



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:00 AM EDT

PDB ID : 2JBU / pdb_00002jbu
Title : Crystal structure of human insulin degrading enzyme complexed with co-purified peptides.
Authors : Im, H.; Shen, Y.; Tang, W.J.
Deposited on : 2006-12-11
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

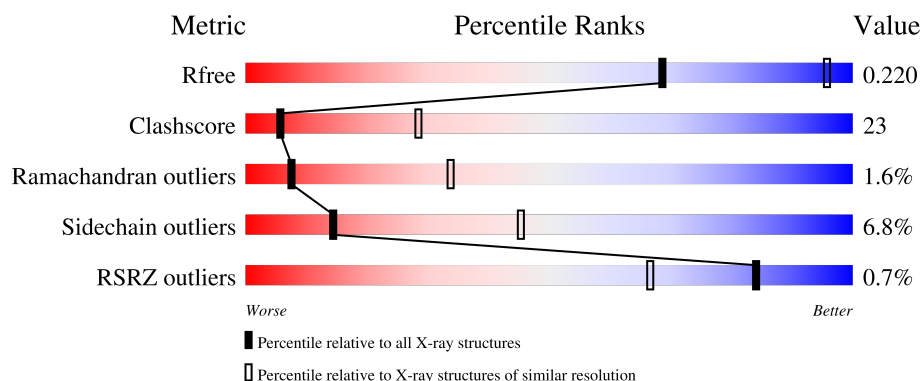
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	990	17% 54% 37% 6% .
1	B	990	51% 39% 6% . .
2	C	12	17% 75% 8% 17%
2	D	12	8% 58% 25% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15897 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 INSULIN-DEGRADING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	963	Total	C	N	O	S	0	0	1
			7859	5058	1318	1448	35			
1	B	961	Total	C	N	O	S	0	0	1
			7846	5049	1316	1446	35			

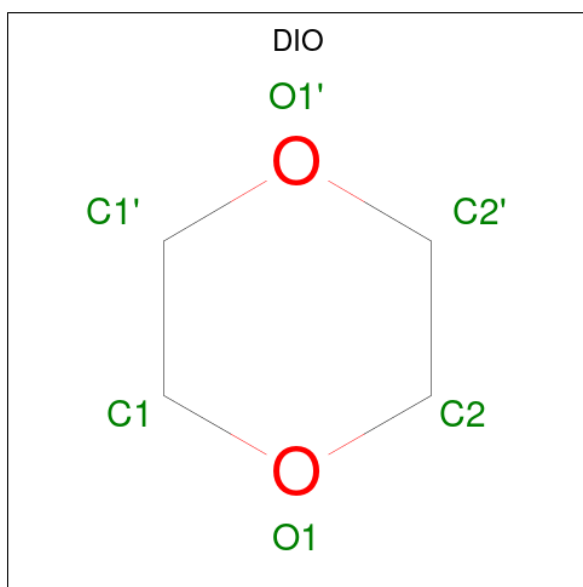
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	GLN	GLU	engineered mutation	UNP Q5T5N2
B	111	GLN	GLU	engineered mutation	UNP Q5T5N2

- Molecule 2 is a protein called CO-PURIFIED PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			50	30	10	10			
2	D	10	Total	C	N	O	0	0	0
			50	30	10	10			

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		

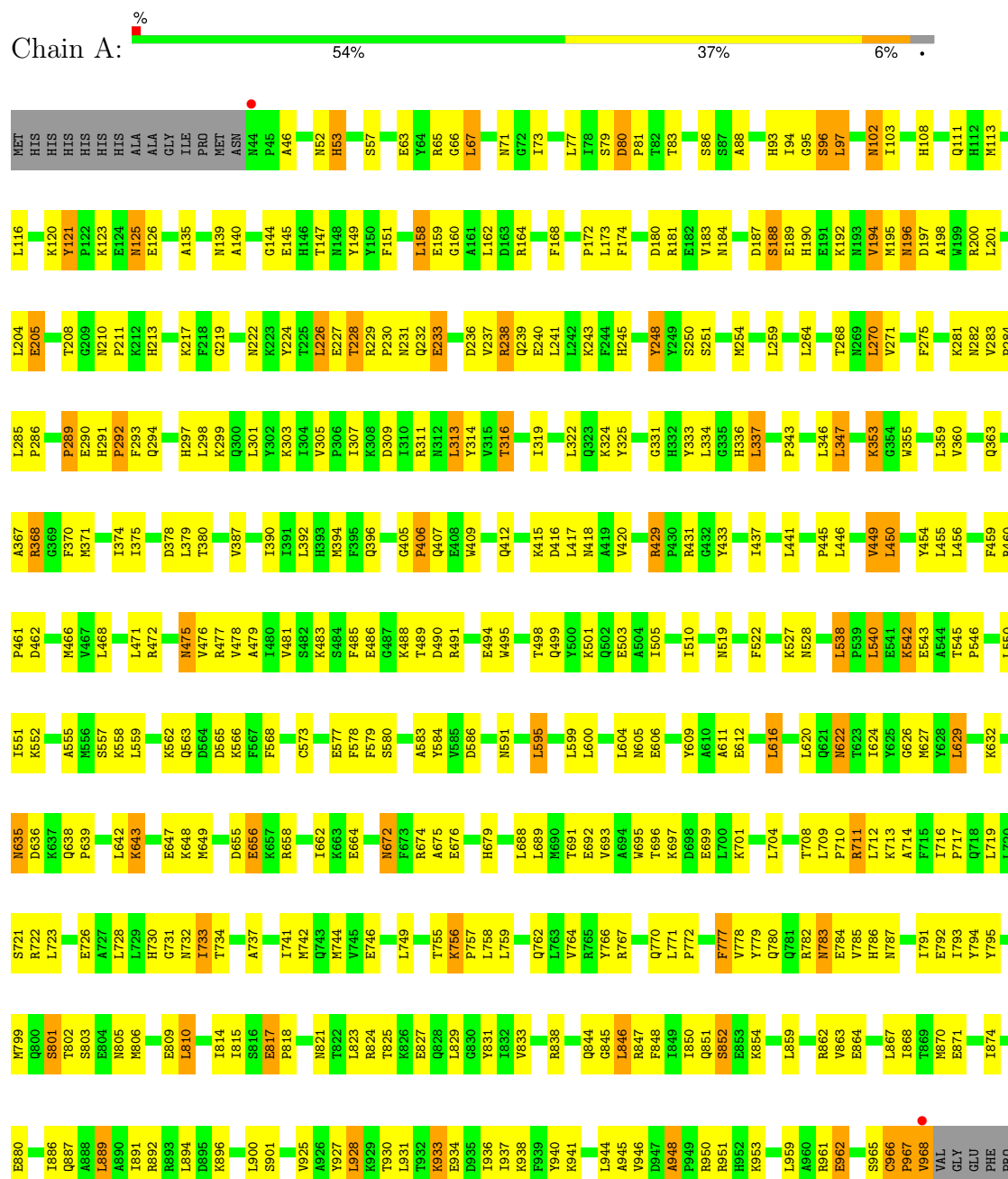
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	35	Total	O	0	0
			35	35		
4	D	1	Total	O	0	0
			1	1		

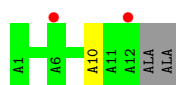
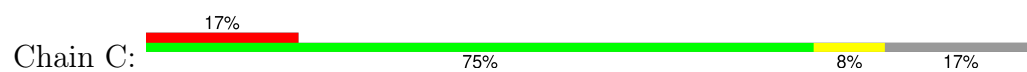
3 Residue-property plots

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

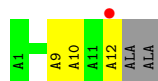
• Molecule 1: INSULIN-DEGRADING ENZYME







● Molecule 2: CO-PURIFIED PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.28Å 263.28Å 90.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 3.00 29.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.86-3.00) 97.9 (29.86-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.240 0.172 , 0.220	Depositor DCC
R_{free} test set	3670 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15897	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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

5.1 Standard geometry

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

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	0.62	1/8056 (0.0%)	1.07	50/10896 (0.5%)
1	B	0.55	1/8043 (0.0%)	1.04	40/10877 (0.4%)
2	C	1.03	0/48	1.07	0/64
2	D	1.01	0/48	1.19	1/64 (1.6%)
All	All	0.59	2/16195 (0.0%)	1.05	91/21901 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1016	ALA	C-N	-6.05	1.24	1.33
1	B	1016	ALA	C-N	-5.73	1.25	1.33

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	PHE	N-CA-C	-15.03	91.55	110.19
1	A	121	TYR	CA-C-N	10.11	130.27	119.05
1	A	121	TYR	C-N-CA	10.11	130.27	119.05
1	A	429	ARG	N-CA-C	-8.86	96.47	109.50
1	B	219	GLY	N-CA-C	7.96	122.96	112.77
1	B	494	GLU	N-CA-C	7.91	120.81	111.71
1	B	116	LEU	N-CA-C	7.21	121.67	113.02
1	B	380	THR	N-CA-C	-7.12	100.94	110.55
1	A	854	LYS	CA-C-N	6.93	124.72	119.66
1	A	854	LYS	C-N-CA	6.93	124.72	119.66
1	A	557	SER	N-CA-C	6.93	119.70	108.76
1	B	307	ILE	N-CA-C	-6.89	105.04	111.45
1	B	86	SER	N-CA-C	-6.87	101.67	110.53
1	B	559	LEU	N-CA-C	6.72	119.47	108.52
1	B	677	GLN	N-CA-C	6.71	118.53	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	LEU	CA-C-N	6.66	127.19	119.99
1	A	771	LEU	C-N-CA	6.66	127.19	119.99
1	A	353	LYS	N-CA-C	-6.52	105.08	113.16
1	A	568	PHE	N-CA-C	6.50	120.14	111.30
1	B	654	ILE	N-CA-C	6.46	118.00	109.21
1	B	822	THR	N-CA-C	6.46	118.20	111.03
1	B	715	PHE	N-CA-C	6.42	118.27	111.28
1	A	307	ILE	N-CA-C	-6.41	104.91	110.74
1	A	966	CYS	CA-C-N	6.35	127.78	119.84
1	A	966	CYS	C-N-CA	6.35	127.78	119.84
1	B	590	CYS	N-CA-C	-6.31	104.33	111.14
1	A	113	MET	N-CA-C	6.26	118.11	111.28
1	A	494	GLU	N-CA-C	6.23	118.87	111.33
1	B	953	LYS	N-CA-C	6.17	119.30	109.24
1	B	785	VAL	N-CA-C	6.10	117.05	111.81
1	A	721	SER	N-CA-C	6.03	117.94	111.36
1	A	219	GLY	N-CA-C	6.00	121.41	113.37
1	B	455	LEU	N-CA-C	5.97	119.99	109.96
1	B	121	TYR	CA-C-N	5.93	125.64	119.05
1	B	121	TYR	C-N-CA	5.93	125.64	119.05
1	A	380	THR	N-CA-C	-5.93	102.17	110.35
1	B	827	GLU	N-CA-C	5.93	119.77	112.54
1	A	731	GLY	N-CA-C	5.92	118.01	110.20
2	D	9	ALA	N-CA-C	5.87	119.20	110.52
1	A	194	VAL	N-CA-C	5.79	117.22	110.62
1	A	1009	LYS	CA-C-N	5.77	125.70	119.76
1	A	1009	LYS	C-N-CA	5.77	125.70	119.76
1	B	580	SER	CA-C-N	5.76	125.45	119.05
1	B	580	SER	C-N-CA	5.76	125.45	119.05
1	A	116	LEU	N-CA-C	5.71	119.23	112.72
1	B	288	PHE	CA-C-N	5.69	125.05	118.85
1	B	288	PHE	C-N-CA	5.69	125.05	118.85
1	B	353	LYS	N-CA-C	-5.68	106.39	113.15
1	B	429	ARG	N-CA-C	-5.68	100.78	109.64
1	A	46	ALA	N-CA-C	-5.64	106.24	113.23
1	A	953	LYS	N-CA-C	5.64	118.09	108.90
1	A	378	ASP	N-CA-C	-5.62	102.45	110.59
1	A	948	ALA	CA-C-N	5.59	125.26	119.05
1	A	948	ALA	C-N-CA	5.59	125.26	119.05
1	B	444	TYR	CA-C-N	5.59	125.52	119.76
1	B	444	TYR	C-N-CA	5.59	125.52	119.76
1	B	637	LYS	N-CA-C	5.58	119.79	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	557	SER	N-CA-C	5.58	118.29	108.75
1	A	289	PRO	N-CA-C	-5.54	102.76	111.34
1	A	455	LEU	N-CA-C	5.54	117.75	108.73
1	B	357	ASN	N-CA-C	-5.53	106.58	113.55
1	A	217	LYS	N-CA-C	5.51	117.65	110.43
1	A	505	ILE	CA-C-N	5.49	126.70	119.84
1	A	505	ILE	C-N-CA	5.49	126.70	119.84
1	A	944	LEU	N-CA-C	5.48	119.97	113.12
1	B	853	GLU	N-CA-C	-5.45	106.13	112.89
1	A	292	PRO	N-CA-C	-5.43	107.07	113.86
1	A	80	ASP	CA-C-N	5.43	126.62	119.84
1	A	80	ASP	C-N-CA	5.43	126.62	119.84
1	A	248	TYR	N-CA-C	5.40	120.74	114.04
1	B	569	LEU	N-CA-C	-5.33	102.78	110.40
1	A	764	VAL	N-CA-C	5.32	116.23	108.58
1	A	333	TYR	N-CA-C	-5.27	105.43	111.07
1	B	896	LYS	N-CA-C	5.27	117.93	110.24
1	A	962	GLU	N-CA-C	5.25	117.08	111.36
1	B	83	THR	N-CA-C	5.21	118.03	110.42
1	A	538	LEU	N-CA-C	5.19	115.57	109.60
1	A	254	MET	N-CA-C	5.17	117.82	109.40
1	A	205	GLU	N-CA-C	-5.17	105.30	111.03
1	A	429	ARG	CA-C-N	5.16	124.61	119.24
1	A	429	ARG	C-N-CA	5.16	124.61	119.24
1	B	545	THR	CA-C-N	5.15	124.47	118.85
1	B	545	THR	C-N-CA	5.15	124.47	118.85
1	A	275	PHE	N-CA-C	5.14	120.94	114.31
1	B	724	HIS	N-CA-C	-5.10	100.73	109.24
1	A	704	LEU	N-CA-C	5.07	117.46	111.33
1	A	814	ILE	N-CA-C	5.03	115.75	110.62
1	B	329	ASN	CA-C-N	-5.03	113.47	119.05
1	B	329	ASN	C-N-CA	-5.03	113.47	119.05
1	A	495	TRP	N-CA-C	5.01	117.85	111.69
1	B	379	LEU	N-CA-C	5.00	117.60	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7859	0	7788	336	0
1	B	7846	0	7776	401	0
2	C	50	0	51	3	0
2	D	50	0	51	3	0
3	A	6	0	8	3	0
3	B	6	0	8	2	0
4	A	44	0	0	2	0
4	B	35	0	0	4	0
4	D	1	0	0	0	0
All	All	15897	0	15682	734	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (734) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:LEU:HD23	1:B:928:LEU:HD21	1.30	1.12
1:A:538:LEU:HD23	1:A:734:THR:HG23	1.38	1.06
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.39	1.01
1:A:309:ASP:H	1:A:672:ASN:HD21	1.11	0.98
1:B:309:ASP:H	1:B:672:ASN:HD21	1.02	0.98
1:A:162:LEU:HD23	1:A:270:LEU:HD11	1.47	0.96
1:A:622:ASN:HD22	1:A:622:ASN:H	1.03	0.94
1:A:604:LEU:HD21	1:A:648:LYS:HG3	1.49	0.94
1:B:711:ARG:HH21	1:B:711:ARG:HG3	1.32	0.92
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.50	0.91
1:A:111:GLN:HE22	2:C:10:ALA:HB2	1.35	0.91
1:A:429:ARG:HH11	1:A:431:ARG:HB3	1.33	0.91
1:B:363:GLN:NE2	1:B:371:MET:HE1	1.86	0.90
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.53	0.90
1:B:446:LEU:HD22	1:B:446:LEU:H	1.35	0.88
1:A:829:LEU:O	1:A:852:SER:HB2	1.73	0.88
1:B:309:ASP:H	1:B:672:ASN:ND2	1.69	0.88
1:B:1014:PHE:O	1:B:1015:MET:HB2	1.72	0.88
1:B:815:ILE:HA	1:B:870:MET:HE2	1.56	0.87
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.73	0.87
1:A:449:VAL:HG23	1:A:450:LEU:HD13	1.56	0.85
1:A:111:GLN:NE2	2:C:10:ALA:HB2	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:H	1:A:297:HIS:HD2	1.20	0.84
1:A:783:ASN:ND2	1:A:786:HIS:H	1.77	0.82
1:B:311:ARG:NH2	1:B:668:ARG:HE	1.77	0.82
1:B:540:LEU:HD12	1:B:563:GLN:OE1	1.81	0.80
1:B:783:ASN:ND2	1:B:786:HIS:H	1.79	0.80
1:A:125:ASN:H	1:A:125:ASN:HD22	1.30	0.80
1:B:65:ARG:HB2	1:B:264:LEU:HD13	1.64	0.80
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.63	0.79
1:B:798:ASP:CG	1:B:799:MET:H	1.89	0.79
1:B:534:ASN:HD21	1:B:536:GLU:HG2	1.45	0.78
1:A:490:ASP:OD1	1:A:491:ARG:HG3	1.84	0.78
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.20	0.77
1:A:309:ASP:H	1:A:672:ASN:ND2	1.82	0.77
1:B:196:ASN:ND2	1:B:198:ALA:H	1.81	0.77
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.68	0.76
1:A:316:THR:HG23	1:A:374:ILE:HG22	1.65	0.76
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.66	0.76
1:B:575:ASN:HD22	1:B:575:ASN:N	1.84	0.76
1:A:609:TYR:O	1:A:612:GLU:HB3	1.85	0.76
1:B:534:ASN:C	1:B:534:ASN:HD22	1.93	0.76
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.17	0.75
1:A:622:ASN:HD22	1:A:622:ASN:N	1.82	0.75
1:A:289:PRO:O	1:A:290:GLU:HB3	1.87	0.75
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.32	0.75
1:B:363:GLN:HE21	1:B:371:MET:HE1	1.50	0.75
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.69	0.74
1:A:236:ASP:CG	1:A:239:GLN:HG2	2.12	0.74
1:B:810:LEU:CD2	1:B:928:LEU:HD21	2.15	0.74
1:A:656:GLU:OE1	1:A:709:LEU:HD22	1.87	0.74
1:B:574:LEU:C	1:B:575:ASN:HD22	1.95	0.74
1:B:251:SER:HB3	1:B:278:VAL:HG12	1.69	0.74
1:B:466:MET:HE2	1:B:466:MET:O	1.88	0.74
1:B:689:LEU:HG	1:B:995:MET:HE2	1.69	0.73
1:A:538:LEU:HD23	1:A:734:THR:CG2	2.16	0.73
1:A:195:MET:HB2	1:A:786:HIS:CE1	2.23	0.73
1:A:196:ASN:HD22	1:A:197:ASP:N	1.86	0.73
1:A:71:ASN:HB2	1:A:251:SER:OG	1.88	0.72
1:B:90:LEU:HD11	1:B:254:MET:CE	2.19	0.72
1:B:782:ARG:HG3	1:B:959:LEU:HB2	1.71	0.72
1:B:960:ALA:HB3	1:B:963:MET:HB2	1.72	0.72
1:A:145:GLU:OE2	1:A:367:ALA:HB1	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:VAL:HG21	1:B:968:VAL:HG21	1.71	0.72
1:A:863:VAL:O	1:A:867:LEU:HD23	1.89	0.71
1:B:422:PHE:CZ	1:B:451:THR:HG22	2.24	0.71
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.36	0.71
1:B:604:LEU:HD21	1:B:648:LYS:HG3	1.70	0.71
1:A:392:LEU:O	1:A:396:GLN:HG3	1.91	0.71
1:B:677:GLN:HG3	1:B:786:HIS:CE1	2.26	0.71
1:B:805:ASN:ND2	1:B:844:GLN:HE22	1.89	0.71
1:B:517:ASP:HB2	4:B:1232:HOH:O	1.90	0.70
1:B:818:PRO:HG2	1:B:870:MET:HE1	1.74	0.70
1:A:205:GLU:HG3	3:A:1101:DIO:H1'2	1.74	0.69
1:A:799:MET:HE3	1:A:1008:VAL:HA	1.74	0.69
1:B:47:ILE:O	1:B:47:ILE:HG22	1.90	0.69
1:B:172:PRO:HB2	1:B:174:PHE:CE1	2.27	0.69
1:B:174:PHE:O	1:B:238:ARG:HD3	1.92	0.69
1:B:311:ARG:HA	1:B:481:VAL:O	1.93	0.69
1:B:205:GLU:HG3	3:B:1101:DIO:H1'2	1.73	0.69
1:A:783:ASN:HD21	1:A:786:HIS:H	1.36	0.68
1:B:679:HIS:O	1:B:683:MET:HG3	1.93	0.68
1:B:770:GLN:HB3	1:B:1003:PRO:HG2	1.76	0.67
1:A:196:ASN:HD22	1:A:196:ASN:C	2.02	0.67
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.25	0.67
1:A:449:VAL:HG23	1:A:450:LEU:CD1	2.25	0.67
1:B:331:GLY:HA3	1:B:363:GLN:OE1	1.95	0.67
1:B:475:ASN:HD22	1:B:475:ASN:H	1.43	0.67
1:A:102:ASN:ND2	1:A:103:ILE:HG13	2.11	0.66
1:A:805:ASN:ND2	1:A:844:GLN:HE22	1.92	0.66
1:B:416:ASP:O	1:B:420:VAL:HG23	1.95	0.66
1:B:629:LEU:HD22	1:B:630:SER:N	2.09	0.66
1:B:446:LEU:H	1:B:446:LEU:CD2	2.08	0.66
1:B:200:ARG:NH2	1:B:498:THR:HA	2.11	0.66
1:A:180:ASP:O	1:A:183:VAL:HG12	1.95	0.66
1:B:600:LEU:HD21	1:B:649:MET:HB3	1.78	0.66
1:A:204:LEU:HG	3:A:1101:DIO:H22	1.78	0.65
1:A:172:PRO:HB2	1:A:174:PHE:CE1	2.32	0.65
1:A:538:LEU:CD2	1:A:734:THR:HG23	2.23	0.65
1:B:90:LEU:HD21	1:B:254:MET:HE3	1.77	0.65
1:B:874:ILE:O	1:B:933:LYS:HE3	1.96	0.65
1:B:510:ILE:O	1:B:514:GLN:HG3	1.97	0.65
1:B:196:ASN:ND2	1:B:198:ALA:N	2.45	0.65
1:A:63:GLU:HB2	1:A:79:SER:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:HD13	1:A:475:ASN:HB3	1.77	0.65
1:B:967:PRO:HD3	4:B:1234:HOH:O	1.95	0.65
1:A:162:LEU:HD23	1:A:270:LEU:CD1	2.25	0.65
1:A:174:PHE:O	1:A:238:ARG:HD3	1.97	0.64
1:A:222:ASN:O	1:A:226:LEU:HB2	1.98	0.64
1:A:359:LEU:HD23	1:A:360:VAL:N	2.13	0.64
1:A:565:ASP:OD2	1:A:566:LYS:HE3	1.97	0.64
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.31	0.64
1:B:349:GLU:OE2	1:B:349:GLU:HA	1.97	0.64
1:A:622:ASN:H	1:A:622:ASN:ND2	1.81	0.64
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.78	0.64
1:B:599:LEU:CD2	1:B:662:ILE:HD12	2.22	0.64
1:B:864:GLU:HG2	1:B:986:LEU:HD21	1.79	0.64
1:B:711:ARG:HH21	1:B:711:ARG:CG	2.10	0.64
1:B:846:LEU:HD23	1:B:847:ARG:N	2.12	0.64
1:B:475:ASN:HD22	1:B:475:ASN:N	1.96	0.64
1:A:846:LEU:HD23	1:A:847:ARG:N	2.12	0.63
1:A:874:ILE:O	1:A:933:LYS:HD3	1.98	0.63
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.80	0.63
1:B:245:HIS:O	1:B:249:TYR:HB2	1.98	0.63
1:B:733:ILE:HG13	1:B:737:ALA:HB3	1.78	0.63
1:B:407:GLN:HG3	1:B:409:TRP:NE1	2.14	0.63
1:B:622:ASN:HD22	1:B:622:ASN:H	1.46	0.63
1:A:67:LEU:HD12	1:A:67:LEU:C	2.23	0.63
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.81	0.63
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.80	0.63
1:B:298:LEU:HD21	1:B:318:PRO:HG2	1.80	0.63
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.80	0.62
1:B:80:ASP:O	1:B:83:THR:HG22	1.98	0.62
1:B:597:LEU:HG	1:B:620:LEU:HG	1.81	0.62
1:B:994:ASN:HB3	1:B:997:GLU:HB2	1.81	0.62
1:A:227:GLU:C	1:A:230:PRO:HD2	2.25	0.62
1:B:591:ASN:ND2	1:B:700:LEU:HD22	2.14	0.62
1:B:846:LEU:HD23	1:B:847:ARG:H	1.64	0.62
1:B:407:GLN:HG3	1:B:409:TRP:CD1	2.35	0.62
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.35	0.62
1:A:779:TYR:CZ	1:A:995:MET:HE3	2.35	0.62
1:B:309:ASP:N	1:B:672:ASN:HD21	1.84	0.61
1:B:868:ILE:HD12	1:B:984:PRO:HD3	1.82	0.61
1:A:805:ASN:HD22	1:A:844:GLN:NE2	1.97	0.61
1:B:776:TRP:NE1	1:B:953:LYS:HE2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:SER:HA	1:B:927:TYR:CE2	2.35	0.61
1:B:167:GLN:C	1:B:168:PHE:O	2.35	0.61
1:B:806:MET:HE3	1:B:806:MET:HA	1.81	0.61
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.00	0.61
1:A:770:GLN:HA	1:A:1005:PHE:CE1	2.35	0.61
1:B:671:ASN:O	1:B:674:ARG:HG2	2.00	0.61
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.82	0.61
1:B:102:ASN:HD22	1:B:102:ASN:H	1.47	0.61
1:A:303:LYS:HD3	1:A:485:PHE:CE2	2.35	0.61
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.36	0.61
1:B:798:ASP:CG	1:B:799:MET:N	2.59	0.60
1:B:196:ASN:HD21	1:B:198:ALA:HB3	1.67	0.60
1:A:643:LYS:HE2	1:A:647:GLU:OE2	2.02	0.60
1:B:119:LYS:HB2	1:B:171:CYS:SG	2.41	0.60
1:B:329:ASN:HB3	1:B:332:HIS:HB2	1.83	0.60
1:B:541:GLU:HB3	1:B:543:GLU:OE2	2.02	0.60
1:B:77:LEU:HD21	1:B:271:VAL:HG21	1.83	0.60
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.82	0.60
1:B:789:CYS:SG	1:B:963:MET:SD	2.99	0.60
1:A:201:LEU:HD21	1:A:481:VAL:HG21	1.83	0.59
1:A:577:GLU:HG2	1:A:579:PHE:CZ	2.37	0.59
1:B:79:SER:HB2	1:B:264:LEU:HD23	1.83	0.59
1:B:542:LYS:HB2	1:B:542:LYS:NZ	2.17	0.59
1:A:294:GLN:H	1:A:297:HIS:CD2	2.12	0.59
1:A:476:VAL:HG22	1:A:477:ARG:N	2.16	0.59
1:B:47:ILE:O	1:B:48:LYS:C	2.45	0.59
1:B:102:ASN:HD22	1:B:102:ASN:N	1.99	0.59
1:B:556:MET:HG2	1:B:746:GLU:HG2	1.84	0.59
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.01	0.59
1:A:545:THR:HB	1:A:546:PRO:HD2	1.85	0.59
1:B:854:LYS:HB2	1:B:859:LEU:HD21	1.84	0.59
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.85	0.59
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.67	0.59
1:B:428:GLU:HG2	1:B:433:TYR:CD1	2.38	0.59
1:B:135:ALA:HA	1:B:892:ARG:NH2	2.18	0.59
1:A:709:LEU:HD11	1:A:713:LYS:HE3	1.85	0.59
1:A:777:PHE:N	1:A:777:PHE:CD1	2.71	0.59
1:A:552:LYS:NZ	1:A:746:GLU:OE1	2.35	0.58
1:B:683:MET:HA	1:B:792:GLU:OE2	2.02	0.58
1:A:870:MET:O	1:A:874:ILE:HG13	2.03	0.58
1:B:783:ASN:ND2	1:B:785:VAL:H	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:HD22	1:A:125:ASN:N	2.01	0.58
1:A:550:LEU:N	1:A:1015:MET:SD	2.62	0.58
1:B:600:LEU:CD2	1:B:649:MET:HB3	2.33	0.58
1:A:227:GLU:O	1:A:230:PRO:HD2	2.04	0.58
1:B:810:LEU:HD21	1:B:886:ILE:HG12	1.85	0.58
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.85	0.58
1:A:375:ILE:HG22	1:A:394:MET:HE2	1.86	0.58
1:A:689:LEU:HD23	1:A:995:MET:HG2	1.84	0.58
1:B:654:ILE:HD13	1:B:712:LEU:HD13	1.85	0.58
1:A:162:LEU:CD2	1:A:270:LEU:HD11	2.28	0.58
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.34	0.58
1:A:164:ARG:HG3	1:A:164:ARG:HH11	1.68	0.58
1:B:800:GLN:HA	1:B:844:GLN:NE2	2.18	0.58
1:A:205:GLU:HG2	1:A:293:PHE:HZ	1.69	0.58
1:A:880:GLU:CB	1:B:457:GLU:HG2	2.34	0.58
1:B:268:THR:O	1:B:272:VAL:HG23	2.04	0.57
1:B:375:ILE:CG2	1:B:394:MET:HE2	2.33	0.57
1:A:359:LEU:HD23	1:A:359:LEU:C	2.29	0.57
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.39	0.57
1:A:197:ASP:O	1:A:201:LEU:HD13	2.03	0.57
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.85	0.57
1:B:591:ASN:O	1:B:595:LEU:HB2	2.04	0.57
1:B:858:TYR:CZ	1:B:862:ARG:HD2	2.39	0.57
1:B:961:ARG:NH1	1:B:962:GLU:OE1	2.36	0.57
1:A:611:ALA:HB1	1:A:616:LEU:HB3	1.87	0.57
1:B:666:TYR:CZ	1:B:670:LEU:HD11	2.38	0.57
1:A:471:LEU:HD23	1:A:471:LEU:N	2.20	0.57
1:A:135:ALA:HA	1:A:892:ARG:NH2	2.19	0.57
1:A:778:VAL:HG21	1:A:968:VAL:HG11	1.86	0.57
1:B:817:GLU:CB	1:B:818:PRO:HD3	2.34	0.57
1:B:384:LEU:HD12	1:B:384:LEU:O	2.04	0.57
1:B:831:TYR:CE2	2:D:12:ALA:HB2	2.39	0.57
1:A:196:ASN:C	1:A:196:ASN:ND2	2.61	0.57
1:B:54:ILE:HD12	1:B:446:LEU:O	2.05	0.56
1:B:534:ASN:ND2	1:B:536:GLU:H	2.02	0.56
1:A:159:GLU:HG3	1:A:270:LEU:HD21	1.86	0.56
1:A:696:THR:OG1	1:A:699:GLU:HG3	2.03	0.56
1:B:675:ALA:HA	1:B:785:VAL:HG21	1.87	0.56
1:A:868:ILE:HD11	1:A:984:PRO:HB3	1.88	0.56
1:A:980:LEU:N	4:A:1201:HOH:O	2.38	0.56
1:B:147:THR:HG21	1:B:249:TYR:OH	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:CYS:SG	1:A:967:PRO:HD2	2.45	0.56
1:B:408:GLU:HB2	1:B:459:PHE:CE2	2.40	0.56
1:B:387:VAL:HG21	1:B:480:ILE:HD13	1.87	0.56
1:B:689:LEU:CG	1:B:995:MET:HE2	2.36	0.56
1:A:231:ASN:C	1:A:233:GLU:H	2.13	0.56
1:A:767:ARG:HD3	1:A:1005:PHE:O	2.06	0.56
1:B:864:GLU:OE1	1:B:951:ARG:NH2	2.35	0.56
1:A:479:ALA:HB2	3:A:1101:DIO:H12	1.88	0.56
1:B:446:LEU:HD22	1:B:446:LEU:N	2.15	0.56
1:B:706:ASP:O	1:B:708:THR:HG23	2.06	0.56
1:B:812:CYS:SG	1:B:837:PRO:HD3	2.45	0.56
1:A:181:ARG:O	1:A:184:ASN:HB2	2.06	0.56
1:B:160:GLY:O	1:B:164:ARG:HG3	2.05	0.56
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.88	0.56
1:B:538:LEU:HD12	1:B:538:LEU:H	1.70	0.56
1:B:48:LYS:HD2	1:B:68:GLU:CD	2.30	0.55
1:A:204:LEU:O	1:A:208:THR:HG23	2.07	0.55
1:B:413:GLU:OE2	1:B:527:LYS:HD2	2.06	0.55
1:B:534:ASN:C	1:B:534:ASN:ND2	2.58	0.55
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.41	0.55
1:A:196:ASN:ND2	1:A:198:ALA:H	2.04	0.55
1:A:805:ASN:ND2	1:A:844:GLN:NE2	2.55	0.55
1:A:93:HIS:HD2	1:A:145:GLU:O	1.90	0.55
1:B:722:ARG:NH1	1:B:756:LYS:HB2	2.21	0.55
1:A:540:LEU:HD12	1:A:563:GLN:OE1	2.05	0.55
1:B:66:GLY:O	1:B:67:LEU:HB3	2.06	0.55
1:B:656:GLU:HG3	1:B:709:LEU:CD2	2.36	0.55
1:A:229:ARG:HB3	1:A:230:PRO:HD3	1.87	0.55
1:B:71:ASN:HB2	1:B:251:SER:OG	2.06	0.55
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.55	0.55
1:A:616:LEU:HD21	1:A:638:GLN:HG2	1.89	0.55
1:A:823:LEU:HD12	1:A:829:LEU:CD1	2.37	0.55
1:A:562:LYS:HD3	1:A:730:HIS:CE1	2.42	0.55
1:B:119:LYS:HD2	1:B:171:CYS:HB2	1.89	0.55
1:B:172:PRO:HB2	1:B:174:PHE:HE1	1.71	0.55
1:B:778:VAL:HG23	1:B:989:PRO:HB2	1.89	0.54
1:B:946:VAL:HA	1:B:951:ARG:CZ	2.37	0.54
1:A:322:LEU:HD12	1:A:363:GLN:NE2	2.21	0.54
1:B:479:ALA:HB2	3:B:1101:DIO:H12	1.90	0.54
1:B:789:CYS:SG	1:B:856:PRO:HD3	2.48	0.54
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:ILE:HD11	1:B:984:PRO:HB3	1.89	0.54
1:A:236:ASP:OD1	1:A:239:GLN:HG2	2.08	0.54
1:A:459:PHE:CE2	1:A:461:PRO:HG3	2.43	0.54
1:A:868:ILE:CD1	1:A:984:PRO:HD3	2.38	0.54
1:B:316:THR:HG23	1:B:374:ILE:HG22	1.90	0.54
1:A:224:TYR:HA	1:A:228:THR:HB	1.89	0.54
1:A:77:LEU:HD11	1:A:268:THR:HA	1.90	0.54
1:A:102:ASN:N	1:A:102:ASN:HD22	2.06	0.54
1:A:240:GLU:OE2	1:A:243:LYS:HD2	2.08	0.54
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.42	0.54
1:A:200:ARG:NH2	1:A:498:THR:HA	2.23	0.54
1:B:111:GLN:HE21	2:D:10:ALA:HB2	1.73	0.54
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.90	0.53
1:B:134:HIS:HD2	1:B:157:HIS:CD2	2.26	0.53
1:A:655:ASP:HB3	1:A:658:ARG:HB2	1.90	0.53
1:B:49:ARG:HG2	1:B:50:ILE:H	1.74	0.53
1:B:770:GLN:HA	1:B:1005:PHE:CE1	2.43	0.53
1:A:86:SER:HB3	1:A:158:LEU:HG	1.91	0.53
1:A:196:ASN:O	1:A:200:ARG:HG3	2.09	0.53
1:A:722:ARG:C	1:A:758:LEU:HD13	2.33	0.53
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.89	0.53
1:B:259:LEU:HD23	1:B:259:LEU:C	2.33	0.53
1:B:449:VAL:HG23	1:B:450:LEU:H	1.74	0.53
1:B:742:MET:HA	1:B:742:MET:HE3	1.90	0.53
1:B:287:GLU:OE1	1:B:289:PRO:HD3	2.09	0.53
1:B:417:LEU:HD21	1:B:531:ILE:HG12	1.89	0.53
1:A:331:GLY:HA3	1:A:363:GLN:NE2	2.23	0.53
1:A:375:ILE:CG2	1:A:394:MET:HE2	2.38	0.53
1:B:823:LEU:HB2	1:B:833:VAL:HG11	1.91	0.53
1:A:52:ASN:O	1:A:53:HIS:C	2.52	0.53
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.90	0.53
1:B:540:LEU:HA	1:B:563:GLN:OE1	2.09	0.53
1:A:483:LYS:O	1:A:486:GLU:HB2	2.09	0.52
1:B:187:ASP:OD1	1:B:222:ASN:HB2	2.09	0.52
1:A:927:TYR:O	1:A:930:THR:HB	2.09	0.52
1:B:1014:PHE:O	1:B:1015:MET:CB	2.51	0.52
1:A:580:SER:HB2	1:A:723:LEU:HD23	1.90	0.52
1:A:231:ASN:O	1:A:233:GLU:N	2.36	0.52
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.17	0.52
1:B:78:ILE:O	1:B:259:LEU:HA	2.10	0.52
1:B:1012:ILE:HD11	1:B:1014:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLN:HG3	1:A:409:TRP:CD1	2.44	0.52
1:A:558:LYS:HB3	1:A:726:GLU:HG3	1.91	0.52
1:B:392:LEU:O	1:B:396:GLN:HG3	2.10	0.52
1:B:409:TRP:CE2	1:B:410:VAL:HG23	2.44	0.52
1:B:119:LYS:CD	1:B:171:CYS:HB2	2.40	0.52
1:B:733:ILE:CG1	1:B:737:ALA:HB3	2.39	0.52
1:B:179:LYS:HB3	1:B:179:LYS:HZ3	1.75	0.52
1:B:733:ILE:HG13	1:B:737:ALA:CB	2.40	0.52
1:A:693:VAL:HB	1:A:766:TYR:CE2	2.44	0.52
1:A:324:LYS:HE3	1:A:325:TYR:CZ	2.45	0.52
1:A:810:LEU:HD13	1:A:936:ILE:HG13	1.92	0.52
1:A:1013:ASN:OD1	1:A:1015:MET:HE3	2.10	0.52
1:B:733:ILE:HG12	1:B:734:THR:N	2.25	0.51
1:B:151:PHE:CD1	1:B:151:PHE:C	2.88	0.51
1:A:429:ARG:NH1	1:A:431:ARG:HB3	2.16	0.51
1:B:179:LYS:HB3	1:B:179:LYS:NZ	2.24	0.51
1:B:806:MET:SD	1:B:924:GLU:HB3	2.50	0.51
1:B:882:PHE:CE1	1:B:933:LYS:HA	2.46	0.51
1:B:466:MET:HE2	1:B:466:MET:C	2.35	0.51
1:B:968:VAL:HG22	1:B:989:PRO:HG3	1.92	0.51
1:A:894:LEU:HG	1:A:925:VAL:HG21	1.92	0.51
1:B:831:TYR:HE2	2:D:12:ALA:HB2	1.75	0.51
1:B:86:SER:HB3	1:B:158:LEU:HG	1.93	0.51
1:B:196:ASN:HD22	1:B:198:ALA:N	2.09	0.51
1:A:406:PRO:HG3	1:A:461:PRO:HB3	1.93	0.50
1:A:550:LEU:HB3	1:A:1015:MET:HB2	1.92	0.50
1:A:697:LYS:O	1:A:701:LYS:HG2	2.11	0.50
1:A:723:LEU:HD12	1:A:755:THR:HG21	1.93	0.50
1:B:102:ASN:H	1:B:102:ASN:ND2	2.09	0.50
1:B:574:LEU:CD2	1:B:729:LEU:HD22	2.41	0.50
1:A:787:ASN:HB2	1:A:961:ARG:NH2	2.26	0.50
1:B:407:GLN:O	1:B:410:VAL:HB	2.11	0.50
1:B:800:GLN:HA	1:B:805:ASN:HD21	1.75	0.50
1:A:194:VAL:HG12	1:A:195:MET:HE2	1.93	0.50
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.44	0.50
1:A:189:GLU:O	1:A:192:LYS:HG2	2.11	0.50
1:A:183:VAL:HG23	1:A:226:LEU:HB3	1.94	0.50
1:B:449:VAL:HG23	1:B:450:LEU:N	2.27	0.50
1:B:882:PHE:CZ	1:B:933:LYS:HA	2.46	0.50
1:B:1015:MET:HE2	1:B:1015:MET:HA	1.94	0.50
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LEU:HD12	1:A:563:GLN:CD	2.36	0.50
1:A:733:ILE:HD11	1:A:741:ILE:HD12	1.93	0.50
1:A:213:HIS:CE1	1:A:292:PRO:HG3	2.47	0.50
1:A:499:GLN:HA	1:A:499:GLN:OE1	2.11	0.50
1:A:791:ILE:HG21	1:A:859:LEU:HD23	1.93	0.50
1:B:262:GLU:CD	1:B:262:GLU:H	2.19	0.50
1:B:328:SER:HB3	1:B:458:GLU:O	2.12	0.50
1:B:685:TYR:CZ	1:B:781:GLN:HG3	2.46	0.50
1:B:773:ASP:O	1:B:774:ARG:HB2	2.11	0.50
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.94	0.49
1:A:334:LEU:HD22	1:A:468:LEU:HD13	1.94	0.49
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.95	0.49
1:B:251:SER:HB3	1:B:278:VAL:CG1	2.39	0.49
1:B:158:LEU:HD23	1:B:158:LEU:O	2.12	0.49
1:B:285:LEU:HD22	1:B:286:PRO:HD2	1.93	0.49
1:A:259:LEU:C	1:A:259:LEU:HD23	2.37	0.49
1:A:555:ALA:HB1	1:A:757:PRO:HB3	1.93	0.49
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.94	0.49
1:A:578:PHE:HB2	1:A:627:MET:HB2	1.93	0.49
1:A:827:GLU:OE2	1:A:862:ARG:NH1	2.45	0.49
1:A:313:LEU:HD22	1:A:387:VAL:HG13	1.94	0.49
1:A:759:LEU:HD13	1:A:762:GLN:OE1	2.12	0.49
1:A:313:LEU:HD12	1:A:314:TYR:N	2.28	0.49
1:A:799:MET:SD	1:A:1006:PRO:HG2	2.53	0.49
1:B:311:ARG:HH21	1:B:668:ARG:HE	1.56	0.49
1:B:565:ASP:OD2	1:B:566:LYS:HG3	2.12	0.49
1:A:584:TYR:CZ	1:A:624:ILE:HG22	2.48	0.49
1:A:786:HIS:O	1:A:961:ARG:HB2	2.13	0.49
1:B:93:HIS:HD2	1:B:145:GLU:O	1.96	0.49
1:B:357:ASN:HB2	1:B:378:ASP:OD1	2.13	0.49
1:B:490:ASP:OD1	1:B:491:ARG:HG3	2.12	0.49
1:B:49:ARG:HG2	1:B:50:ILE:N	2.28	0.48
1:B:189:GLU:O	1:B:192:LYS:HG3	2.13	0.48
1:A:164:ARG:HG3	1:A:164:ARG:NH1	2.28	0.48
1:A:237:VAL:O	1:A:240:GLU:N	2.47	0.48
1:A:780:GLN:CD	1:A:959:LEU:HD11	2.38	0.48
1:A:374:ILE:HD12	1:A:374:ILE:C	2.39	0.48
1:B:854:LYS:HA	1:B:854:LYS:HE2	1.95	0.48
1:A:809:GLU:HB3	1:A:889:LEU:HD11	1.95	0.48
1:B:311:ARG:NH2	1:B:668:ARG:NE	2.56	0.48
1:B:793:ILE:HG22	1:B:795:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:ILE:HG22	1:B:844:GLN:N	2.29	0.48
1:A:950:ARG:HB3	1:A:950:ARG:HH11	1.79	0.48
1:B:820:PHE:CZ	1:B:824:ARG:HD3	2.48	0.48
1:B:823:LEU:HD12	1:B:829:LEU:HD12	1.96	0.48
1:A:334:LEU:CD2	1:A:468:LEU:HD13	2.44	0.48
1:A:679:HIS:ND1	1:A:851:GLN:OE1	2.47	0.48
1:B:686:LEU:HD23	1:B:838:ARG:NH1	2.29	0.48
1:B:942:GLU:O	1:B:942:GLU:HG2	2.14	0.48
1:A:600:LEU:HD21	1:A:649:MET:HB3	1.95	0.48
1:B:294:GLN:O	1:B:298:LEU:HG	2.12	0.48
1:A:783:ASN:ND2	1:A:786:HIS:N	2.56	0.48
1:B:538:LEU:HD12	1:B:538:LEU:N	2.28	0.48
1:A:151:PHE:CD1	1:A:151:PHE:C	2.92	0.47
1:A:445:PRO:O	1:A:446:LEU:C	2.57	0.47
1:B:56:LYS:NZ	1:B:62:ARG:O	2.38	0.47
1:B:251:SER:OG	1:B:280:ASN:HB2	2.14	0.47
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.96	0.47
1:B:667:MET:HE2	1:B:704:LEU:HD23	1.95	0.47
1:B:733:ILE:CG1	1:B:734:THR:N	2.77	0.47
1:A:314:TYR:HB2	1:A:479:ALA:HB3	1.95	0.47
1:B:204:LEU:CD2	1:B:304:ILE:HG12	2.44	0.47
1:B:475:ASN:N	1:B:475:ASN:ND2	2.62	0.47
1:B:802:THR:O	1:B:806:MET:HG2	2.14	0.47
1:B:821:ASN:O	1:B:825:THR:HB	2.13	0.47
1:B:842:GLY:C	1:B:843:ILE:HD13	2.39	0.47
1:A:864:GLU:HG3	1:A:986:LEU:HD21	1.95	0.47
1:B:530:PHE:O	1:B:531:ILE:C	2.58	0.47
1:B:575:ASN:N	1:B:575:ASN:ND2	2.55	0.47
1:B:622:ASN:H	1:B:622:ASN:ND2	2.12	0.47
1:B:868:ILE:O	1:B:871:GLU:HB3	2.15	0.47
1:B:871:GLU:O	1:B:875:GLU:HG3	2.15	0.47
1:A:674:ARG:HG3	1:A:674:ARG:HH11	1.80	0.47
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.96	0.47
1:B:299:LYS:HA	1:B:505:ILE:HD12	1.96	0.47
1:B:914:GLN:HA	1:B:916:TYR:CE1	2.50	0.47
1:A:120:LYS:HE3	1:B:409:TRP:CD1	2.50	0.47
1:A:803:SER:HA	1:A:927:TYR:CE2	2.49	0.47
1:A:823:LEU:HD12	1:A:829:LEU:HD11	1.95	0.47
1:A:896:LYS:HD3	1:A:896:LYS:HA	1.59	0.47
1:B:123:LYS:HB3	1:B:126:GLU:HG2	1.97	0.47
1:B:823:LEU:HD12	1:B:829:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:O	1:A:83:THR:HG22	2.14	0.47
1:A:367:ALA:HB3	1:A:370:PHE:CE2	2.50	0.47
1:A:550:LEU:HD11	1:A:558:LYS:HG2	1.97	0.47
1:B:114:LEU:HD13	1:B:168:PHE:HB3	1.97	0.47
1:B:196:ASN:HD22	1:B:196:ASN:C	2.23	0.47
1:B:223:LYS:HE3	1:B:227:GLU:OE1	2.14	0.47
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.47	0.47
1:B:329:ASN:CG	1:B:332:HIS:HD2	2.23	0.47
1:B:830:GLY:HA3	1:B:851:GLN:O	2.15	0.47
1:A:817:GLU:N	1:A:818:PRO:CD	2.77	0.47
1:B:643:LYS:O	1:B:647:GLU:HB2	2.15	0.47
1:B:789:CYS:O	1:B:851:GLN:HG3	2.15	0.47
1:A:123:LYS:HG2	1:A:125:ASN:ND2	2.30	0.47
1:A:558:LYS:HB2	1:A:558:LYS:HE3	1.80	0.47
1:A:722:ARG:CG	1:A:758:LEU:HD12	2.45	0.47
1:A:880:GLU:HG3	1:B:327:LYS:HD3	1.97	0.47
1:B:90:LEU:C	1:B:90:LEU:HD23	2.40	0.47
1:B:624:ILE:HG13	1:B:625:TYR:CD2	2.50	0.47
1:A:418:ASN:HB3	1:A:454:TYR:O	2.15	0.46
1:B:49:ARG:CG	1:B:50:ILE:H	2.28	0.46
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.96	0.46
1:B:822:THR:O	1:B:827:GLU:HG3	2.15	0.46
1:B:988:GLN:NE2	1:B:989:PRO:HD2	2.30	0.46
1:A:722:ARG:HG2	1:A:758:LEU:HD12	1.97	0.46
1:B:688:LEU:O	1:B:999:LYS:HE2	2.15	0.46
1:B:852:SER:OG	1:B:853:GLU:N	2.48	0.46
1:B:103:ILE:HD11	1:B:235:ILE:HG21	1.98	0.46
1:B:134:HIS:HD2	1:B:157:HIS:CG	2.34	0.46
1:B:280:ASN:OD1	1:B:282:ASN:N	2.48	0.46
1:B:708:THR:O	1:B:709:LEU:C	2.58	0.46
1:A:174:PHE:CD2	1:A:241:LEU:HB3	2.51	0.46
1:A:708:THR:OG1	1:A:711:ARG:HB2	2.15	0.46
1:A:742:MET:HE3	1:A:742:MET:HA	1.97	0.46
1:A:838:ARG:O	1:A:844:GLN:HA	2.16	0.46
1:A:66:GLY:O	1:A:67:LEU:HB3	2.16	0.46
1:A:933:LYS:O	1:A:937:ILE:HG12	2.16	0.46
1:B:116:LEU:CD1	1:B:178:CYS:HB3	2.45	0.46
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.97	0.46
1:A:172:PRO:HG2	1:A:245:HIS:NE2	2.30	0.46
1:A:767:ARG:NH1	1:A:1006:PRO:HA	2.31	0.46
1:B:352:SER:C	1:B:354:GLY:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LEU:O	1:B:466:MET:HB3	2.16	0.46
1:A:551:ILE:HD11	1:A:559:LEU:CD2	2.46	0.45
1:B:67:LEU:C	1:B:67:LEU:HD12	2.40	0.45
1:B:751:GLU:O	1:B:751:GLU:HG2	2.16	0.45
1:A:194:VAL:HG12	1:A:195:MET:CE	2.47	0.45
1:A:838:ARG:HG3	1:A:847:ARG:HD3	1.98	0.45
1:A:887:GLN:HE21	1:A:891:ILE:HD11	1.81	0.45
1:B:196:ASN:HD21	1:B:198:ALA:H	1.61	0.45
1:B:291:HIS:ND1	1:B:292:PRO:HD2	2.31	0.45
1:B:336:HIS:HD2	1:B:337:LEU:HD12	1.81	0.45
1:B:561:PHE:CG	1:B:562:LYS:N	2.85	0.45
1:B:655:ASP:HB3	1:B:658:ARG:HB2	1.98	0.45
1:B:800:GLN:CA	1:B:805:ASN:HD21	2.29	0.45
1:B:928:LEU:HD22	1:B:928:LEU:O	2.16	0.45
1:A:817:GLU:CG	1:A:818:PRO:HD3	2.37	0.45
1:B:90:LEU:HD11	1:B:254:MET:HE2	1.96	0.45
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.99	0.45
1:B:417:LEU:HD13	1:B:417:LEU:HA	1.78	0.45
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.51	0.45
1:A:708:THR:HB	1:A:710:PRO:HD2	1.97	0.45
1:A:817:GLU:HG3	1:A:818:PRO:N	2.32	0.45
1:B:296:GLU:HG2	1:B:297:HIS:CD2	2.51	0.45
1:B:528:ASN:HB3	1:B:531:ILE:CD1	2.47	0.45
1:B:783:ASN:HD22	1:B:786:HIS:H	1.62	0.45
1:A:285:LEU:HD23	1:A:286:PRO:N	2.31	0.45
1:A:299:LYS:HD2	1:A:510:ILE:HG13	1.98	0.45
1:A:433:TYR:O	1:A:437:ILE:HG12	2.17	0.45
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.17	0.45
1:B:558:LYS:HB3	1:B:726:GLU:HG3	1.96	0.45
1:B:794:TYR:CE1	1:B:838:ARG:HD3	2.52	0.45
1:B:1015:MET:O	1:B:1016:ALA:HB2	2.17	0.45
1:A:472:ARG:NH1	1:A:472:ARG:HG2	2.32	0.45
1:A:573:CYS:SG	1:A:632:LYS:HD3	2.56	0.45
1:A:583:ALA:HB3	1:A:626:GLY:HA2	1.99	0.45
1:A:871:GLU:OE2	1:A:941:LYS:HE3	2.17	0.45
1:B:674:ARG:NH1	4:B:1201:HOH:O	2.28	0.45
1:B:771:LEU:HB2	1:B:952:HIS:HB3	1.98	0.45
1:A:674:ARG:HD3	1:A:784:GLU:OE2	2.17	0.44
1:B:116:LEU:HD12	1:B:178:CYS:HB3	1.99	0.44
1:B:227:GLU:C	1:B:230:PRO:HD2	2.42	0.44
1:B:793:ILE:CG2	1:B:795:TYR:CE1	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LYS:HE2	1:B:129:GLN:OE1	2.17	0.44
1:B:379:LEU:HD13	1:B:384:LEU:HA	1.99	0.44
1:B:445:PRO:O	1:B:446:LEU:C	2.61	0.44
1:B:643:LYS:HB2	1:B:744:MET:SD	2.58	0.44
1:B:689:LEU:CD2	1:B:995:MET:HE2	2.47	0.44
1:A:346:LEU:HA	1:A:522:PHE:CE2	2.52	0.44
1:A:756:LYS:HB3	1:A:756:LYS:HE2	1.71	0.44
1:A:782:ARG:NH1	1:A:961:ARG:O	2.50	0.44
1:B:83:THR:OG1	1:B:85:LYS:O	2.32	0.44
1:A:147:THR:CG2	1:A:149:TYR:CE1	2.97	0.44
1:B:196:ASN:ND2	1:B:196:ASN:C	2.75	0.44
1:B:548:PRO:HA	1:B:562:LYS:HB2	1.99	0.44
1:B:858:TYR:OH	1:B:862:ARG:HD2	2.17	0.44
1:A:173:LEU:O	1:A:174:PHE:C	2.61	0.44
1:A:779:TYR:CE1	1:A:995:MET:HE3	2.53	0.44
1:B:65:ARG:HH21	1:B:65:ARG:HG3	1.82	0.44
1:A:73:ILE:HG13	1:A:251:SER:HB2	1.99	0.44
1:A:239:GLN:O	1:A:243:LYS:N	2.44	0.44
1:A:801:SER:O	1:A:802:THR:C	2.58	0.44
1:A:986:LEU:HA	1:A:987:PRO:HD3	1.85	0.44
1:B:53:HIS:N	1:B:53:HIS:CD2	2.84	0.44
1:B:191:GLU:HA	1:B:194:VAL:HG23	1.98	0.44
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.47	0.44
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.52	0.44
1:A:174:PHE:CE2	1:A:241:LEU:HB3	2.53	0.44
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.17	0.44
1:A:102:ASN:HD22	1:A:102:ASN:H	1.65	0.44
1:A:459:PHE:CZ	1:A:461:PRO:HG3	2.53	0.44
1:B:721:SER:O	1:B:755:THR:HA	2.18	0.44
1:B:71:ASN:ND2	1:B:276:SER:HA	2.33	0.43
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.83	0.43
1:A:635:ASN:O	1:A:636:ASP:C	2.61	0.43
1:A:65:ARG:HB2	1:A:264:LEU:HD13	2.00	0.43
1:A:97:LEU:HB2	1:A:144:GLY:O	2.18	0.43
1:B:201:LEU:HD12	1:B:201:LEU:HA	1.87	0.43
1:B:711:ARG:CG	1:B:711:ARG:NH2	2.75	0.43
1:A:231:ASN:C	1:A:233:GLU:N	2.75	0.43
1:A:542:LYS:HB2	1:A:542:LYS:NZ	2.33	0.43
1:A:787:ASN:OD1	1:A:962:GLU:HG2	2.17	0.43
1:B:153:VAL:O	1:B:154:SER:C	2.60	0.43
1:B:538:LEU:H	1:B:538:LEU:CD1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:GLU:O	1:B:961:ARG:HD3	2.18	0.43
1:B:801:SER:H	1:B:805:ASN:ND2	2.15	0.43
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.73	0.43
1:A:656:GLU:OE1	1:A:656:GLU:HA	2.18	0.43
1:A:900:LEU:O	1:A:901:SER:C	2.59	0.43
1:B:158:LEU:C	1:B:158:LEU:CD2	2.92	0.43
1:B:168:PHE:N	1:B:168:PHE:CD1	2.86	0.43
1:B:405:GLY:O	1:B:406:PRO:C	2.60	0.43
1:B:759:LEU:HD12	1:B:759:LEU:HA	1.84	0.43
1:B:967:PRO:C	1:B:968:VAL:HG12	2.43	0.43
1:A:227:GLU:O	1:A:228:THR:C	2.61	0.43
1:A:305:VAL:HG23	1:A:489:THR:HG21	2.00	0.43
1:A:638:GLN:HB2	1:A:639:PRO:HD3	2.01	0.43
1:A:827:GLU:CD	1:A:862:ARG:HH11	2.26	0.43
1:B:411:PHE:CD2	1:B:459:PHE:HB2	2.53	0.43
1:B:611:ALA:HB1	1:B:616:LEU:HB3	2.00	0.43
1:B:733:ILE:HD11	1:B:738:ALA:N	2.32	0.43
1:B:833:VAL:O	1:B:833:VAL:HG12	2.17	0.43
1:A:934:GLU:O	1:A:938:LYS:HG3	2.18	0.43
1:B:116:LEU:HD13	1:B:178:CYS:SG	2.59	0.43
1:B:407:GLN:HG3	1:B:409:TRP:HE1	1.82	0.43
1:B:429:ARG:HG2	1:B:429:ARG:HH11	1.84	0.43
1:B:843:ILE:HG22	1:B:844:GLN:H	1.82	0.43
1:A:824:ARG:HB2	1:A:833:VAL:HG21	2.00	0.43
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.54	0.43
1:B:228:THR:HG23	4:B:1222:HOH:O	2.18	0.43
1:B:270:LEU:O	1:B:274:LEU:HG	2.19	0.43
1:B:346:LEU:HD23	1:B:359:LEU:HD11	2.01	0.43
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.51	0.43
1:B:685:TYR:O	1:B:686:LEU:C	2.61	0.43
1:A:490:ASP:C	1:A:491:ARG:HG3	2.44	0.43
1:A:714:ALA:O	1:A:717:PRO:HD2	2.19	0.43
1:B:174:PHE:HE2	1:B:241:LEU:HD22	1.84	0.43
1:B:860:GLU:OE1	1:B:957:HIS:CE1	2.72	0.43
1:A:200:ARG:HH21	1:A:498:THR:HA	1.82	0.42
1:A:806:MET:CE	1:A:928:LEU:HG	2.49	0.42
1:A:992:ILE:HD11	1:A:998:PHE:CE1	2.54	0.42
1:B:162:LEU:HG	1:B:274:LEU:HD12	2.00	0.42
1:B:779:TYR:CZ	1:B:995:MET:HE3	2.54	0.42
1:B:896:LYS:HA	1:B:896:LYS:HD3	1.68	0.42
1:A:236:ASP:OD1	1:A:236:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:VAL:HA	1:A:951:ARG:CZ	2.49	0.42
1:B:304:ILE:HB	1:B:481:VAL:HG22	2.00	0.42
1:B:823:LEU:CB	1:B:833:VAL:HG11	2.49	0.42
1:A:237:VAL:C	1:A:239:GLN:N	2.76	0.42
1:A:635:ASN:OD1	1:A:732:ASN:HB3	2.19	0.42
1:A:868:ILE:HD11	1:A:984:PRO:HD3	2.00	0.42
1:B:783:ASN:HD22	1:B:785:VAL:H	1.66	0.42
1:A:139:ASN:OD1	2:C:10:ALA:HB3	2.20	0.42
1:A:412:GLN:NE2	1:A:415:LYS:NZ	2.67	0.42
1:A:965:SER:O	1:A:966:CYS:HB2	2.19	0.42
1:B:407:GLN:CG	1:B:409:TRP:HE1	2.31	0.42
1:B:786:HIS:CD2	1:B:786:HIS:N	2.86	0.42
1:B:846:LEU:CD2	1:B:847:ARG:N	2.81	0.42
1:B:77:LEU:HD21	1:B:271:VAL:CG2	2.49	0.42
1:B:686:LEU:HD12	1:B:686:LEU:HA	1.80	0.42
1:B:928:LEU:HD22	1:B:928:LEU:C	2.44	0.42
1:A:77:LEU:HD21	1:A:271:VAL:HG21	2.02	0.42
1:A:604:LEU:O	1:A:605:ASN:C	2.61	0.42
1:A:674:ARG:NH1	1:A:675:ALA:HB2	2.35	0.42
1:B:364:LYS:HB3	1:B:372:PHE:HB2	2.02	0.42
1:B:849:ILE:C	1:B:850:ILE:HG13	2.44	0.42
1:A:347:LEU:HD22	1:A:347:LEU:O	2.20	0.42
1:A:353:LYS:HD3	1:A:355:TRP:CZ3	2.54	0.42
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.87	0.42
1:B:90:LEU:HD23	1:B:91:ASP:N	2.34	0.42
1:A:600:LEU:HD11	1:A:648:LYS:HB3	2.00	0.42
1:A:791:ILE:HG22	1:A:850:ILE:O	2.20	0.42
1:A:810:LEU:HD12	1:A:931:LEU:HD23	2.01	0.42
1:A:948:ALA:HB3	1:A:951:ARG:HB2	2.01	0.42
1:B:459:PHE:O	1:B:461:PRO:HD2	2.20	0.42
1:B:882:PHE:CE2	1:B:886:ILE:HD11	2.55	0.42
1:B:899:LYS:O	1:B:900:LEU:C	2.63	0.42
1:A:527:LYS:HD3	1:A:528:ASN:N	2.34	0.42
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.55	0.42
1:B:281:LYS:O	1:B:282:ASN:C	2.62	0.42
1:B:424:PHE:CE1	1:B:535:PHE:CD2	3.08	0.42
1:B:767:ARG:NH1	1:B:1006:PRO:HA	2.35	0.42
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.89	0.42
1:A:783:ASN:ND2	1:A:785:VAL:H	2.18	0.42
1:A:792:GLU:HA	1:A:848:PHE:O	2.20	0.42
1:B:153:VAL:HG22	1:B:154:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASN:O	1:B:330:PRO:C	2.63	0.42
1:B:422:PHE:CE2	1:B:451:THR:HG22	2.54	0.42
1:B:793:ILE:O	1:B:847:ARG:HA	2.20	0.42
1:B:886:ILE:HG23	1:B:928:LEU:HD13	2.01	0.42
1:A:93:HIS:CD2	1:A:145:GLU:O	2.72	0.41
1:A:190:HIS:O	1:A:194:VAL:HG23	2.21	0.41
1:A:301:LEU:HA	1:A:478:VAL:O	2.20	0.41
1:A:355:TRP:HB3	1:A:390:ILE:HD11	2.01	0.41
1:A:476:VAL:CG2	1:A:477:ARG:N	2.82	0.41
1:A:733:ILE:HG12	1:A:737:ALA:HB3	2.02	0.41
1:B:288:PHE:O	1:B:369:GLY:HA3	2.20	0.41
1:A:121:TYR:HB3	1:A:126:GLU:HG2	2.02	0.41
1:A:343:PRO:HD3	1:A:606:GLU:HG2	2.02	0.41
1:A:821:ASN:O	1:A:825:THR:HB	2.20	0.41
1:B:49:ARG:CG	1:B:50:ILE:N	2.83	0.41
1:B:114:LEU:HD12	1:B:149:TYR:CZ	2.55	0.41
1:B:125:ASN:ND2	1:B:817:GLU:OE1	2.54	0.41
1:A:405:GLY:O	1:A:406:PRO:C	2.62	0.41
1:A:551:ILE:HD11	1:A:559:LEU:HD21	2.02	0.41
1:B:301:LEU:HD12	1:B:302:TYR:H	1.85	0.41
1:A:501:LYS:NZ	1:A:503:GLU:HG2	2.36	0.41
1:A:591:ASN:O	1:A:595:LEU:CD2	2.68	0.41
1:B:90:LEU:HD11	1:B:254:MET:HE3	1.97	0.41
1:B:168:PHE:N	1:B:168:PHE:HD1	2.18	0.41
1:B:862:ARG:CZ	1:B:862:ARG:HA	2.51	0.41
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.51	0.41
1:A:591:ASN:O	1:A:595:LEU:HD22	2.20	0.41
1:B:94:ILE:HG13	1:B:248:TYR:HB3	2.02	0.41
1:B:259:LEU:HD23	1:B:260:GLY:N	2.36	0.41
1:B:540:LEU:HD12	1:B:540:LEU:HA	1.92	0.41
1:A:281:LYS:O	1:A:282:ASN:C	2.64	0.41
1:A:283:VAL:HA	1:A:284:PRO:HD3	1.85	0.41
1:A:622:ASN:N	1:A:622:ASN:ND2	2.51	0.41
1:A:676:GLU:OE2	1:A:676:GLU:HA	2.21	0.41
1:B:78:ILE:HB	1:B:259:LEU:HB2	2.03	0.41
1:B:119:LYS:CG	1:B:171:CYS:HB2	2.50	0.41
1:B:591:ASN:HD21	1:B:700:LEU:HB3	1.86	0.41
1:B:870:MET:O	1:B:874:ILE:HG13	2.20	0.41
1:A:108:HIS:O	1:A:111:GLN:HB3	2.21	0.41
1:A:168:PHE:O	1:A:172:PRO:HG3	2.20	0.41
1:A:767:ARG:HG2	1:A:1007:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:TYR:HD2	1:B:76:LEU:HD11	1.85	0.41
1:B:213:HIS:ND1	1:B:214:PRO:HD2	2.35	0.41
1:B:315:VAL:HG21	1:B:394:MET:SD	2.60	0.41
1:B:616:LEU:HA	1:B:616:LEU:HD23	1.75	0.41
1:A:102:ASN:ND2	1:A:102:ASN:H	2.19	0.41
1:A:285:LEU:HD23	1:A:285:LEU:C	2.46	0.41
1:A:415:LYS:HA	1:A:456:LEU:HD12	2.03	0.41
1:A:488:LYS:HD2	1:A:488:LYS:N	2.36	0.41
1:A:519:ASN:OD1	1:A:519:ASN:C	2.64	0.41
1:A:656:GLU:HB2	4:A:1212:HOH:O	2.21	0.41
1:A:889:LEU:HA	1:A:889:LEU:HD23	1.76	0.41
1:B:337:LEU:HD23	1:B:401:LEU:CD2	2.51	0.41
1:B:504:ALA:O	1:B:505:ILE:C	2.64	0.41
1:B:542:LYS:HB2	1:B:542:LYS:HZ3	1.85	0.41
1:B:728:LEU:C	1:B:728:LEU:CD2	2.93	0.41
1:A:794:TYR:HE1	1:A:845:GLY:HA3	1.86	0.41
1:B:176:GLU:OE1	1:B:179:LYS:NZ	2.45	0.41
1:B:858:TYR:O	1:B:861:SER:OG	2.22	0.41
1:A:67:LEU:C	1:A:67:LEU:CD1	2.93	0.40
1:A:95:GLY:O	1:A:96:SER:C	2.64	0.40
1:A:159:GLU:O	1:A:160:GLY:C	2.61	0.40
1:A:184:ASN:HD22	1:A:184:ASN:HA	1.70	0.40
1:A:928:LEU:O	1:A:928:LEU:HD22	2.20	0.40
1:B:96:SER:HA	1:B:107:SER:OG	2.21	0.40
1:B:173:LEU:O	1:B:174:PHE:HB2	2.21	0.40
1:B:711:ARG:HG3	1:B:711:ARG:NH2	2.12	0.40
1:B:722:ARG:HB3	1:B:758:LEU:HD12	2.04	0.40
1:B:821:ASN:HA	1:B:825:THR:OG1	2.20	0.40
1:B:834:PHE:CD2	1:B:834:PHE:C	2.99	0.40
1:A:248:TYR:O	1:A:250:SER:N	2.49	0.40
1:B:285:LEU:HD22	1:B:286:PRO:CD	2.51	0.40
1:B:523:LYS:HD2	1:B:523:LYS:N	2.35	0.40
1:B:576:PHE:CD1	1:B:576:PHE:N	2.89	0.40
1:B:629:LEU:HD22	1:B:629:LEU:C	2.46	0.40
1:B:779:TYR:CE2	1:B:995:MET:HE3	2.55	0.40
1:B:846:LEU:HD22	1:B:848:PHE:CE1	2.56	0.40
1:A:93:HIS:CE1	1:A:368:ARG:HE	2.38	0.40
1:A:111:GLN:NE2	1:A:140:ALA:HB3	2.35	0.40
1:A:303:LYS:NZ	1:A:503:GLU:OE1	2.45	0.40
1:B:209:GLY:O	1:B:210:ASN:C	2.63	0.40
1:B:459:PHE:O	1:B:461:PRO:CD	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:840:ALA:C	1:B:842:GLY:H	2.28	0.40
1:A:311:ARG:NH1	1:A:379:LEU:O	2.43	0.40
1:A:319:ILE:HG13	1:A:371:MET:HB2	2.03	0.40
1:A:793:ILE:HG22	1:A:795:TYR:CE1	2.57	0.40
1:B:460:ARG:NH1	1:B:462:ASP:OD2	2.54	0.40
1:B:576:PHE:CE2	1:B:745:VAL:HG21	2.56	0.40
1:B:591:ASN:ND2	1:B:700:LEU:CD2	2.84	0.40
1:B:856:PRO:HB2	1:B:957:HIS:CD2	2.57	0.40
1:A:210:ASN:HA	1:A:211:PRO:HD3	1.89	0.40
1:A:412:GLN:HE21	1:A:415:LYS:NZ	2.19	0.40
1:A:416:ASP:O	1:A:420:VAL:HG23	2.21	0.40
1:A:823:LEU:HD22	1:A:823:LEU:N	2.37	0.40
1:B:483:LYS:HD3	1:B:483:LYS:HA	1.97	0.40
1:B:505:ILE:H	1:B:505:ILE:HG13	1.73	0.40
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.56	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	959/990 (97%)	885 (92%)	61 (6%)	13 (1%)	9	36
1	B	957/990 (97%)	861 (90%)	79 (8%)	17 (2%)	6	31
2	C	6/12 (50%)	5 (83%)	1 (17%)	0	100	100
2	D	6/12 (50%)	6 (100%)	0	0	100	100
All	All	1928/2004 (96%)	1757 (91%)	141 (7%)	30 (2%)	7	34

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	981	SER
1	B	48	LYS
1	B	52	ASN
1	B	984	PRO
1	B	1012	ILE
1	B	1015	MET
1	B	1016	ALA
1	B	721	SER
1	A	228	THR
1	A	232	GLN
1	A	233	GLU
1	A	368	ARG
1	A	672	ASN
1	A	987	PRO
1	B	484	SER
1	B	967	PRO
1	A	53	HIS
1	A	449	VAL
1	A	1014	PHE
1	B	67	LEU
1	A	96	SER
1	B	430	PRO
1	B	965	SER
1	B	368	ARG
1	B	405	GLY
1	A	406	PRO
1	A	967	PRO
1	B	366	GLY
1	B	449	VAL
1	B	833	VAL

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	859/883 (97%)	805 (94%)	54 (6%)	16	48
1	B	858/883 (97%)	795 (93%)	63 (7%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1717/1766 (97%)	1600 (93%)	117 (7%)	14	45

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	67	LEU
1	A	81	PRO
1	A	97	LEU
1	A	102	ASN
1	A	125	ASN
1	A	158	LEU
1	A	188	SER
1	A	196	ASN
1	A	226	LEU
1	A	238	ARG
1	A	270	LEU
1	A	313	LEU
1	A	316	THR
1	A	337	LEU
1	A	347	LEU
1	A	417	LEU
1	A	450	LEU
1	A	466	MET
1	A	475	ASN
1	A	540	LEU
1	A	542	LYS
1	A	543	GLU
1	A	595	LEU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	635	ASN
1	A	642	LEU
1	A	643	LYS
1	A	656	GLU
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	719	LEU
1	A	728	LEU
1	A	733	ILE

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Mol	Chain	Res	Type
1	A	744	MET
1	A	756	LYS
1	A	772	PRO
1	A	777	PHE
1	A	783	ASN
1	A	801	SER
1	A	810	LEU
1	A	817	GLU
1	A	846	LEU
1	A	852	SER
1	A	889	LEU
1	A	928	LEU
1	A	933	LYS
1	A	968	VAL
1	A	993	GLN
1	A	1007	LEU
1	A	1013	ASN
1	B	74	LYS
1	B	102	ASN
1	B	126	GLU
1	B	128	SER
1	B	158	LEU
1	B	168	PHE
1	B	179	LYS
1	B	196	ASN
1	B	201	LEU
1	B	226	LEU
1	B	238	ARG
1	B	243	LYS
1	B	270	LEU
1	B	285	LEU
1	B	287	GLU
1	B	347	LEU
1	B	356	VAL
1	B	417	LEU
1	B	431	ARG
1	B	446	LEU
1	B	450	LEU
1	B	457	GLU
1	B	466	MET
1	B	475	ASN
1	B	488	LYS

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Mol	Chain	Res	Type
1	B	507	ASP
1	B	512	LYS
1	B	523	LYS
1	B	524	LEU
1	B	540	LEU
1	B	542	LYS
1	B	543	GLU
1	B	575	ASN
1	B	595	LEU
1	B	597	LEU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	657	LYS
1	B	677	GLN
1	B	678	PRO
1	B	687	ARG
1	B	711	ARG
1	B	712	LEU
1	B	722	ARG
1	B	728	LEU
1	B	733	ILE
1	B	744	MET
1	B	759	LEU
1	B	768	GLU
1	B	783	ASN
1	B	825	THR
1	B	846	LEU
1	B	862	ARG
1	B	880	GLU
1	B	928	LEU
1	B	964	ASP
1	B	966	CYS
1	B	968	VAL
1	B	1007	LEU
1	B	1012	ILE
1	B	1015	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	102	ASN
1	A	111	GLN
1	A	125	ASN
1	A	129	GLN
1	A	167	GLN
1	A	184	ASN
1	A	196	ASN
1	A	203	GLN
1	A	231	ASN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	332	HIS
1	A	336	HIS
1	A	363	GLN
1	A	376	ASN
1	A	412	GLN
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	622	ASN
1	A	672	ASN
1	A	718	GLN
1	A	730	HIS
1	A	736	GLN
1	A	743	GLN
1	A	780	GLN
1	A	781	GLN
1	A	783	ASN
1	A	805	ASN
1	A	813	GLN
1	A	828	GLN
1	A	922	ASN
1	B	52	ASN
1	B	53	HIS
1	B	93	HIS
1	B	102	ASN
1	B	134	HIS
1	B	157	HIS
1	B	184	ASN
1	B	190	HIS
1	B	196	ASN

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Mol	Chain	Res	Type
1	B	231	ASN
1	B	239	GLN
1	B	297	HIS
1	B	300	GLN
1	B	332	HIS
1	B	336	HIS
1	B	386	HIS
1	B	393	HIS
1	B	399	GLN
1	B	475	ASN
1	B	502	GLN
1	B	515	ASN
1	B	534	ASN
1	B	575	ASN
1	B	591	ASN
1	B	605	ASN
1	B	622	ASN
1	B	672	ASN
1	B	718	GLN
1	B	743	GLN
1	B	783	ASN
1	B	786	HIS
1	B	805	ASN
1	B	828	GLN
1	B	887	GLN
1	B	917	ASN
1	B	922	ASN
1	B	957	HIS
1	B	982	GLN
1	B	988	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	DIO	A	1101	-	6,6,6	0.75	0	6,6,6	0.27	0
3	DIO	B	1101	-	6,6,6	0.77	0	6,6,6	0.25	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	DIO	A	1101	-	-	-	0/1/1/1
3	DIO	B	1101	-	-	-	0/1/1/1

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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	DIO	3	0
3	B	1101	DIO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3:ALA	C	6:ALA	N	12.43
1	C	3:ALA	C	6:ALA	N	12.25

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	963/990 (97%)	-0.79	7 (0%) 84 66	15, 34, 60, 96	0
1	B	961/990 (97%)	-0.61	4 (0%) 88 76	19, 44, 71, 98	0
2	C	10/12 (83%)	1.10	2 (20%) 3 2	30, 60, 73, 75	0
2	D	10/12 (83%)	1.01	1 (10%) 12 7	29, 61, 76, 80	0
All	All	1944/2004 (97%)	-0.68	14 (0%) 84 66	15, 39, 68, 98	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1016	ALA	3.4
1	A	980	LEU	3.3
1	A	1014	PHE	3.2
1	B	1017	ALA	3.1
1	A	44	ASN	3.1
1	B	45	PRO	2.9
1	A	968	VAL	2.8
1	B	967	PRO	2.6
2	C	6	ALA	2.6
2	D	12	ALA	2.6
2	C	12	ALA	2.5
1	A	1015	MET	2.3
1	B	968	VAL	2.3
1	A	1013	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	DIO	A	1101	6/6	0.96	0.11	45,55,60,61	0
3	DIO	B	1101	6/6	0.97	0.09	26,34,43,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.