:O	1:A:252:TYR:HB3	2.12	0.49
1:A:333:ARG:NH1	1:A:333:ARG:CG	2.70	0.49
1:A:118:LEU:N	1:A:118:LEU:CD2	2.75	0.49
1:A:132:GLN:O	1:A:154:ARG:HG3	2.13	0.49
1:C:2093:LEU:HD21	1:C:2172:VAL:HG11	1.93	0.49
1:A:348:ARG:HG3	1:A:348:ARG:HH11	1.78	0.49
1:A:117:PHE:CZ	1:A:121:ILE:HD11	2.47	0.48
1:A:169:VAL:HG21	1:A:186:ASN:CB	2.43	0.48
1:A:217:ARG:HG2	1:A:217:ARG:NH1	2.28	0.48
1:A:248:VAL:HG22	1:A:266:ILE:HD11	1.95	0.48
1:C:2038:SER:C	1:C:2040:ASP:N	2.66	0.48
1:C:2076:VAL:HG22	1:C:2117:PHE:CE1	2.48	0.48
1:A:347:GLU:HG2	1:A:348:ARG:H	1.78	0.48
1:A:38:SER:OG	1:A:43:GLY:HA3	2.13	0.48
1:C:2237:GLN:HB2	1:C:2242:ARG:NH2	2.28	0.48
1:C:2304:GLN:HA	1:C:2307:GLN:OE1	2.13	0.48
1:A:58:SER:HB3	1:A:62:CYS:HB3	1.94	0.48
1:A:192:LYS:O	1:A:198:LEU:HD12	2.13	0.48
1:C:2345:GLY:HA2	1:C:2349:ALA:HB2	1.95	0.48
1:A:361:LEU:C	1:A:361:LEU:HD23	2.34	0.48
2:B:1091:ARG:HG2	2:B:1091:ARG:NH1	2.29	0.48
1:C:2046:SER:C	1:C:2047:HIS:ND1	2.67	0.48
1:C:2356:GLU:HG2	1:C:2357:ASP:N	2.27	0.48
1:A:95:ALA:HB3	1:A:97:HIS:HD2	1.78	0.48
1:C:2090:LEU:N	1:C:2092:GLN:HE22	2.12	0.48
1:C:2121:ILE:HD12	1:C:2246:TYR:HD1	1.78	0.48
1:C:2068:PHE:N	1:C:2068:PHE:CD1	2.81	0.47
1:A:245:ASP:CG	1:A:248:VAL:HG12	2.35	0.47
1:C:2075:ARG:NH2	1:C:2117:PHE:HE1	2.12	0.47
1:C:2255:ILE:N	1:C:2255:ILE:HD12	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLY:C	1:A:43:GLY:N	2.68	0.47
1:C:2038:SER:HB2	1:C:2043:GLY:HA3	1.97	0.47
1:A:107:LEU:HD23	1:A:272:ILE:HD11	1.97	0.47
1:A:88:LEU:HD21	1:A:109:ALA:HB1	1.96	0.47
1:A:288:MET:CE	1:A:293:TYR:HB3	2.44	0.47
1:A:163:SER:OG	1:A:247:LYS:HD2	2.14	0.47
2:B:1071:ASP:OD1	2:B:1071:ASP:C	2.52	0.47
1:C:2021:LEU:HB2	1:C:2022:PRO:CD	2.40	0.47
1:C:2153:GLU:O	1:C:2153:GLU:HG2	2.15	0.47
1:C:2026:LEU:O	1:C:2363:ARG:HD3	2.14	0.47
1:A:235:CYS:O	1:A:237:GLN:N	2.48	0.47
1:A:345:GLY:HA2	1:A:349:ALA:HB2	1.96	0.47
1:A:343:ALA:C	1:A:345:GLY:H	2.18	0.47
2:B:1095:GLY:C	2:B:1097:TYR:H	2.19	0.47
1:A:169:VAL:HG23	1:A:186:ASN:CB	2.35	0.47
1:A:347:GLU:HG2	1:A:348:ARG:N	2.30	0.47
1:C:2184:GLY:N	1:C:2207:HIS:HD2	1.91	0.47
1:C:2175:ASN:N	1:C:2175:ASN:ND2	2.62	0.46
2:D:3091:ARG:O	2:D:3094:ASN:N	2.43	0.46
1:A:95:ALA:HB3	1:A:97:HIS:CD2	2.50	0.46
1:C:2063:PHE:HB3	1:C:2065:TYR:CE1	2.50	0.46
1:A:316:GLU:HG2	1:A:329:ALA:CB	2.45	0.46
1:C:2191:CYS:O	1:C:2283:GLY:HA3	2.15	0.46
1:C:2312:MET:HG2	1:C:2333:ARG:NH2	2.31	0.46
1:A:174:LEU:O	1:A:175:ASN:HB2	2.15	0.46
1:A:87:GLU:C	1:A:88:LEU:HD22	2.36	0.46
1:A:96:GLU:HG3	1:A:96:GLU:O	2.16	0.46
2:D:3061:VAL:O	2:D:3069:ALA:HA	2.15	0.46
2:B:1061:VAL:O	2:B:1069:ALA:HA	2.16	0.46
1:A:152:LEU:C	1:A:154:ARG:N	2.68	0.46
2:B:1062:ARG:HG2	2:B:1067:HIS:C	2.36	0.46
1:A:41:GLY:C	1:A:43:GLY:H	2.19	0.46
1:C:2097:HIS:HB3	1:C:2101:ASP:HB3	1.97	0.46
1:C:2312:MET:O	1:C:2316:GLU:HG2	2.16	0.46
1:C:2037:TYR:OH	1:C:2339:SER:HB3	2.16	0.46
2:B:1062:ARG:HA	2:B:1068:ALA:O	2.16	0.46
2:B:1065:SER:HB3	2:B:1090:CYS:SG	2.56	0.46
1:C:2054:LEU:O	1:C:2065:TYR:HA	2.16	0.46
1:A:323:LEU:O	1:A:326:VAL:N	2.49	0.45
2:B:1028:ASN:N	2:B:1028:ASN:ND2	2.61	0.45
1:C:2063:PHE:N	1:C:2063:PHE:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1057:GLU:N	2:B:1057:GLU:OE2	2.49	0.45
1:C:2090:LEU:H	1:C:2092:GLN:HE22	1.64	0.45
1:C:2343:ALA:C	1:C:2345:GLY:H	2.19	0.45
1:A:153:GLU:HA	1:A:156:LYS:HE2	1.97	0.45
1:C:2036:SER:CB	1:C:2045:GLU:HG2	2.43	0.45
1:C:2021:LEU:CD1	1:C:2089:LEU:HD13	2.44	0.45
1:A:42:LYS:HZ2	1:A:42:LYS:HA	1.76	0.45
1:A:191:CYS:O	1:A:283:GLY:HA3	2.16	0.45
1:A:290:GLU:O	1:A:294:LYS:HB2	2.17	0.45
1:C:2036:SER:HA	1:C:2354:ARG:HB2	1.99	0.45
1:C:2178:LEU:HB3	1:C:2276:GLN:HB3	1.98	0.45
1:A:333:ARG:HH11	1:A:333:ARG:CG	2.09	0.45
1:A:361:LEU:HD23	1:A:362:VAL:N	2.32	0.45
1:C:2038:SER:O	1:C:2040:ASP:N	2.49	0.45
1:C:2290:GLU:O	1:C:2294:LYS:HB2	2.16	0.45
1:C:2064:LEU:HD12	1:C:2172:VAL:HG22	1.99	0.44
1:A:316:GLU:HG2	1:A:329:ALA:HB1	1.98	0.44
1:A:176:ASN:O	1:A:278:LEU:HB2	2.18	0.44
1:A:345:GLY:CA	1:A:349:ALA:HB2	2.48	0.44
1:C:2084:LEU:HD21	1:C:2170:VAL:HG21	1.99	0.44
1:C:2245:ASP:CG	1:C:2248:VAL:HG12	2.37	0.44
1:A:57:ARG:HG3	1:A:63:PHE:CE1	2.52	0.44
1:C:2194:THR:HG22	1:C:2196:ASP:H	1.82	0.44
1:C:2234:ILE:O	1:C:2235:CYS:HB2	2.18	0.44
1:C:2347:GLU:N	1:C:2347:GLU:OE1	2.49	0.44
1:A:71:TYR:CZ	1:A:165:GLY:HA3	2.53	0.44
2:D:3062:ARG:HG2	2:D:3068:ALA:O	2.18	0.44
1:C:2050:GLU:HG3	1:C:2070:GLY:O	2.18	0.43
1:C:2235:CYS:O	1:C:2237:GLN:N	2.51	0.43
1:C:2267:ILE:CG1	1:C:2268:ALA:N	2.81	0.43
1:A:42:LYS:O	1:A:44:THR:HG23	2.18	0.43
1:C:2345:GLY:CA	1:C:2349:ALA:HB2	2.47	0.43
1:A:45:GLU:O	1:A:46:SER:HB2	2.18	0.43
1:A:169:VAL:HG22	1:A:182:ASN:ND2	2.33	0.43
1:A:321:THR:O	1:A:369:LEU:HD21	2.17	0.43
1:A:184:GLY:H	1:A:207:HIS:CD2	2.36	0.43
1:A:297:GLU:CG	1:A:302:PRO:HA	2.48	0.43
1:A:286:VAL:HG13	1:A:360:LEU:HD11	2.00	0.43
1:C:2058:SER:HB2	1:C:2062:CYS:HB3	2.00	0.43
1:A:292:LEU:C	1:A:292:LEU:CD2	2.87	0.43
1:A:84:LEU:HD21	1:A:170:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2192:LYS:HG2	1:C:2281:VAL:HG13	1.99	0.43
1:A:248:VAL:O	1:A:266:ILE:HD11	2.19	0.43
1:C:2036:SER:HA	1:C:2354:ARG:HB3	2.01	0.43
1:A:78:ASN:N	1:A:78:ASN:ND2	2.67	0.43
1:A:34:ASN:O	1:A:35:ARG:HG2	2.19	0.42
2:B:1055:THR:OG1	2:B:1056:GLY:N	2.52	0.42
1:C:2060:ASN:O	1:C:2061:ASN:HB3	2.19	0.42
1:C:2290:GLU:HA	1:C:2293:TYR:CE2	2.54	0.42
1:C:2190:LEU:HD12	1:C:2191:CYS:N	2.35	0.42
1:C:2121:ILE:CD1	1:C:2246:TYR:HD1	2.30	0.42
1:C:2292:LEU:HD12	1:C:2358:MET:HE1	2.01	0.42
1:C:2300:HIS:CE1	1:C:2337:ILE:HG21	2.53	0.42
1:C:2337:ILE:O	1:C:2341:THR:HG23	2.19	0.42
1:A:103:ARG:NH2	1:A:274:GLY:CA	2.81	0.42
1:A:103:ARG:CZ	1:A:274:GLY:HA2	2.50	0.42
1:C:2173:LEU:HA	1:C:2173:LEU:HD12	1.86	0.42
1:A:194:THR:C	1:A:196:ASP:H	2.20	0.42
1:C:2068:PHE:CD2	1:C:2168:ALA:HB2	2.54	0.42
2:D:3095:GLY:C	2:D:3097:TYR:H	2.23	0.42
1:A:195:VAL:O	1:A:195:VAL:HG12	2.19	0.42
1:A:24:CYS:O	1:A:55:LYS:NZ	2.53	0.42
1:C:2175:ASN:N	1:C:2175:ASN:HD22	2.16	0.42
1:C:2241:ARG:C	1:C:2242:ARG:HG2	2.40	0.42
1:A:37:TYR:OH	1:A:338:HIS:HD2	2.02	0.42
1:C:2309:ILE:O	1:C:2313:ILE:HG13	2.20	0.42
1:C:2319:LYS:NZ	1:C:2319:LYS:HB3	2.34	0.42
1:A:35:ARG:O	1:A:354:ARG:HB2	2.19	0.42
1:C:2192:LYS:O	1:C:2198:LEU:HD12	2.20	0.42
1:C:2317:PHE:CD2	1:C:2367:TYR:HD2	2.38	0.42
1:C:2316:GLU:HG3	1:C:2330:VAL:HG22	2.02	0.42
2:D:3070:VAL:HG22	2:D:3086:VAL:HG21	2.01	0.42
1:A:246:TYR:HE2	1:A:250:TYR:CG	2.38	0.42
1:C:2019:ASP:N	1:C:2019:ASP:OD1	2.53	0.42
1:C:2044:THR:HG23	1:C:2044:THR:O	2.19	0.42
1:C:2173:LEU:HD11	1:C:2278:LEU:HD12	2.02	0.42
1:A:188:ALA:N	1:A:204:ASN:HD21	2.11	0.42
1:C:2057:ARG:HE	1:C:2061:ASN:HA	1.85	0.42
1:C:2063:PHE:HD1	1:C:2173:LEU:HB3	1.85	0.42
1:C:2243:ILE:HD13	1:C:2243:ILE:N	2.34	0.42
1:A:223:LEU:HD13	1:A:228:ILE:HD11	2.02	0.41
1:A:215:LEU:HD21	1:A:229:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3082:ARG:CG	2:D:3082:ARG:NH1	2.81	0.41
2:D:3097:TYR:C	2:D:3098:LEU:HD22	2.40	0.41
1:A:265:PRO:HG2	1:A:266:ILE:HG13	2.02	0.41
2:B:1080:VAL:CG1	2:B:1084:ARG:HH12	2.30	0.41
2:B:1087:SER:C	2:B:1089:ASN:H	2.23	0.41
1:A:246:TYR:HD2	1:A:246:TYR:O	2.02	0.41
1:A:293:TYR:C	1:A:293:TYR:CD1	2.94	0.41
1:A:30:GLY:HA2	1:A:328:GLN:NE2	2.34	0.41
1:A:347:GLU:O	1:A:350:ARG:CD	2.69	0.41
1:C:2034:ASN:O	1:C:2035:ARG:HG3	2.20	0.41
1:C:2338:HIS:HD2	1:C:2355:HIS:HD2	1.68	0.41
1:A:75:ARG:HG2	1:A:75:ARG:O	2.20	0.41
1:C:2194:THR:C	1:C:2196:ASP:H	2.24	0.41
1:A:107:LEU:HD23	1:A:272:ILE:CD1	2.51	0.41
1:A:50:GLU:O	1:A:51:ASP:OD1	2.39	0.41
2:B:1053:LEU:HD12	2:B:1053:LEU:C	2.41	0.41
1:A:215:LEU:HA	1:A:215:LEU:HD12	1.72	0.41
1:A:152:LEU:HD13	1:A:152:LEU:O	2.21	0.40
1:A:188:ALA:C	1:A:189:LEU:HD23	2.41	0.40
1:A:183:VAL:CG2	1:A:270:PRO:HB3	2.51	0.40
1:C:2057:ARG:NE	1:C:2061:ASN:HA	2.36	0.40
1:C:2093:LEU:HG	1:C:2174:LEU:HD11	2.02	0.40
1:C:2316:GLU:O	1:C:2320:GLN:HG2	2.20	0.40
2:D:3062:ARG:HA	2:D:3068:ALA:O	2.20	0.40
1:A:248:VAL:CG2	1:A:266:ILE:HG12	2.51	0.40
1:A:285:LEU:HA	1:A:285:LEU:HD22	1.88	0.40
1:A:80:VAL:O	1:A:84:LEU:HB2	2.21	0.40
2:B:1090:CYS:O	2:B:1091:ARG:C	2.59	0.40
1:C:2046:SER:O	1:C:2047:HIS:ND1	2.55	0.40
1:C:2190:LEU:HD12	1:C:2191:CYS:H	1.86	0.40
2:D:3054:TYR:CD2	2:D:3055:THR:N	2.90	0.40
2:B:1022:GLU:C	2:B:1024:VAL:N	2.74	0.40
1:C:2195:VAL:HG12	1:C:2195:VAL:O	2.21	0.40
1:C:2338:HIS:O	1:C:2341:THR:OG1	2.36	0.40
1:A:18:THR:CG2	1:A:19:ASP:H	2.27	0.40
1:C:2319:LYS:HZ2	1:C:2319:LYS:HB2	1.86	0.40
1:C:2323:LEU:O	1:C:2326:VAL:N	2.54	0.40
1:C:2292:LEU:CD1	1:C:2358:MET:HB3	2.41	0.40
1:A:116:SER:OG	1:A:117:PHE:N	2.54	0.40
1:A:252:TYR:HA	1:A:255:ILE:HD12	2.04	0.40
1:A:304:GLN:HA	1:A:307:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:N	1:A:78:ASN:HD22	2.18	0.40
2:B:1054:TYR:HD2	2:B:1055:THR:N	2.20	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	322/353 (91%)	258 (80%)	53 (16%)	11 (3%)	4	24
1	C	321/353 (91%)	258 (80%)	52 (16%)	11 (3%)	4	24
2	B	77/95 (81%)	63 (82%)	9 (12%)	5 (6%)	1	9
2	D	78/95 (82%)	65 (83%)	9 (12%)	4 (5%)	2	15
All	All	798/896 (89%)	644 (81%)	123 (15%)	31 (4%)	3	21

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
2	B	1090	CYS
2	B	1091	ARG
1	C	2092	GLN
2	D	3090	CYS
2	D	3091	ARG
1	A	42	LYS
1	A	274	GLY
2	B	1023	PHE
1	C	2041	GLY
1	C	2274	GLY
1	A	121	ILE
1	A	153	GLU

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Mol	Chain	Res	Type
1	A	291	GLY
1	C	2039	ALA
1	C	2121	ILE
1	C	2159	GLU
1	A	95	ALA
1	A	159	GLU
1	A	350	ARG
1	C	2094	ASN
1	C	2095	ALA
1	A	346	GLY
2	B	1088	PRO
2	D	3088	PRO
1	C	2291	GLY
1	C	2346	GLY
2	D	3041	PRO
1	A	236	GLY
2	B	1041	PRO
1	C	2236	GLY

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	267/289 (92%)	234 (88%)	33 (12%)	5	23
1	C	267/289 (92%)	233 (87%)	34 (13%)	5	21
2	B	65/79 (82%)	57 (88%)	8 (12%)	5	23
2	D	66/79 (84%)	61 (92%)	5 (8%)	15	49
All	All	665/736 (90%)	585 (88%)	80 (12%)	6	24

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	24	CYS
1	A	42	LYS

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Mol	Chain	Res	Type
1	A	50	GLU
1	A	61	ASN
1	A	68	PHE
1	A	77	THR
1	A	78	ASN
1	A	92	GLN
1	A	94	ASN
1	A	107	LEU
1	A	115	ARG
1	A	118	LEU
1	A	152	LEU
1	A	173	LEU
1	A	178	LEU
1	A	190	LEU
1	A	214	GLU
1	A	215	LEU
1	A	246	TYR
1	A	264	LYS
1	A	266	ILE
1	A	279	ASP
1	A	292	LEU
1	A	293	TYR
1	A	316	GLU
1	A	317	PHE
1	A	324	ASP
1	A	340	ASP
1	A	347	GLU
1	A	350	ARG
1	A	354	ARG
1	A	363	ARG
2	B	1022	GLU
2	B	1028	ASN
2	B	1045	SER
2	B	1082	ARG
2	B	1084	ARG
2	B	1090	CYS
2	B	1097	TYR
2	B	1099	GLU
1	C	2020	ASP
1	C	2034	ASN
1	C	2045	GLU
1	C	2051	ASP

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Mol	Chain	Res	Type
1	C	2057	ARG
1	C	2075	ARG
1	C	2083	ARG
1	C	2092	GLN
1	C	2103	ARG
1	C	2107	LEU
1	C	2118	LEU
1	C	2156	LYS
1	C	2158	LEU
1	C	2169	VAL
1	C	2174	LEU
1	C	2175	ASN
1	C	2189	LEU
1	C	2196	ASP
1	C	2201	THR
1	C	2214	GLU
1	C	2215	LEU
1	C	2219	SER
1	C	2242	ARG
1	C	2253	THR
1	C	2285	LEU
1	C	2296	LEU
1	C	2317	PHE
1	C	2321	THR
1	C	2333	ARG
1	C	2336	ARG
1	C	2354	ARG
1	C	2357	ASP
1	C	2363	ARG
1	C	2369	LEU
2	D	3020	GLU
2	D	3053	LEU
2	D	3062	ARG
2	D	3082	ARG
2	D	3090	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	78	ASN
1	A	82	GLN

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Mol	Chain	Res	Type
1	A	92	GLN
1	A	94	ASN
1	A	204	ASN
1	A	207	HIS
1	A	300	HIS
1	A	328	GLN
1	A	338	HIS
2	B	1028	ASN
2	B	1074	GLN
1	C	2034	ASN
1	C	2069	ASN
1	C	2092	GLN
1	C	2175	ASN
1	C	2182	ASN
1	C	2186	ASN
1	C	2202	GLN
1	C	2207	HIS
1	C	2211	ASN
1	C	2276	GLN
1	C	2300	HIS
2	D	3094	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [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	326/353 (92%)	-0.19	2 (0%) 89 77	38, 76, 120, 162	0
1	C	325/353 (92%)	-0.01	12 (3%) 42 21	43, 90, 149, 195	0
2	B	79/95 (83%)	-0.32	0 100 100	42, 67, 137, 157	0
2	D	80/95 (84%)	-0.40	0 100 100	45, 66, 114, 147	0
All	All	810/896 (90%)	-0.15	14 (1%) 70 49	38, 80, 137, 195	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	LYS	3.2
1	C	2041	GLY	2.5
1	A	260	ALA	2.5
1	C	2195	VAL	2.4
1	C	2370	GLY	2.3
1	C	2182	ASN	2.2
1	C	2037	TYR	2.2
1	C	2346	GLY	2.2
1	C	2034	ASN	2.2
1	C	2094	ASN	2.1
1	C	2347	GLU	2.1
1	C	2042	LYS	2.1
1	C	2039	ALA	2.0
1	C	2194	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
3	ZN	D	3500	1/1	1.00	0.12	-0.67	85,85,85,85	0
3	ZN	B	1500	1/1	0.99	0.10	-1.07	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.