



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:04 PM GMT

PDB ID : 1WDM  
Title : fatty acid beta-oxidation multienzyme complex from Pseudomonas fragi, form I (native3)  
Authors : Ishikawa, M.; Tsuchiya, D.; Oyama, T.; Tsunaka, Y.; Morikawa, K.  
Deposited on : 2004-05-17  
Resolution : 3.80 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 (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

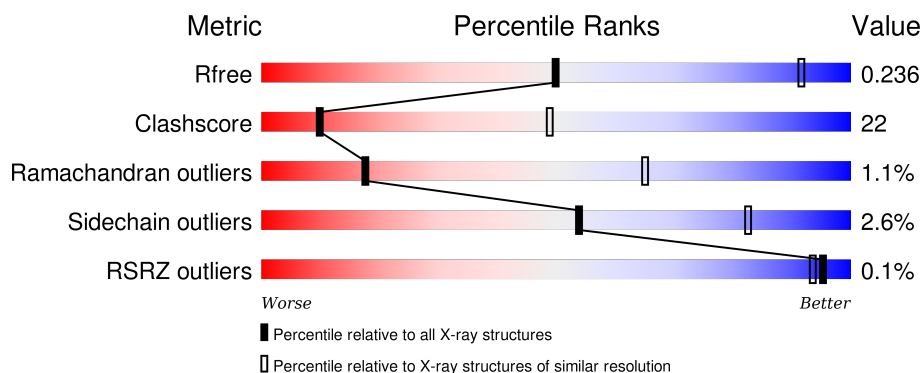
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	715	 61% 37% ..
1	B	715	 59% 39% ..
2	C	390	 56% 42% .
2	D	390	 55% 43% .

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
4	ACO	A	1002	-	-	-	X
4	ACO	C	3001	-	-	-	X
4	ACO	D	4001	-	-	-	X
5	NAD	A	1001	-	-	-	X
5	NAD	B	2001	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16541 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 Fatty oxidation complex alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	0	0
			5257	3355	878	997	27			
1	B	710	Total	C	N	O	S	0	0	0
			5302	3383	889	1003	27			

- Molecule 2 is a protein called 3-ketoacyl-CoA thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	390	Total	C	N	O	S	0	0	0
			2871	1786	508	548	29			
2	D	390	Total	C	N	O	S	0	0	0
			2869	1785	510	545	29			

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

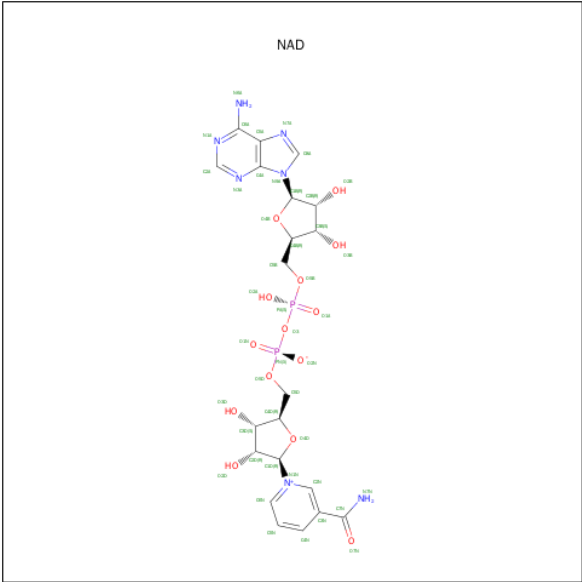
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).

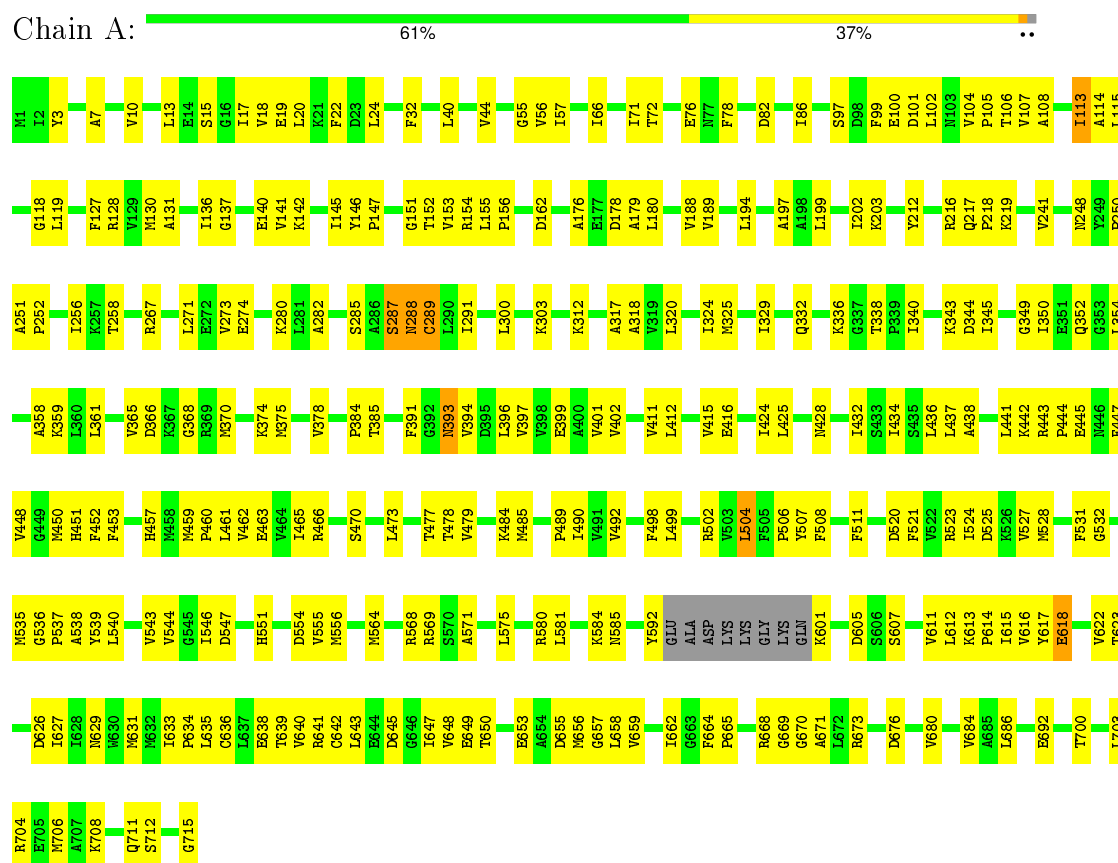


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

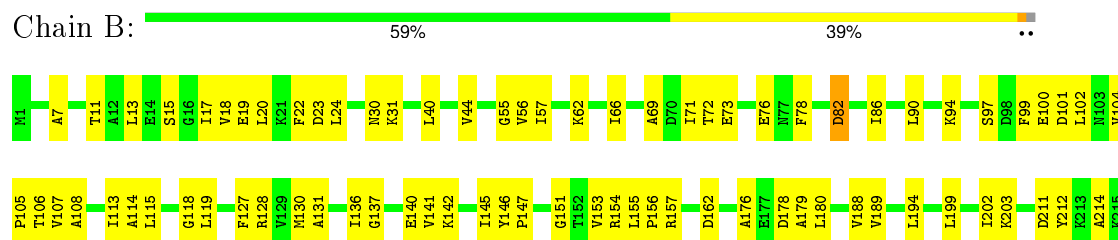
### 3 Residue-property plots

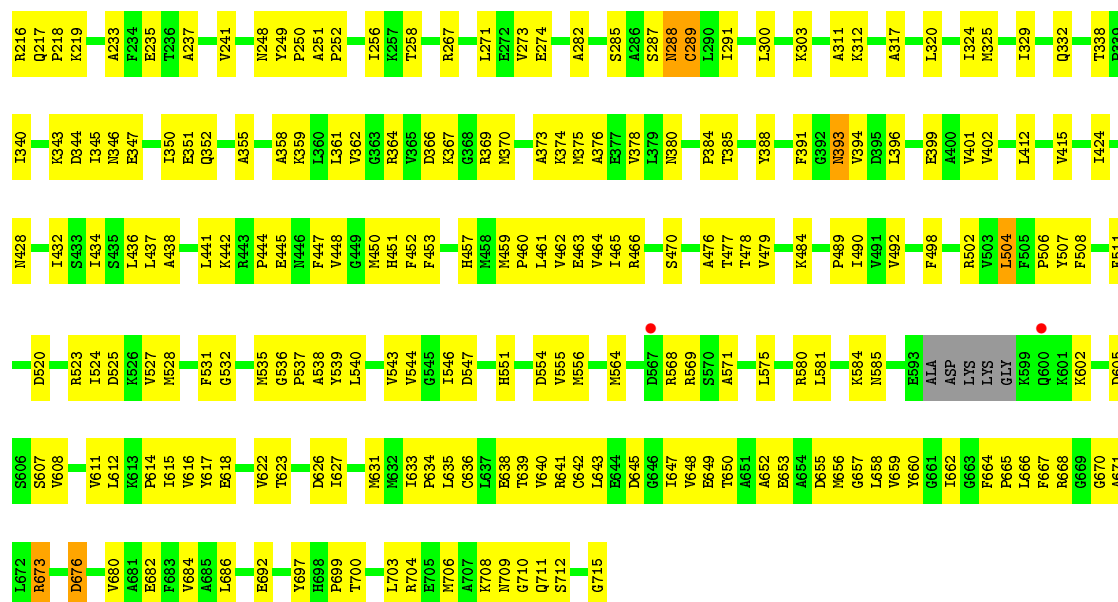
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Fatty oxidation complex alpha subunit

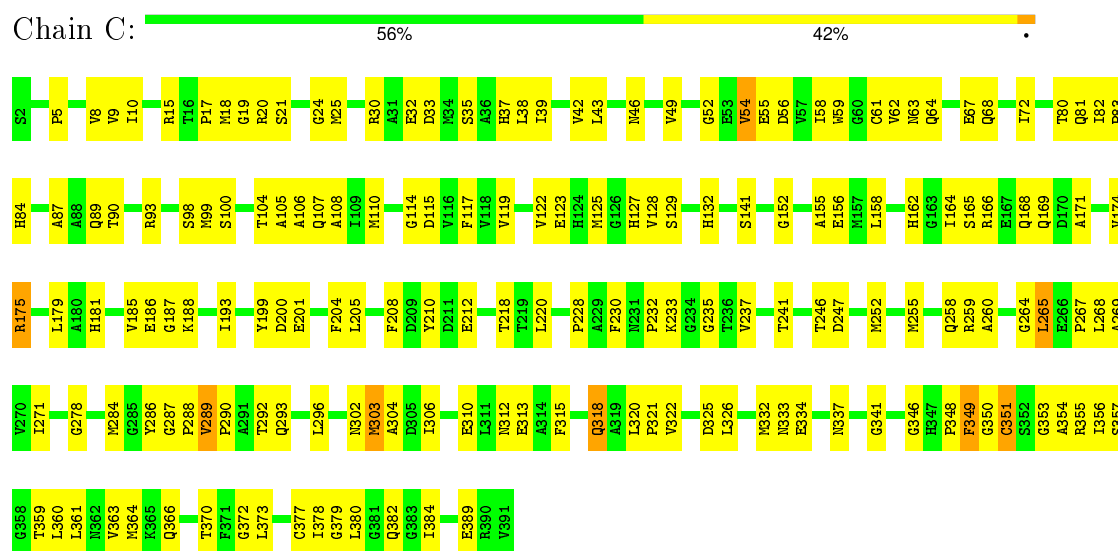


#### • Molecule 1: Fatty oxidation complex alpha subunit

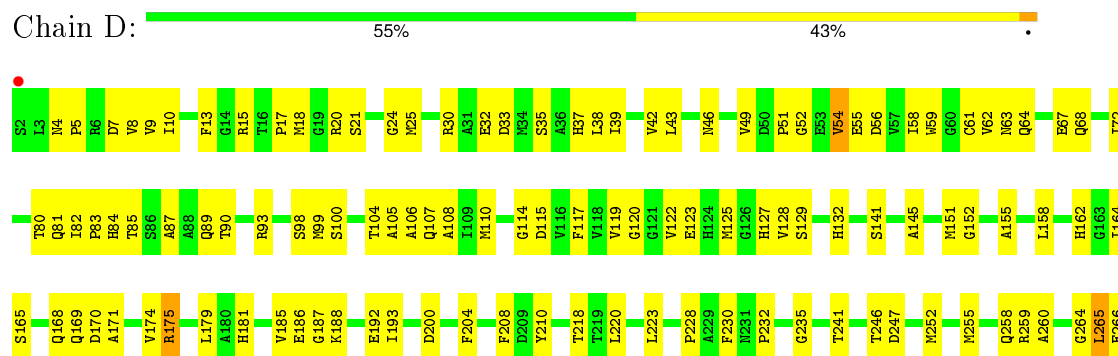




• Molecule 2: 3-ketoacyl-CoA thiolase



• Molecule 2: 3-ketoacyl-CoA thiolase





C351	S352	G353	A354	R355	L356	S357	G358	T359	L360	L361	M362	G363	M364	K365	Q366	T370	L373	G374	T375	K376	G377	L378	G379	Q382	G383	L384	E389	R390	V391																													
P267	L268	A269	V270	L271		G278		M284	G285	V286	G287	P288	V289	P290		Q293	K294	L296	K297	R298		M302	M303	A304	G305	L306		L309	E310	L311	M312	E313	A314	F315		Q318	A319	L320	P321	V322		D325	L326		L329		M332	M333		M337		G341		G346	E347	P348	C349	C350

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.45Å 95.46Å 161.32Å 90.00° 111.79° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80 19.99 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.80) 98.4 (19.99-3.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.39 (at 3.82Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.262 0.194 , 0.236	Depositor DCC
$R_{free}$ test set	1709 reflections (6.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 21.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 24902 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.29	0/5343	0.51	0/7237
1	B	0.28	0/5388	0.51	0/7291
2	C	0.29	0/2919	0.52	0/3944
2	D	0.30	0/2917	0.52	0/3941
All	All	0.29	0/16567	0.51	0/22413

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5257	0	5243	217	0
1	B	5302	0	5314	232	0
2	C	2871	0	2848	146	0
2	D	2869	0	2849	152	0
3	A	1	0	0	0	0
4	A	51	0	34	2	0
4	C	51	0	34	0	0
4	D	51	0	34	0	0
5	A	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	44	0	26	1	0
All	All	16541	0	16408	727	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 22.

All (727) 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:525:ASP:HB2	1:A:536:GLY:HA3	1.34	1.09
1:B:525:ASP:HB2	1:B:536:GLY:HA3	1.36	1.07
2:D:289:VAL:HG13	2:D:290:PRO:HD3	1.55	0.87
2:D:98:SER:HB3	2:D:353:GLY:HA3	1.59	0.85
1:B:130:MET:HE1	1:B:176:ALA:HA	1.57	0.84
1:B:401:VAL:HG12	1:B:402:VAL:H	1.42	0.84
2:D:125:MET:HE2	2:D:348:PRO:HA	1.57	0.83
2:C:289:VAL:HG13	2:C:290:PRO:HD3	1.60	0.83
2:C:125:MET:HE2	2:C:348:PRO:HA	1.62	0.82
1:B:673:ARG:HH11	1:B:673:ARG:HB2	1.43	0.82
1:A:401:VAL:HG12	1:A:402:VAL:H	1.45	0.81
2:C:378:ILE:HB	2:C:382:GLN:HB2	1.62	0.80
1:A:71:ILE:HD11	1:A:291:ILE:HG23	1.64	0.80
2:C:287:GLY:O	2:C:290:PRO:HD2	1.80	0.80
2:D:306:ILE:HD13	2:D:373:LEU:HB2	1.63	0.79
2:D:378:ILE:HB	2:D:382:GLN:HB2	1.66	0.77
1:A:251:ALA:HB3	1:A:252:PRO:HD3	1.67	0.76
1:B:71:ILE:HD11	1:B:291:ILE:HG23	1.66	0.76
1:A:343:LYS:HD3	1:A:344:ASP:N	2.01	0.76
1:A:416:GLU:OE1	1:A:442:LYS:HG2	1.85	0.76
2:D:287:GLY:O	2:D:290:PRO:HD2	1.85	0.76
2:C:98:SER:HB3	2:C:353:GLY:HA3	1.67	0.76
1:B:361:LEU:HD21	1:B:378:VAL:HG11	1.67	0.75
1:A:581:LEU:HB2	1:A:585:ASN:HB2	1.69	0.74
1:A:113:ILE:CD1	1:A:113:ILE:H	2.01	0.74
1:B:343:LYS:HD3	1:B:344:ASP:N	2.02	0.73
2:D:80:THR:HG22	2:D:81:GLN:H	1.53	0.73
2:C:8:VAL:HG21	2:C:106:ALA:HB1	1.69	0.73
1:B:251:ALA:HB3	1:B:252:PRO:HD3	1.69	0.72
1:B:241:VAL:HG21	1:B:256:ILE:HD11	1.72	0.72
1:B:581:LEU:HB2	1:B:585:ASN:HB2	1.71	0.72
1:A:361:LEU:HD21	1:A:378:VAL:HG11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:306:ILE:HD13	2:C:373:LEU:HB2	1.71	0.72
1:A:350:ILE:HG21	1:A:384:PRO:HB3	1.72	0.71
2:D:43:LEU:HD11	2:D:82:ILE:HD11	1.71	0.71
1:A:241:VAL:HG21	1:A:256:ILE:HD11	1.71	0.71
1:A:130:MET:HE1	1:A:176:ALA:HA	1.72	0.70
1:A:199:LEU:HD11	1:A:203:LYS:HE3	1.73	0.70
2:C:296:LEU:HD21	2:C:306:ILE:HD11	1.72	0.70
2:D:8:VAL:HG21	2:D:106:ALA:HB1	1.72	0.70
1:A:450:MET:HG2	1:A:452:PHE:CE1	2.26	0.69
1:B:130:MET:CE	1:B:176:ALA:HA	2.22	0.69
1:A:504:LEU:HD13	4:A:1002:ACO:HH33	1.73	0.69
2:D:152:GLY:HA3	2:D:230:PHE:CE2	2.27	0.69
1:A:673:ARG:HH11	1:A:673:ARG:HB2	1.55	0.69
2:C:46:ASN:O	2:C:49:VAL:HG22	1.92	0.69
1:B:325:MET:HE2	1:B:428:ASN:HD21	1.55	0.69
1:B:350:ILE:HG21	1:B:384:PRO:HB3	1.75	0.69
2:C:55:GLU:HG3	2:C:114:GLY:HA2	1.74	0.69
1:A:401:VAL:HG12	1:A:402:VAL:N	2.06	0.69
2:C:80:THR:HG22	2:C:81:GLN:H	1.57	0.69
1:B:546:ILE:HD12	1:B:546:ILE:H	1.58	0.69
1:A:180:LEU:HD23	1:A:180:LEU:O	1.93	0.69
2:C:43:LEU:HD11	2:C:82:ILE:HD11	1.75	0.69
1:B:450:MET:HG2	1:B:452:PHE:CE1	2.28	0.69
1:A:108:ALA:HB3	1:A:128:ARG:HG2	1.74	0.68
2:C:188:LYS:HD3	2:C:366:GLN:OE1	1.94	0.68
1:B:401:VAL:HG12	1:B:402:VAL:N	2.07	0.68
1:A:546:ILE:H	1:A:546:ILE:HD12	1.57	0.67
1:A:113:ILE:HD12	1:A:113:ILE:N	2.09	0.67
1:A:130:MET:CE	1:A:176:ALA:HA	2.24	0.67
1:A:320:LEU:HD11	1:A:415:VAL:HG21	1.76	0.67
2:D:289:VAL:HG23	2:D:293:GLN:HE21	1.59	0.67
2:C:289:VAL:HG23	2:C:293:GLN:HE21	1.59	0.67
2:D:55:GLU:HG3	2:D:114:GLY:HA2	1.77	0.67
2:C:54:VAL:HG21	2:C:82:ILE:HD12	1.76	0.67
1:B:320:LEU:HD11	1:B:415:VAL:HG21	1.77	0.67
1:B:199:LEU:HD11	1:B:203:LYS:HE3	1.76	0.66
2:D:152:GLY:HA3	2:D:230:PHE:CD2	2.30	0.66
2:D:348:PRO:HB2	2:D:351:CYS:HB3	1.77	0.66
2:D:98:SER:HB3	2:D:353:GLY:CA	2.26	0.66
1:A:113:ILE:HD12	1:A:113:ILE:H	1.61	0.66
2:C:255:MET:HE3	2:C:259:ARG:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HG21	1:B:271:LEU:HD23	1.77	0.65
1:B:108:ALA:HB3	1:B:128:ARG:HG2	1.77	0.65
1:B:539:TYR:O	1:B:543:VAL:HG23	1.96	0.65
2:D:54:VAL:HG21	2:D:82:ILE:HD12	1.79	0.65
2:C:89:GLN:HB3	2:D:93:ARG:NH1	2.11	0.65
1:B:325:MET:CE	1:B:428:ASN:HD21	2.08	0.65
2:D:21:SER:HA	2:D:247:ASP:OD2	1.96	0.65
1:A:56:VAL:HB	1:A:106:THR:HG22	1.77	0.65
1:A:546:ILE:N	1:A:546:ILE:HD12	2.11	0.65
1:B:180:LEU:HD23	1:B:180:LEU:O	1.96	0.65
1:B:502:ARG:NH1	1:B:647:ILE:HG12	2.12	0.64
1:B:706:MET:HB2	1:B:711:GLN:HB2	1.80	0.64
2:D:98:SER:HB2	2:D:350:GLY:O	1.98	0.64
2:C:35:SER:O	2:C:39:ILE:HG13	1.97	0.64
2:C:63:ASN:HB3	2:C:128:VAL:HG11	1.80	0.64
1:B:300:LEU:HD11	1:B:656:MET:HG3	1.80	0.64
2:D:46:ASN:O	2:D:49:VAL:HG22	1.96	0.64
2:C:9:VAL:HG13	2:C:267:PRO:HB3	1.80	0.63
1:A:424:ILE:HD12	1:A:424:ILE:N	2.13	0.63
1:B:113:ILE:N	1:B:113:ILE:HD13	2.14	0.63
1:B:303:LYS:HE3	1:B:650:THR:HG21	1.80	0.63
1:A:592:TYR:HA	1:A:601:LYS:O	1.99	0.63
2:D:9:VAL:HG13	2:D:267:PRO:HB3	1.80	0.63
1:B:525:ASP:CB	1:B:536:GLY:HA3	2.22	0.62
1:B:631:MET:O	1:B:634:PRO:HD2	1.99	0.62
1:B:622:VAL:CG2	1:B:626:ASP:HB2	2.29	0.62
1:B:285:SER:O	1:B:289:CYS:HB2	1.98	0.62
2:C:246:THR:OG1	2:C:346:GLY:HA3	1.98	0.62
1:A:633:ILE:HB	1:A:634:PRO:HD3	1.80	0.62
1:A:525:ASP:CB	1:A:536:GLY:HA3	2.20	0.62
2:C:348:PRO:HB2	2:C:351:CYS:HB3	1.82	0.62
1:A:706:MET:HB2	1:A:711:GLN:HB2	1.80	0.62
1:A:189:VAL:HG21	1:A:194:LEU:HA	1.82	0.62
2:C:87:ALA:HB1	2:D:93:ARG:HH21	1.64	0.61
1:B:424:ILE:HD12	1:B:424:ILE:N	2.14	0.61
2:C:58:ILE:HD12	2:C:105:ALA:HB2	1.81	0.61
2:D:188:LYS:HD2	2:D:366:GLN:OE1	2.01	0.61
2:C:18:MET:HB3	2:C:246:THR:HG21	1.81	0.61
2:D:296:LEU:HD21	2:D:306:ILE:HD11	1.82	0.61
1:A:465:ILE:N	1:A:465:ILE:HD12	2.15	0.61
1:B:56:VAL:HB	1:B:106:THR:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:SER:O	2:D:39:ILE:HG13	2.00	0.61
2:C:152:GLY:HA3	2:C:230:PHE:CE2	2.36	0.61
1:A:40:LEU:HD23	1:A:40:LEU:O	2.01	0.61
1:B:288:ASN:N	1:B:288:ASN:HD22	1.97	0.61
2:C:265:LEU:HD23	2:C:265:LEU:N	2.16	0.61
2:D:18:MET:HB3	2:D:246:THR:HG21	1.83	0.61
1:A:546:ILE:H	1:A:546:ILE:CD1	2.13	0.61
1:B:546:ILE:N	1:B:546:ILE:HD12	2.16	0.60
2:D:58:ILE:HD12	2:D:105:ALA:HB2	1.83	0.60
2:C:21:SER:HA	2:C:247:ASP:OD2	2.01	0.60
1:A:82:ASP:O	1:A:86:ILE:HG13	2.01	0.60
2:C:174:VAL:HG22	2:C:218:THR:HG22	1.81	0.60
1:A:537:PRO:HG2	1:A:631:MET:CE	2.32	0.60
1:B:155:LEU:HB3	1:B:156:PRO:HD3	1.84	0.60
1:A:465:ILE:HG12	1:A:498:PHE:CE2	2.37	0.60
1:B:622:VAL:HG23	1:B:626:ASP:HB2	1.84	0.60
1:B:673:ARG:HB2	1:B:673:ARG:NH1	2.17	0.60
2:D:62:VAL:HG21	2:D:349:PHE:HB3	1.83	0.60
1:A:285:SER:O	1:A:289:CYS:HB2	2.01	0.60
1:A:40:LEU:HD23	1:A:44:VAL:HG23	1.84	0.60
2:D:175:ARG:NE	2:D:179:LEU:HD12	2.16	0.60
1:B:22:PHE:CD2	1:B:66:ILE:HD11	2.37	0.59
1:B:105:PRO:HG3	1:B:212:TYR:CD2	2.37	0.59
1:A:680:VAL:O	1:A:684:VAL:HG23	2.01	0.59
1:A:97:SER:HB3	1:A:267:ARG:NH1	2.18	0.59
1:B:40:LEU:HD23	1:B:44:VAL:HG23	1.84	0.59
2:C:315:PHE:O	2:C:318:GLN:HG3	2.02	0.59
2:C:20:ARG:O	2:C:24:GLY:HA3	2.02	0.59
2:D:246:THR:OG1	2:D:346:GLY:HA3	2.02	0.59
1:A:622:VAL:CG2	1:A:626:ASP:HB2	2.33	0.59
2:D:255:MET:HE3	2:D:259:ARG:HG3	1.85	0.59
1:B:465:ILE:HG12	1:B:498:PHE:CE2	2.38	0.59
2:C:93:ARG:HH21	2:D:87:ALA:HB1	1.66	0.58
1:B:40:LEU:O	1:B:40:LEU:HD23	2.02	0.58
2:C:106:ALA:O	2:C:110:MET:HG3	2.03	0.58
1:B:668:ARG:HH11	1:B:668:ARG:HG2	1.67	0.58
2:D:313:GLU:CD	2:D:341:GLY:HA3	2.23	0.58
2:C:62:VAL:HG21	2:C:349:PHE:HB3	1.84	0.58
2:C:30:ARG:HB2	2:C:33:ASP:OD2	2.03	0.58
2:C:98:SER:HB2	2:C:350:GLY:O	2.04	0.58
1:A:101:ASP:CG	1:A:267:ARG:HH22	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:OG1	1:A:484:LYS:HE3	2.03	0.58
1:A:361:LEU:HB3	1:A:375:MET:HG3	1.86	0.58
1:B:399:GLU:HG2	1:B:401:VAL:HG23	1.84	0.58
1:A:55:GLY:HA2	1:A:104:VAL:HG13	1.84	0.57
2:D:63:ASN:HB3	2:D:128:VAL:HG11	1.86	0.57
2:D:265:LEU:N	2:D:265:LEU:HD23	2.19	0.57
1:B:249:TYR:OH	1:B:666:LEU:HB2	2.04	0.57
2:D:329:LEU:O	2:D:329:LEU:HD23	2.04	0.57
1:A:631:MET:O	1:A:634:PRO:HD2	2.05	0.57
1:B:465:ILE:HD12	1:B:465:ILE:N	2.20	0.57
1:B:338:THR:OG1	1:B:484:LYS:HE3	2.04	0.57
1:B:649:GLU:HB3	1:B:653:GLU:OE1	2.05	0.57
1:B:461:LEU:HD12	1:B:462:VAL:H	1.69	0.57
1:A:673:ARG:NH1	1:A:673:ARG:HB2	2.20	0.57
1:B:645:ASP:HB2	1:B:647:ILE:HD13	1.86	0.57
1:B:537:PRO:HG2	1:B:631:MET:CE	2.35	0.57
2:D:38:LEU:O	2:D:42:VAL:HG23	2.05	0.57
1:A:399:GLU:HG2	1:A:401:VAL:HG23	1.87	0.56
2:C:98:SER:HB3	2:C:353:GLY:CA	2.32	0.56
2:C:152:GLY:HA3	2:C:230:PHE:CD2	2.39	0.56
1:B:465:ILE:HG12	1:B:498:PHE:CZ	2.40	0.56
2:D:359:THR:O	2:D:363:VAL:HG23	2.05	0.56
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.85	0.56
1:A:704:ARG:O	1:A:708:LYS:HG3	2.05	0.56
1:B:140:GLU:HB2	1:B:146:TYR:HA	1.86	0.56
1:B:99:PHE:HA	1:B:102:LEU:HD13	1.86	0.56
2:C:61:CYS:SG	2:C:68:GLN:HB3	2.46	0.56
1:B:684:VAL:HG22	1:B:703:LEU:HD22	1.88	0.56
2:D:10:ILE:HD12	2:D:10:ILE:N	2.19	0.56
2:D:33:ASP:O	2:D:37:HIS:HB2	2.06	0.56
2:D:17:PRO:HB2	2:D:25:MET:CE	2.35	0.56
2:D:320:LEU:HB2	2:D:321:PRO:HD3	1.86	0.56
2:C:38:LEU:O	2:C:42:VAL:HG23	2.04	0.56
1:A:146:TYR:HB2	1:A:147:PRO:HD2	1.87	0.56
2:C:125:MET:HE3	2:C:246:THR:N	2.20	0.56
2:D:80:THR:HG22	2:D:81:GLN:N	2.20	0.56
1:A:523:ARG:O	1:A:527:VAL:HG23	2.06	0.56
1:B:569:ARG:O	1:B:615:ILE:HD12	2.06	0.56
1:A:288:ASN:N	1:A:288:ASN:HD22	2.04	0.56
1:B:107:VAL:HG22	1:B:127:PHE:HB2	1.88	0.55
2:C:360:LEU:HG	2:C:364:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:LEU:HD23	2:D:364:MET:HE3	1.87	0.55
2:D:93:ARG:HD2	2:D:100:SER:OG	2.06	0.55
1:B:502:ARG:HA	1:B:556:MET:CE	2.36	0.55
2:C:17:PRO:HB3	2:C:210:TYR:O	2.06	0.55
2:C:320:LEU:HB2	2:C:321:PRO:HD3	1.87	0.55
2:D:17:PRO:HB3	2:D:210:TYR:O	2.07	0.55
1:A:712:SER:OG	1:A:715:GLY:HA3	2.07	0.55
1:A:676:ASP:OD2	1:A:712:SER:HB2	2.07	0.55
2:D:125:MET:HE3	2:D:246:THR:N	2.21	0.55
1:B:180:LEU:HD12	1:B:188:VAL:HG23	1.88	0.55
1:B:40:LEU:O	1:B:44:VAL:HG23	2.07	0.55
2:C:181:HIS:O	2:C:185:VAL:HG23	2.07	0.55
2:C:52:GLY:HA2	2:C:83:PRO:HG2	1.87	0.55
1:A:686:LEU:HD23	1:A:686:LEU:O	2.06	0.55
1:A:502:ARG:NH1	1:A:647:ILE:HG12	2.22	0.55
1:A:401:VAL:CG1	1:A:402:VAL:H	2.19	0.55
1:B:546:ILE:H	1:B:546:ILE:CD1	2.19	0.55
2:C:67:GLU:OE2	2:C:127:HIS:HB3	2.07	0.55
2:D:67:GLU:OE2	2:D:127:HIS:HB3	2.07	0.55
1:B:680:VAL:O	1:B:684:VAL:HG23	2.07	0.55
1:B:101:ASP:CG	1:B:267:ARG:HH22	2.10	0.55
1:A:525:ASP:OD2	1:A:538:ALA:HB3	2.07	0.54
2:D:286:TYR:O	2:D:289:VAL:HG13	2.06	0.54
1:A:547:ASP:OD2	1:A:584:LYS:HD2	2.08	0.54
1:B:66:ILE:O	1:B:118:GLY:HA3	2.07	0.54
2:C:313:GLU:CD	2:C:341:GLY:HA3	2.26	0.54
1:B:347:GLU:O	1:B:351:GLU:HG2	2.08	0.54
1:B:464:VAL:HG21	1:B:479:VAL:HG22	1.89	0.54
1:A:130:MET:HE1	1:A:179:ALA:HB3	1.90	0.54
2:C:30:ARG:NH1	2:C:32:GLU:OE1	2.41	0.54
1:B:140:GLU:HG3	1:B:147:PRO:N	2.22	0.54
1:B:504:LEU:HG	1:B:662:ILE:HD11	1.90	0.54
1:B:130:MET:HE1	1:B:179:ALA:HB3	1.89	0.54
2:D:59:TRP:CZ3	2:D:120:GLY:HA3	2.42	0.54
2:C:10:ILE:HD12	2:C:10:ILE:N	2.23	0.54
2:C:255:MET:HE1	2:C:260:ALA:HA	1.88	0.54
1:A:140:GLU:HB2	1:A:146:TYR:HA	1.89	0.54
1:A:520:ASP:O	1:A:524:ILE:HG13	2.07	0.54
1:A:66:ILE:O	1:A:118:GLY:HA3	2.08	0.54
2:D:165:SER:OG	2:D:168:GLN:HG3	2.07	0.54
1:A:40:LEU:O	1:A:44:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:ASP:O	2:C:37:HIS:HB2	2.06	0.54
1:B:623:THR:O	1:B:627:ILE:HG13	2.08	0.54
2:D:20:ARG:O	2:D:24:GLY:HA3	2.06	0.54
1:A:668:ARG:HG2	1:A:668:ARG:HH11	1.72	0.54
1:B:525:ASP:OD2	1:B:538:ALA:HB3	2.07	0.54
1:A:490:ILE:HD12	1:A:657:GLY:HA2	1.90	0.54
1:A:300:LEU:HD11	1:A:656:MET:HG3	1.89	0.54
1:B:686:LEU:HD23	1:B:686:LEU:O	2.07	0.53
2:D:181:HIS:O	2:D:185:VAL:HG23	2.08	0.53
2:D:246:THR:HB	2:D:348:PRO:HG3	1.90	0.53
2:C:246:THR:HB	2:C:348:PRO:HG3	1.90	0.53
1:B:146:TYR:HB2	1:B:147:PRO:HD2	1.90	0.53
1:A:22:PHE:CD2	1:A:66:ILE:HD11	2.44	0.53
2:D:58:ILE:HB	2:D:119:VAL:HG12	1.91	0.53
2:D:106:ALA:O	2:D:110:MET:HG3	2.09	0.53
1:B:31:LYS:HB2	1:B:69:ALA:HA	1.91	0.53
1:B:13:LEU:HD11	1:B:19:GLU:HB2	1.91	0.53
1:B:55:GLY:HA2	1:B:104:VAL:HG13	1.89	0.53
2:D:318:GLN:O	2:D:322:VAL:HG23	2.08	0.53
1:B:523:ARG:NH2	1:B:627:ILE:HD11	2.24	0.53
2:C:359:THR:O	2:C:363:VAL:HG23	2.09	0.53
1:B:535:MET:SD	1:B:543:VAL:HG21	2.49	0.53
1:B:658:LEU:O	1:B:662:ILE:HG22	2.09	0.53
1:A:506:PRO:HG3	1:A:564:MET:CE	2.39	0.53
1:A:537:PRO:HG2	1:A:631:MET:HE2	1.90	0.52
1:A:412:LEU:HB3	1:A:441:LEU:HD21	1.91	0.52
1:B:343:LYS:HD3	1:B:344:ASP:H	1.73	0.52
1:A:611:VAL:O	1:A:614:PRO:HD2	2.09	0.52
1:A:539:TYR:O	1:A:543:VAL:HG23	2.09	0.52
1:A:465:ILE:HA	1:A:492:VAL:O	2.09	0.52
2:C:93:ARG:HD2	2:C:100:SER:OG	2.10	0.52
1:A:194:LEU:O	1:A:194:LEU:HD23	2.10	0.52
2:C:58:ILE:HB	2:C:119:VAL:HG12	1.92	0.52
1:A:280:LYS:HB2	1:A:280:LYS:NZ	2.25	0.52
1:A:622:VAL:HG23	1:A:626:ASP:HB2	1.91	0.52
1:B:465:ILE:HA	1:B:492:VAL:O	2.09	0.52
2:D:52:GLY:HA2	2:D:83:PRO:HG2	1.90	0.52
1:B:401:VAL:CG1	1:B:402:VAL:H	2.19	0.52
2:C:122:VAL:HG22	2:C:123:GLU:N	2.25	0.52
2:C:286:TYR:CE1	2:C:289:VAL:HG11	2.45	0.52
2:D:315:PHE:O	2:D:318:GLN:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PRO:HB3	1:A:151:GLY:HA3	1.92	0.52
1:B:72:THR:O	1:B:76:GLU:HG3	2.09	0.52
2:C:59:TRP:HE1	2:C:122:VAL:HB	1.75	0.51
1:A:180:LEU:HD12	1:A:188:VAL:HG23	1.93	0.51
1:B:147:PRO:HB3	1:B:151:GLY:HA3	1.92	0.51
2:C:292:THR:HG23	2:C:373:LEU:HD21	1.92	0.51
1:B:189:VAL:HG21	1:B:194:LEU:HA	1.92	0.51
2:C:252:MET:CE	2:C:354:ALA:HB1	2.40	0.51
1:B:633:ILE:HB	1:B:634:PRO:HD3	1.90	0.51
2:D:175:ARG:HE	2:D:179:LEU:HD12	1.75	0.51
2:C:360:LEU:HG	2:C:364:MET:CE	2.39	0.51
1:A:571:ALA:HB1	1:A:612:LEU:HD22	1.93	0.51
1:B:391:PHE:HA	1:B:394:VAL:HG23	1.91	0.51
2:D:286:TYR:CZ	2:D:289:VAL:HG11	2.46	0.51
1:A:317:ALA:O	1:A:340:ILE:HA	2.10	0.51
2:D:228:PRO:HB3	2:D:235:GLY:HA3	1.92	0.51
1:B:312:LYS:O	1:B:477:THR:HG23	2.10	0.51
2:D:125:MET:HE3	2:D:246:THR:H	1.76	0.51
1:A:684:VAL:HG22	1:A:703:LEU:HD22	1.92	0.51
1:A:613:LYS:HB3	1:A:614:PRO:HD3	1.91	0.51
1:A:568:ARG:HD2	1:A:617:TYR:CE1	2.46	0.51
1:B:57:ILE:HG12	1:B:202:ILE:HG13	1.91	0.51
1:A:32:PHE:CE1	1:A:66:ILE:HG21	2.45	0.51
2:D:174:VAL:HG22	2:D:218:THR:HG22	1.93	0.51
2:C:318:GLN:C	2:C:321:PRO:HD2	2.31	0.51
1:B:448:VAL:HG12	1:B:470:SER:HB3	1.92	0.51
1:B:113:ILE:HD13	1:B:113:ILE:H	1.74	0.51
1:A:465:ILE:HG12	1:A:498:PHE:CZ	2.46	0.51
2:C:312:ASN:HB2	2:C:356:ILE:HD13	1.93	0.51
1:B:568:ARG:HD2	1:B:617:TYR:CE1	2.46	0.51
1:A:391:PHE:HA	1:A:394:VAL:HG23	1.93	0.51
1:A:99:PHE:HA	1:A:102:LEU:HD13	1.93	0.51
1:A:374:LYS:O	1:A:378:VAL:HG23	2.11	0.51
1:B:502:ARG:HA	1:B:556:MET:HE1	1.93	0.51
1:B:708:LYS:C	1:B:710:GLY:H	2.13	0.51
1:A:504:LEU:O	1:A:507:TYR:HB3	2.11	0.50
1:A:436:LEU:HD23	1:A:436:LEU:O	2.11	0.50
2:C:80:THR:HG22	2:C:81:GLN:N	2.24	0.50
1:B:237:ALA:O	1:B:241:VAL:HG23	2.10	0.50
1:A:72:THR:O	1:A:76:GLU:HG3	2.11	0.50
1:A:461:LEU:HD12	1:A:462:VAL:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:HIS:HB3	1:B:463:GLU:HB2	1.93	0.50
1:A:643:LEU:O	1:A:643:LEU:HD23	2.12	0.50
2:C:93:ARG:NH1	2:D:89:GLN:HB3	2.26	0.50
2:C:310:GLU:OE2	2:C:337:ASN:HA	2.12	0.50
2:D:192:GLU:HB3	2:D:362:ASN:ND2	2.27	0.50
1:A:194:LEU:C	1:A:194:LEU:HD23	2.32	0.50
1:A:13:LEU:HD11	1:A:19:GLU:HB2	1.93	0.50
2:C:171:ALA:HA	2:C:220:LEU:HD21	1.92	0.50
1:B:105:PRO:HG3	1:B:212:TYR:CE2	2.47	0.50
1:B:479:VAL:HG13	1:B:489:PRO:CG	2.42	0.50
1:A:57:ILE:HG12	1:A:202:ILE:HG13	1.93	0.50
2:D:169:GLN:HB3	2:D:241:THR:HG21	1.94	0.50
1:A:645:ASP:HB2	1:A:647:ILE:HD13	1.93	0.50
1:B:194:LEU:HD23	1:B:194:LEU:O	2.12	0.50
1:B:547:ASP:HB3	1:B:581:LEU:HD22	1.94	0.49
1:A:199:LEU:CD1	1:A:203:LYS:HE3	2.42	0.49
1:A:647:ILE:HG22	1:A:648:VAL:HG23	1.94	0.49
1:B:154:ARG:HD3	1:B:219:LYS:HD2	1.93	0.49
1:B:622:VAL:HG22	1:B:623:THR:O	2.12	0.49
2:D:255:MET:HE1	2:D:260:ALA:HA	1.94	0.49
1:B:643:LEU:O	1:B:643:LEU:HD23	2.12	0.49
1:B:350:ILE:HD11	1:B:385:THR:O	2.13	0.49
1:B:504:LEU:O	1:B:507:TYR:HB3	2.12	0.49
2:C:129:SER:OG	2:C:132:HIS:HB2	2.13	0.49
1:B:358:ALA:O	1:B:362:VAL:HG23	2.12	0.49
2:C:200:ASP:OD2	2:C:204:PHE:HB2	2.12	0.49
2:C:105:ALA:O	2:C:108:ALA:HB3	2.13	0.49
1:A:636:CYS:O	1:A:640:VAL:HG23	2.12	0.49
2:C:175:ARG:NE	2:C:179:LEU:HD12	2.27	0.49
2:C:99:MET:HB3	2:C:384:ILE:HD13	1.95	0.49
1:A:217:GLN:HB3	1:A:218:PRO:HD3	1.94	0.49
2:D:122:VAL:HG22	2:D:123:GLU:N	2.28	0.49
2:C:185:VAL:C	2:C:187:GLY:H	2.16	0.49
1:B:668:ARG:NH1	1:B:668:ARG:HG2	2.28	0.49
1:A:623:THR:O	1:A:627:ILE:HG13	2.13	0.49
1:A:7:ALA:HA	1:A:24:LEU:HA	1.95	0.49
1:A:448:VAL:HG21	1:A:478:THR:OG1	2.13	0.49
1:A:325:MET:O	1:A:329:ILE:HG13	2.13	0.49
2:C:125:MET:HE3	2:C:246:THR:H	1.76	0.48
1:B:361:LEU:HB3	1:B:375:MET:HG3	1.94	0.48
1:B:345:ILE:HG13	1:B:346:ASN:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:ASN:HB2	2:D:356:ILE:HD13	1.95	0.48
1:B:82:ASP:O	1:B:86:ILE:HG13	2.13	0.48
1:B:700:THR:OG1	1:B:703:LEU:HB2	2.13	0.48
1:B:248:ASN:O	1:B:250:PRO:HD3	2.13	0.48
1:A:312:LYS:O	1:A:477:THR:HG23	2.13	0.48
2:C:348:PRO:O	2:C:349:PHE:C	2.51	0.48
1:A:303:LYS:HE3	1:A:650:THR:HG21	1.94	0.48
1:A:451:HIS:HB3	1:A:463:GLU:HB2	1.95	0.48
1:A:105:PRO:HG3	1:A:212:TYR:CD2	2.48	0.48
1:B:436:LEU:HD23	1:B:436:LEU:O	2.13	0.48
2:C:286:TYR:O	2:C:289:VAL:HG13	2.12	0.48
1:A:130:MET:HE1	1:A:179:ALA:CB	2.43	0.48
1:B:271:LEU:O	1:B:274:GLU:HB3	2.14	0.48
1:B:520:ASP:O	1:B:524:ILE:HG13	2.13	0.48
2:D:348:PRO:O	2:D:349:PHE:C	2.51	0.48
1:A:401:VAL:CG1	1:A:402:VAL:N	2.76	0.48
1:B:652:ALA:O	1:B:656:MET:HG2	2.13	0.48
2:D:302:ASN:O	2:D:304:ALA:N	2.46	0.48
1:A:350:ILE:HD11	1:A:385:THR:O	2.14	0.48
1:B:288:ASN:N	1:B:288:ASN:ND2	2.60	0.48
1:A:605:ASP:OD2	1:A:607:SER:OG	2.32	0.48
1:B:388:TYR:HE2	1:B:415:VAL:HG22	1.78	0.48
2:C:302:ASN:O	2:C:304:ALA:N	2.47	0.48
2:D:370:THR:O	2:D:389:GLU:HA	2.13	0.48
2:D:123:GLU:HG2	2:D:349:PHE:HB2	1.95	0.48
2:C:286:TYR:CZ	2:C:289:VAL:HG11	2.49	0.48
1:A:78:PHE:CD1	1:A:282:ALA:HB1	2.48	0.48
2:D:171:ALA:HA	2:D:220:LEU:HD21	1.94	0.48
1:B:374:LYS:O	1:B:378:VAL:HG23	2.13	0.48
1:B:114:ALA:HB3	1:B:136:ILE:HG22	1.96	0.48
1:A:271:LEU:O	1:A:274:GLU:HB3	2.14	0.48
2:C:8:VAL:HG11	2:C:271:ILE:HD12	1.96	0.48
1:B:285:SER:HA	1:B:288:ASN:HD21	1.79	0.48
1:B:448:VAL:HG21	1:B:478:THR:OG1	2.13	0.48
2:D:129:SER:OG	2:D:132:HIS:HB2	2.14	0.48
1:B:393:ASN:C	1:B:393:ASN:HD22	2.17	0.47
1:B:20:LEU:HD23	1:B:20:LEU:C	2.35	0.47
2:C:370:THR:O	2:C:389:GLU:HA	2.14	0.47
2:D:59:TRP:HE1	2:D:122:VAL:HB	1.79	0.47
2:C:289:VAL:O	2:C:293:GLN:HG3	2.14	0.47
2:D:114:GLY:HA3	2:D:117:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:CD1	1:B:203:LYS:HE3	2.43	0.47
2:C:25:MET:HG2	2:C:212:GLU:OE1	2.13	0.47
1:B:317:ALA:O	1:B:340:ILE:HA	2.14	0.47
2:C:169:GLN:HB3	2:C:241:THR:HG21	1.95	0.47
2:C:30:ARG:NH1	2:C:67:GLU:HG2	2.30	0.47
1:B:412:LEU:HB3	1:B:441:LEU:HD21	1.96	0.47
1:B:438:ALA:HB2	1:B:447:PHE:HD2	1.79	0.47
1:B:401:VAL:CG1	1:B:402:VAL:N	2.77	0.47
2:D:125:MET:CE	2:D:246:THR:H	2.27	0.47
2:D:318:GLN:C	2:D:321:PRO:HD2	2.35	0.47
1:A:146:TYR:HB2	1:A:147:PRO:CD	2.45	0.47
2:D:30:ARG:NH1	2:D:67:GLU:HG2	2.29	0.47
1:B:532:GLY:C	1:B:665:PRO:HG3	2.34	0.47
2:C:165:SER:OG	2:C:168:GLN:HG3	2.15	0.47
1:B:636:CYS:O	1:B:640:VAL:HG23	2.15	0.47
2:D:286:TYR:CE1	2:D:289:VAL:HG11	2.50	0.47
1:A:504:LEU:HG	1:A:662:ILE:HD11	1.95	0.47
1:A:658:LEU:O	1:A:662:ILE:HG22	2.14	0.47
1:B:523:ARG:O	1:B:527:VAL:HG23	2.15	0.47
2:C:361:LEU:HA	2:C:364:MET:HE2	1.96	0.47
1:B:434:ILE:HG23	1:B:447:PHE:CE2	2.49	0.47
1:A:453:PHE:HB2	1:A:459:MET:HG3	1.96	0.47
1:B:655:ASP:O	1:B:659:VAL:HG23	2.14	0.47
2:D:10:ILE:HD11	2:D:271:ILE:HG13	1.96	0.47
2:D:30:ARG:NH1	2:D:32:GLU:OE1	2.47	0.47
1:A:546:ILE:N	1:A:546:ILE:CD1	2.76	0.47
1:B:684:VAL:CG2	1:B:703:LEU:HD22	2.45	0.47
2:C:17:PRO:HB2	2:C:25:MET:CE	2.45	0.47
1:B:618:GLU:CD	1:B:618:GLU:H	2.18	0.47
2:C:175:ARG:HE	2:C:179:LEU:HD12	1.79	0.47
1:B:638:GLU:HA	1:B:641:ARG:HH11	1.78	0.47
1:B:704:ARG:HG2	1:B:704:ARG:HH11	1.80	0.47
1:A:700:THR:OG1	1:A:703:LEU:HB2	2.15	0.47
2:C:318:GLN:O	2:C:321:PRO:HD2	2.14	0.47
2:D:361:LEU:HD23	2:D:364:MET:CE	2.45	0.47
1:B:528:MET:O	1:B:531:PHE:HB3	2.14	0.47
1:B:23:ASP:OD2	1:B:62:LYS:HE2	2.14	0.47
1:B:537:PRO:HG2	1:B:631:MET:HE2	1.96	0.47
1:A:434:ILE:HG23	1:A:447:PHE:CE2	2.50	0.47
1:B:303:LYS:HE3	1:B:650:THR:CG2	2.45	0.47
2:D:174:VAL:HG13	2:D:218:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLN:O	1:B:355:ALA:HB3	2.15	0.46
1:B:119:LEU:O	1:B:119:LEU:HD23	2.15	0.46
2:C:303:MET:HE3	2:C:306:ILE:HD12	1.97	0.46
2:D:311:LEU:HD13	2:D:375:THR:HG23	1.98	0.46
1:A:664:PHE:CD2	1:A:670:GLY:HA2	2.50	0.46
2:C:318:GLN:O	2:C:322:VAL:HG23	2.15	0.46
2:D:310:GLU:HG3	2:D:360:LEU:HB2	1.98	0.46
1:B:7:ALA:HA	1:B:24:LEU:HA	1.96	0.46
1:A:544:VAL:HG21	4:A:1002:ACO:HH32	1.97	0.46
1:A:140:GLU:HG3	1:A:147:PRO:N	2.31	0.46
1:B:617:TYR:HB3	1:B:618:GLU:OE2	2.15	0.46
1:A:100:GLU:O	1:A:216:ARG:HD3	2.16	0.46
2:C:19:GLY:O	2:C:246:THR:HG23	2.14	0.46
1:A:504:LEU:HD23	1:A:504:LEU:O	2.15	0.46
1:A:332:GLN:OE1	1:A:457:HIS:HA	2.16	0.46
1:B:571:ALA:HB1	1:B:612:LEU:HD22	1.98	0.46
2:C:255:MET:HE3	2:C:259:ARG:CG	2.46	0.46
1:B:642:CYS:O	1:B:647:ILE:HB	2.16	0.46
2:D:105:ALA:O	2:D:108:ALA:HB3	2.15	0.46
1:B:575:LEU:HD22	1:B:580:ARG:HD3	1.98	0.46
1:B:445:GLU:H	1:B:445:GLU:CD	2.19	0.46
1:A:114:ALA:HB3	1:A:136:ILE:HG22	1.97	0.46
1:B:217:GLN:HB3	1:B:218:PRO:HD3	1.98	0.46
2:C:361:LEU:HD23	2:C:364:MET:HE3	1.96	0.46
2:D:59:TRP:O	2:D:90:THR:HA	2.16	0.46
2:C:63:ASN:HB3	2:C:128:VAL:CG1	2.43	0.46
1:B:162:ASP:HB2	2:D:141:SER:HB3	1.98	0.46
1:A:119:LEU:HD23	1:A:119:LEU:O	2.15	0.46
1:B:647:ILE:HG22	1:B:648:VAL:HG23	1.97	0.46
2:C:252:MET:HE3	2:C:354:ALA:HB1	1.97	0.46
1:A:442:LYS:HG3	1:A:443:ARG:HG3	1.98	0.45
1:B:113:ILE:HG22	1:B:115:LEU:HG	1.97	0.45
1:B:580:ARG:CZ	1:B:608:VAL:HG22	2.46	0.45
2:C:199:TYR:CZ	2:C:205:LEU:HD13	2.51	0.45
1:B:490:ILE:HD12	1:B:657:GLY:HA2	1.97	0.45
2:D:62:VAL:CG2	2:D:349:PHE:HB3	2.46	0.45
1:A:180:LEU:C	1:A:180:LEU:HD23	2.36	0.45
1:A:354:LEU:HD22	1:B:380:ASN:OD1	2.15	0.45
1:A:141:VAL:HA	1:A:145:ILE:O	2.16	0.45
2:C:59:TRP:CD1	2:C:122:VAL:HG12	2.52	0.45
1:B:325:MET:HG3	5:B:2001:NAD:O4D	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:ASP:O	2:D:174:VAL:HG23	2.17	0.45
2:C:107:GLN:HB3	2:D:107:GLN:HB3	1.99	0.45
1:A:197:ALA:HB2	2:D:204:PHE:CE1	2.52	0.45
2:C:378:ILE:HG22	2:C:379:GLY:N	2.32	0.45
1:B:128:ARG:HG3	1:B:128:ARG:HH11	1.82	0.45
2:D:25:MET:HE1	2:D:208:PHE:HB2	1.97	0.45
1:A:638:GLU:HA	1:A:641:ARG:HH11	1.81	0.45
1:B:459:MET:HA	1:B:460:PRO:HD3	1.74	0.45
1:B:350:ILE:CG2	1:B:384:PRO:HB3	2.45	0.45
1:A:502:ARG:HA	1:A:556:MET:CE	2.46	0.45
1:B:141:VAL:HA	1:B:145:ILE:O	2.16	0.45
2:C:166:ARG:HH11	2:C:166:ARG:HG2	1.82	0.45
2:C:288:PRO:HD3	2:C:377:CYS:HB3	1.99	0.45
1:B:664:PHE:CD2	1:B:670:GLY:HA2	2.51	0.45
1:A:443:ARG:N	1:A:444:PRO:HD3	2.32	0.45
1:A:107:VAL:HG23	1:A:202:ILE:CD1	2.47	0.45
1:A:432:ILE:HG21	1:A:437:LEU:HD21	1.98	0.45
1:B:639:THR:HG21	1:B:671:ALA:HB3	1.99	0.45
1:B:551:HIS:O	1:B:555:VAL:HG23	2.17	0.45
1:B:525:ASP:HB3	1:B:537:PRO:HD2	1.99	0.45
2:C:9:VAL:CG1	2:C:267:PRO:HB3	2.47	0.45
1:B:194:LEU:HD23	1:B:194:LEU:C	2.37	0.45
1:A:459:MET:HA	1:A:460:PRO:HD3	1.75	0.45
1:A:528:MET:O	1:A:531:PHE:HB3	2.17	0.45
2:C:49:VAL:HG23	2:C:49:VAL:O	2.17	0.45
2:C:93:ARG:NH2	2:D:87:ALA:HB1	2.32	0.45
1:B:146:TYR:HB2	1:B:147:PRO:CD	2.47	0.45
1:A:569:ARG:O	1:A:615:ILE:HD12	2.17	0.45
1:A:199:LEU:C	1:A:199:LEU:HD13	2.38	0.45
2:C:56:ASP:CG	2:D:93:ARG:HH22	2.21	0.45
2:C:322:VAL:HG12	2:C:326:LEU:HD12	1.99	0.45
2:D:17:PRO:HB2	2:D:25:MET:HE2	1.98	0.45
2:D:269:ALA:CB	2:D:361:LEU:HD22	2.47	0.45
1:B:605:ASP:OD2	1:B:607:SER:OG	2.34	0.45
2:C:114:GLY:HA3	2:C:117:PHE:CE1	2.52	0.44
1:B:100:GLU:O	1:B:216:ARG:HD3	2.16	0.44
2:D:151:MET:HE1	2:D:284:MET:SD	2.56	0.44
1:B:396:LEU:C	1:B:396:LEU:HD23	2.37	0.44
1:A:547:ASP:HB3	1:A:581:LEU:HD22	1.98	0.44
1:B:325:MET:O	1:B:329:ILE:HG13	2.17	0.44
1:B:105:PRO:HG3	1:B:212:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:VAL:C	2:D:187:GLY:H	2.19	0.44
1:A:442:LYS:C	1:A:444:PRO:HD3	2.38	0.44
1:A:113:ILE:CG2	1:A:115:LEU:HG	2.47	0.44
1:A:465:ILE:CD1	1:A:465:ILE:N	2.80	0.44
1:B:157:ARG:HD2	1:B:219:LYS:HA	1.99	0.44
1:A:107:VAL:HG22	1:A:127:PHE:HB2	1.98	0.44
2:C:379:GLY:O	2:C:380:LEU:HB2	2.18	0.44
2:D:378:ILE:HG22	2:D:379:GLY:N	2.32	0.44
1:B:180:LEU:C	1:B:180:LEU:HD23	2.37	0.44
2:D:175:ARG:HH11	2:D:175:ARG:HG3	1.81	0.44
1:A:448:VAL:HG12	1:A:470:SER:HB3	1.99	0.44
2:C:302:ASN:C	2:C:304:ALA:N	2.71	0.44
2:D:61:CYS:SG	2:D:68:GLN:HB3	2.57	0.44
2:C:164:ILE:N	2:C:164:ILE:HD12	2.33	0.44
1:B:364:ARG:HB3	1:B:370:MET:HB2	2.00	0.44
1:A:655:ASP:O	1:A:659:VAL:HG23	2.18	0.44
2:D:99:MET:HB3	2:D:384:ILE:HD13	1.99	0.44
1:A:581:LEU:HB2	1:A:585:ASN:CB	2.45	0.44
2:C:93:ARG:HH22	2:D:56:ASP:CG	2.21	0.44
1:B:611:VAL:O	1:B:614:PRO:HD2	2.17	0.44
2:D:289:VAL:CG1	2:D:290:PRO:HD3	2.38	0.44
2:D:348:PRO:O	2:D:351:CYS:N	2.43	0.44
1:A:649:GLU:HB3	1:A:653:GLU:OE1	2.18	0.44
1:B:56:VAL:HG23	1:B:104:VAL:HG11	2.00	0.44
1:B:22:PHE:CE2	1:B:66:ILE:HD11	2.53	0.44
1:A:153:VAL:HG21	1:A:271:LEU:HD23	2.00	0.44
1:B:442:LYS:C	1:B:444:PRO:HD3	2.38	0.44
2:D:51:PRO:HB3	2:D:82:ILE:HD13	2.00	0.44
2:C:155:ALA:HB2	2:C:315:PHE:CD2	2.53	0.44
2:C:310:GLU:HG3	2:C:360:LEU:HB2	2.00	0.44
1:B:11:THR:O	1:B:18:VAL:HG23	2.17	0.44
1:A:629:ASN:HB3	1:A:633:ILE:HD11	2.00	0.44
2:D:302:ASN:C	2:D:304:ALA:N	2.71	0.44
1:B:676:ASP:OD2	1:B:712:SER:HB2	2.17	0.44
1:B:633:ILE:HD11	1:B:686:LEU:HD22	2.00	0.43
1:B:199:LEU:HD13	1:B:199:LEU:C	2.38	0.43
2:D:310:GLU:OE2	2:D:337:ASN:HA	2.17	0.43
2:C:156:GLU:OE2	2:C:237:VAL:HG23	2.18	0.43
1:A:575:LEU:HD22	1:A:580:ARG:HD3	2.00	0.43
1:B:537:PRO:HG2	1:B:631:MET:HE3	1.99	0.43
1:A:424:ILE:HD12	1:A:424:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:VAL:HG12	2:D:326:LEU:HD12	2.00	0.43
2:D:218:THR:HG23	2:D:223:LEU:HD21	2.00	0.43
2:D:252:MET:CE	2:D:354:ALA:HB1	2.48	0.43
2:C:59:TRP:O	2:C:90:THR:HA	2.19	0.43
2:D:266:GLU:HA	2:D:267:PRO:HD3	1.88	0.43
2:C:64:GLN:HA	2:C:68:GLN:O	2.18	0.43
1:A:288:ASN:N	1:A:288:ASN:ND2	2.66	0.43
2:C:228:PRO:HB3	2:C:235:GLY:HA3	1.99	0.43
1:A:499:LEU:HD13	1:A:499:LEU:C	2.39	0.43
1:A:344:ASP:OD1	1:A:345:ILE:N	2.44	0.43
1:B:547:ASP:OD2	1:B:584:LYS:HD2	2.18	0.43
2:C:357:SER:O	2:C:361:LEU:HG	2.18	0.43
1:A:100:GLU:OE1	1:A:154:ARG:NE	2.40	0.43
1:A:162:ASP:HB2	2:C:141:SER:OG	2.19	0.43
2:D:289:VAL:O	2:D:293:GLN:HG3	2.19	0.43
2:C:62:VAL:CG2	2:C:349:PHE:HB3	2.46	0.43
1:B:461:LEU:HB2	1:B:660:TYR:HB3	2.00	0.43
2:D:13:PHE:CE2	2:D:358:GLY:HA3	2.53	0.43
1:B:367:LYS:C	1:B:369:ARG:H	2.22	0.43
1:B:235:GLU:OE2	1:B:235:GLU:HA	2.19	0.43
1:A:396:LEU:HD23	1:A:396:LEU:C	2.39	0.43
1:A:551:HIS:O	1:A:555:VAL:HG23	2.19	0.43
1:B:635:LEU:HD23	1:B:635:LEU:C	2.39	0.43
1:B:78:PHE:CD1	1:B:282:ALA:HB1	2.52	0.43
2:D:49:VAL:HG23	2:D:49:VAL:O	2.19	0.43
1:B:73:GLU:HA	1:B:76:GLU:OE1	2.19	0.43
2:C:84:HIS:O	2:D:278:GLY:HA3	2.19	0.43
1:A:618:GLU:H	1:A:618:GLU:CD	2.22	0.43
2:C:348:PRO:O	2:C:351:CYS:N	2.45	0.43
1:A:56:VAL:HG23	1:A:104:VAL:HG11	2.01	0.43
2:C:72:ILE:HG12	2:C:72:ILE:O	2.19	0.43
1:A:350:ILE:CG2	1:A:384:PRO:HB3	2.45	0.43
1:B:502:ARG:HA	1:B:556:MET:HE2	2.00	0.43
2:D:63:ASN:HB3	2:D:128:VAL:CG1	2.48	0.43
2:D:269:ALA:HB2	2:D:361:LEU:HD22	2.01	0.43
2:C:201:GLU:CD	2:C:201:GLU:H	2.22	0.43
1:B:712:SER:OG	1:B:715:GLY:HA3	2.19	0.42
1:A:130:MET:HG2	1:A:131:ALA:O	2.18	0.42
1:A:508:PHE:HZ	1:A:540:LEU:HD22	1.83	0.42
2:D:162:HIS:CD2	2:D:321:PRO:HB3	2.55	0.42
2:D:200:ASP:OD2	2:D:204:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLN:OE1	1:B:457:HIS:HA	2.19	0.42
1:B:540:LEU:HD23	1:B:544:VAL:HG23	2.01	0.42
1:B:373:ALA:O	1:B:376:ALA:HB3	2.19	0.42
1:B:504:LEU:HG	1:B:662:ILE:CD1	2.49	0.42
1:B:506:PRO:HG3	1:B:564:MET:CE	2.49	0.42
1:A:540:LEU:HD23	1:A:544:VAL:HG23	2.01	0.42
2:D:230:PHE:O	2:D:232:PRO:HD3	2.19	0.42
1:B:539:TYR:CD1	1:B:602:LYS:HD3	2.54	0.42
1:A:521:PHE:HA	1:A:524:ILE:HD12	2.01	0.42
1:A:668:ARG:HG2	1:A:668:ARG:NH1	2.34	0.42
1:B:162:ASP:HB2	2:D:141:SER:CB	2.49	0.42
2:C:278:GLY:O	2:D:85:THR:HA	2.18	0.42
2:D:287:GLY:N	2:D:288:PRO:CD	2.83	0.42
1:B:130:MET:HG2	1:B:131:ALA:O	2.18	0.42
2:C:123:GLU:HG2	2:C:349:PHE:HB2	2.01	0.42
2:D:318:GLN:O	2:D:321:PRO:HD2	2.19	0.42
2:C:25:MET:HE1	2:C:208:PHE:HB2	2.02	0.42
2:D:64:GLN:HA	2:D:68:GLN:O	2.19	0.42
1:A:20:LEU:C	1:A:20:LEU:HD23	2.39	0.42
2:D:4:ASN:N	2:D:7:ASP:OD2	2.51	0.42
1:B:466:ARG:HG3	1:B:470:SER:HB2	2.00	0.42
1:A:105:PRO:HG3	1:A:212:TYR:CG	2.54	0.42
1:B:258:THR:HG23	1:B:273:VAL:HG12	2.02	0.42
1:B:697:TYR:O	1:B:699:PRO:HD3	2.19	0.42
1:B:502:ARG:HH12	1:B:647:ILE:HG12	1.83	0.42
2:C:364:MET:HE1	2:C:372:GLY:HA3	2.02	0.42
1:B:453:PHE:HB2	1:B:459:MET:HG3	2.02	0.42
1:B:508:PHE:O	1:B:511:PHE:HB3	2.20	0.42
2:C:87:ALA:HB1	2:D:93:ARG:NH2	2.32	0.42
1:B:30:ASN:ND2	1:B:62:LYS:HG3	2.35	0.42
1:A:119:LEU:HD12	1:A:137:GLY:N	2.34	0.42
2:D:13:PHE:CD2	2:D:358:GLY:HA3	2.55	0.42
2:C:125:MET:CE	2:C:246:THR:H	2.32	0.42
1:B:673:ARG:HH11	1:B:673:ARG:CB	2.25	0.42
1:B:287:SER:O	1:B:291:ILE:HG13	2.20	0.42
1:A:55:GLY:HA2	1:A:104:VAL:CG1	2.47	0.42
1:B:17:ILE:HG22	1:B:18:VAL:N	2.34	0.42
2:D:354:ALA:O	2:D:358:GLY:N	2.51	0.42
1:A:336:LYS:HG3	1:A:485:MET:HA	2.02	0.42
2:D:294:LYS:HD3	2:D:298:ARG:NH2	2.34	0.42
1:A:318:ALA:HB3	1:A:397:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:GLY:HA3	2:D:84:HIS:O	2.18	0.42
1:B:432:ILE:HG21	1:B:437:LEU:HD21	2.02	0.42
1:A:479:VAL:HG13	1:A:489:PRO:CG	2.49	0.42
1:A:635:LEU:HD23	1:A:635:LEU:C	2.39	0.42
1:A:525:ASP:HB3	1:A:537:PRO:HD2	2.02	0.41
2:C:265:LEU:N	2:C:265:LEU:CD2	2.83	0.41
1:A:642:CYS:O	1:A:647:ILE:HB	2.20	0.41
1:B:97:SER:HB3	1:B:267:ARG:NH1	2.35	0.41
1:B:704:ARG:NH1	1:B:704:ARG:HG2	2.35	0.41
1:B:682:GLU:OE1	1:B:682:GLU:N	2.51	0.41
1:B:211:ASP:OD1	1:B:214:ALA:N	2.50	0.41
1:A:287:SER:C	1:A:289:CYS:H	2.23	0.41
2:C:56:ASP:OD1	2:D:93:ARG:NH2	2.53	0.41
2:D:268:LEU:O	2:D:269:ALA:HB2	2.20	0.41
1:A:643:LEU:C	1:A:643:LEU:HD23	2.41	0.41
1:B:119:LEU:HD12	1:B:137:GLY:N	2.34	0.41
1:B:90:LEU:O	1:B:94:LYS:HG3	2.20	0.41
2:D:72:ILE:O	2:D:72:ILE:HG12	2.19	0.41
2:D:15:ARG:NH2	2:D:193:ILE:HD11	2.35	0.41
1:A:287:SER:O	1:A:291:ILE:HG13	2.21	0.41
1:A:508:PHE:O	1:A:511:PHE:HB3	2.20	0.41
2:D:155:ALA:HB2	2:D:315:PHE:CD2	2.55	0.41
2:D:164:ILE:HD11	2:D:321:PRO:HG3	2.03	0.41
1:A:325:MET:HE2	1:A:428:ASN:HD21	1.85	0.41
2:C:162:HIS:O	2:C:164:ILE:HD12	2.20	0.41
1:A:358:ALA:O	1:A:359:LYS:C	2.58	0.41
2:D:288:PRO:HD3	2:D:377:CYS:HB3	2.01	0.41
1:B:581:LEU:HB2	1:B:585:ASN:CB	2.45	0.41
1:A:3:TYR:HB3	1:A:10:VAL:HB	2.01	0.41
1:B:233:ALA:HB2	2:D:145:ALA:CB	2.51	0.41
2:C:334:GLU:HG2	2:C:334:GLU:O	2.20	0.41
2:C:5:PRO:HA	2:C:258:GLN:HB2	2.02	0.41
1:A:248:ASN:O	1:A:250:PRO:HD3	2.20	0.41
2:C:10:ILE:HD11	2:C:271:ILE:HG13	2.03	0.41
1:A:669:GLY:HA3	1:A:673:ARG:HD2	2.02	0.41
1:A:320:LEU:HD13	1:A:411:VAL:CG1	2.51	0.41
2:C:268:LEU:O	2:C:269:ALA:HB2	2.20	0.41
1:A:445:GLU:CD	1:A:445:GLU:H	2.24	0.41
1:B:344:ASP:OD1	1:B:345:ILE:N	2.50	0.41
1:A:704:ARG:HH11	1:A:704:ARG:HG2	1.86	0.41
1:B:97:SER:O	1:B:100:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:HD3	1:A:219:LYS:HD2	2.02	0.41
1:A:349:GLY:O	1:A:352:GLN:HB2	2.19	0.41
1:A:535:MET:SD	1:A:543:VAL:HG21	2.60	0.41
1:B:617:TYR:CB	1:B:618:GLU:OE2	2.68	0.41
1:B:358:ALA:O	1:B:359:LYS:C	2.59	0.41
1:B:311:ALA:HB2	1:B:476:ALA:HB1	2.03	0.41
2:C:104:THR:HG23	2:D:104:THR:HG23	2.03	0.41
1:A:438:ALA:HB2	1:A:447:PHE:HD2	1.84	0.41
2:C:166:ARG:NH1	2:C:166:ARG:HG2	2.36	0.41
2:D:303:MET:CE	2:D:309:ILE:HD11	2.51	0.41
2:C:287:GLY:C	2:C:290:PRO:HD2	2.41	0.41
2:D:9:VAL:CG1	2:D:267:PRO:HB3	2.48	0.41
1:A:147:PRO:HB2	1:A:152:THR:HG23	2.01	0.41
1:B:100:GLU:OE1	1:B:154:ARG:NE	2.44	0.41
1:A:535:MET:SD	1:A:539:TYR:CE2	3.13	0.41
1:A:325:MET:HG3	5:A:1001:NAD:O4D	2.20	0.41
2:D:310:GLU:CG	2:D:360:LEU:HB2	2.51	0.41
2:C:233:LYS:HG2	2:C:233:LYS:H	1.69	0.41
1:A:393:ASN:H	1:A:393:ASN:HD22	1.68	0.41
2:C:255:MET:HE2	2:C:260:ALA:N	2.35	0.41
1:A:194:LEU:C	1:A:194:LEU:CD2	2.90	0.41
1:B:465:ILE:N	1:B:465:ILE:CD1	2.83	0.41
1:A:365:VAL:HG22	1:A:370:MET:HG2	2.01	0.41
1:A:532:GLY:C	1:A:665:PRO:HG3	2.41	0.41
1:A:639:THR:HG21	1:A:671:ALA:HB3	2.01	0.41
2:C:15:ARG:NH2	2:C:193:ILE:HD11	2.36	0.40
2:D:164:ILE:N	2:D:164:ILE:HD12	2.36	0.40
1:A:466:ARG:HG3	1:A:470:SER:HB2	2.04	0.40
2:D:204:PHE:N	2:D:204:PHE:CD1	2.88	0.40
1:A:473:LEU:HD23	1:A:473:LEU:O	2.20	0.40
2:D:5:PRO:HA	2:D:258:GLN:HB2	2.02	0.40
1:B:128:ARG:HG3	1:B:128:ARG:NH1	2.36	0.40
1:A:434:ILE:N	1:A:434:ILE:HD12	2.37	0.40
1:A:397:VAL:HB	1:A:425:LEU:HD23	2.02	0.40
1:A:258:THR:HG23	1:A:273:VAL:HG12	2.03	0.40
1:A:17:ILE:HG22	1:A:18:VAL:N	2.36	0.40
1:A:18:VAL:HG12	1:A:55:GLY:O	2.21	0.40
1:B:622:VAL:HG23	1:B:626:ASP:CB	2.51	0.40
2:D:164:ILE:HG22	2:D:169:GLN:HG3	2.03	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	703/715 (98%)	632 (90%)	66 (9%)	5 (1%)	26	72
1	B	706/715 (99%)	628 (89%)	73 (10%)	5 (1%)	26	72
2	C	388/390 (100%)	343 (88%)	37 (10%)	8 (2%)	9	53
2	D	388/390 (100%)	346 (89%)	35 (9%)	7 (2%)	11	55
All	All	2185/2210 (99%)	1949 (89%)	211 (10%)	25 (1%)	17	65

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	ILE
2	C	332	MET
2	C	349	PHE
2	D	332	MET
2	D	349	PHE
1	A	15	SER
1	A	324	ILE
1	B	15	SER
2	C	303	MET
2	D	303	MET
1	B	709	ASN
2	C	186	GLU
2	C	333	ASN
2	D	333	ASN
1	A	287	SER
2	C	264	GLY
2	D	186	GLU
1	B	667	PHE
2	C	54	VAL
2	D	54	VAL
2	D	264	GLY
1	A	368	GLY

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Mol	Chain	Res	Type
1	B	616	VAL
1	A	616	VAL
2	C	232	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	532/562 (95%)	521 (98%)	11 (2%)	61	86
1	B	539/562 (96%)	527 (98%)	12 (2%)	60	85
2	C	302/307 (98%)	292 (97%)	10 (3%)	45	79
2	D	301/307 (98%)	291 (97%)	10 (3%)	45	79
All	All	1674/1738 (96%)	1631 (97%)	43 (3%)	54	82

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ILE
1	A	142	LYS
1	A	178	ASP
1	A	288	ASN
1	A	289	CYS
1	A	366	ASP
1	A	393	ASN
1	A	504	LEU
1	A	554	ASP
1	A	618	GLU
1	A	692	GLU
1	B	82	ASP
1	B	142	LYS
1	B	178	ASP
1	B	288	ASN
1	B	289	CYS
1	B	366	ASP
1	B	393	ASN

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Mol	Chain	Res	Type
1	B	504	LEU
1	B	554	ASP
1	B	673	ARG
1	B	676	ASP
1	B	692	GLU
2	C	115	ASP
2	C	158	LEU
2	C	175	ARG
2	C	265	LEU
2	C	284	MET
2	C	289	VAL
2	C	318	GLN
2	C	325	ASP
2	C	351	CYS
2	C	355	ARG
2	D	115	ASP
2	D	158	LEU
2	D	175	ARG
2	D	265	LEU
2	D	284	MET
2	D	289	VAL
2	D	318	GLN
2	D	325	ASP
2	D	351	CYS
2	D	355	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	288	ASN
1	A	296	ASN
1	A	298	GLN
1	A	393	ASN
1	A	409	GLN
1	A	629	ASN
1	A	709	ASN
1	B	30	ASN
1	B	38	ASN
1	B	42	GLN
1	B	288	ASN
1	B	296	ASN

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Mol	Chain	Res	Type
1	B	298	GLN
1	B	393	ASN
1	B	409	GLN
1	B	428	ASN
1	B	629	ASN
2	C	4	ASN
2	C	46	ASN
2	C	89	GLN
2	C	162	HIS
2	C	197	GLN
2	C	293	GLN
2	C	312	ASN
2	C	318	GLN
2	C	362	ASN
2	D	4	ASN
2	D	46	ASN
2	D	89	GLN
2	D	162	HIS
2	D	197	GLN
2	D	293	GLN
2	D	318	GLN
2	D	362	ASN

### 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 ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAD	A	1001	-	38,48,48	1.34	3 (7%)	47,73,73	1.74	8 (17%)
4	ACO	A	1002	-	43,53,53	0.79	1 (2%)	55,79,79	1.00	4 (7%)
5	NAD	B	2001	-	38,48,48	1.31	3 (7%)	47,73,73	1.76	9 (19%)
4	ACO	C	3001	-	43,53,53	0.82	0	55,79,79	1.05	4 (7%)
4	ACO	D	4001	-	43,53,53	0.75	0	55,79,79	0.93	3 (5%)

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
5	NAD	A	1001	-	-	0/22/62/62	0/5/5/5
4	ACO	A	1002	-	-	2/47/67/67	0/3/3/3
5	NAD	B	2001	-	-	0/22/62/62	0/5/5/5
4	ACO	C	3001	-	-	2/47/67/67	0/3/3/3
4	ACO	D	4001	-	-	2/47/67/67	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	ACO	C2A-N3A	2.13	1.36	1.32
5	A	1001	NAD	C6N-N1N	2.90	1.43	1.35
5	B	2001	NAD	C6N-N1N	2.98	1.43	1.35
5	A	1001	NAD	C4N-C3N	3.20	1.44	1.39
5	B	2001	NAD	C4N-C3N	3.25	1.44	1.39
5	B	2001	NAD	C3N-C7N	4.90	1.58	1.50
5	A	1001	NAD	C3N-C7N	5.14	1.58	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	NAD	C5N-C4N-C3N	-5.37	113.58	120.33
5	B	2001	NAD	C5N-C4N-C3N	-5.20	113.80	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ACO	P2A-O3A-P1A	-4.42	120.33	132.73
4	C	3001	ACO	P2A-O3A-P1A	-4.41	120.35	132.73
5	A	1001	NAD	PN-O3-PA	-4.03	121.40	132.73
5	B	2001	NAD	PN-O3-PA	-3.95	121.62	132.73
4	D	4001	ACO	P2A-O3A-P1A	-3.60	122.61	132.73
5	B	2001	NAD	C5N-C6N-N1N	-3.08	115.15	120.47
5	A	1001	NAD	C5N-C6N-N1N	-2.90	115.46	120.47
5	B	2001	NAD	C3N-C7N-N7N	-2.10	115.52	117.82
5	B	2001	NAD	O3-PN-O5D	2.33	109.12	102.94
5	A	1001	NAD	O3-PN-O5D	2.38	109.26	102.94
5	B	2001	NAD	O3-PA-O5B	2.38	109.26	102.94
4	C	3001	ACO	O3A-P2A-O6A	2.41	109.33	102.94
4	A	1002	ACO	O3A-P2A-O6A	2.44	109.41	102.94
4	D	4001	ACO	O3A-P2A-O6A	2.44	109.42	102.94
5	A	1001	NAD	O3-PA-O5B	2.47	109.48	102.94
4	A	1002	ACO	O3A-P1A-O5B	2.48	109.52	102.94
4	C	3001	ACO	C2P-S1P-C	2.85	119.46	101.83
4	D	4001	ACO	C2P-S1P-C	2.89	119.72	101.83
4	A	1002	ACO	C2P-S1P-C	2.96	120.15	101.83
5	B	2001	NAD	C2N-C3N-C4N	3.04	121.67	118.29
4	C	3001	ACO	O3A-P1A-O5B	3.09	111.14	102.94
5	A	1001	NAD	C2N-C3N-C4N	3.20	121.85	118.29
5	A	1001	NAD	O4D-C1D-N1N	4.95	113.56	108.13
5	B	2001	NAD	C6N-C5N-C4N	5.21	127.32	119.44
5	B	2001	NAD	O4D-C1D-N1N	5.23	113.88	108.13
5	A	1001	NAD	C6N-C5N-C4N	5.26	127.39	119.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	ACO	CH3-C-S1P-C2P
4	A	1002	ACO	O-C-S1P-C2P
4	D	4001	ACO	CH3-C-S1P-C2P
4	C	3001	ACO	CH3-C-S1P-C2P
4	D	4001	ACO	O-C-S1P-C2P
4	C	3001	ACO	O-C-S1P-C2P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	NAD	1	0
4	A	1002	ACO	2	0
5	B	2001	NAD	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	707/715 (98%)	-0.65	0 100 100	1, 21, 67, 97	0
1	B	710/715 (99%)	-0.62	2 (0%) 94 89	1, 22, 65, 99	0
2	C	390/390 (100%)	-0.71	0 100 100	1, 8, 45, 83	0
2	D	390/390 (100%)	-0.69	1 (0%) 94 89	1, 11, 45, 97	0
All	All	2197/2210 (99%)	-0.66	3 (0%) 95 93	1, 17, 61, 99	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	GLN	2.2
1	B	567	ASP	2.1
2	D	2	SER	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	ACO	A	1002	51/51	0.57	0.57	8.19	160,160,160,160	0
4	ACO	C	3001	51/51	0.76	0.44	5.74	159,159,159,159	0
4	ACO	D	4001	51/51	0.84	0.39	4.10	133,133,133,133	0
5	NAD	B	2001	44/44	0.81	0.35	2.93	123,123,123,123	0
5	NAD	A	1001	44/44	0.87	0.32	2.28	98,98,98,98	0
3	ZN	A	716	1/1	0.99	0.04	-4.35	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.