



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:54 AM UTC

PDB ID : 3Q2V / pdb_00003q2v
Title : Crystal structure of mouse E-cadherin ectodomain
Authors : Jin, X.; Harrison, O.J.; Shapiro, L.
Deposited on : 2010-12-20
Resolution : 3.40 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

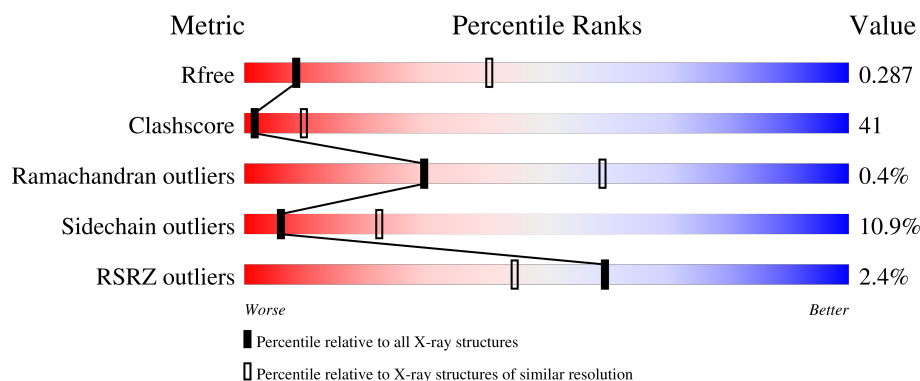
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	550	
1	B	550	

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	MAN	A	802	X	-	-	-
4	MAN	A	804	X	-	-	-
4	MAN	A	805	X	-	-	-
4	MAN	A	806	X	-	-	-
4	MAN	A	807	X	-	-	-
4	MAN	B	801	X	-	-	-
4	MAN	B	803	X	-	-	-
4	MAN	B	804	X	-	-	-
4	MAN	B	805	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7871 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 Cadherin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	1	0
			4113	2581	683	838	11			
1	B	440	Total	C	N	O	S	0	0	0
			3399	2138	553	701	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	HIS	-	expression tag	UNP P09803
A	546	HIS	-	expression tag	UNP P09803
A	547	HIS	-	expression tag	UNP P09803
A	548	HIS	-	expression tag	UNP P09803
A	549	HIS	-	expression tag	UNP P09803
A	550	HIS	-	expression tag	UNP P09803
B	545	HIS	-	expression tag	UNP P09803
B	546	HIS	-	expression tag	UNP P09803
B	547	HIS	-	expression tag	UNP P09803
B	548	HIS	-	expression tag	UNP P09803
B	549	HIS	-	expression tag	UNP P09803
B	550	HIS	-	expression tag	UNP P09803

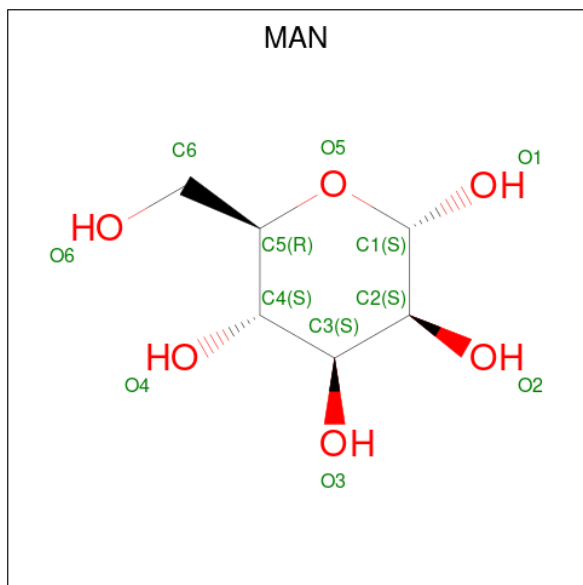
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	Ca	0	0
			12	12		
2	B	12	Total	Ca	0	0
			12	12		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

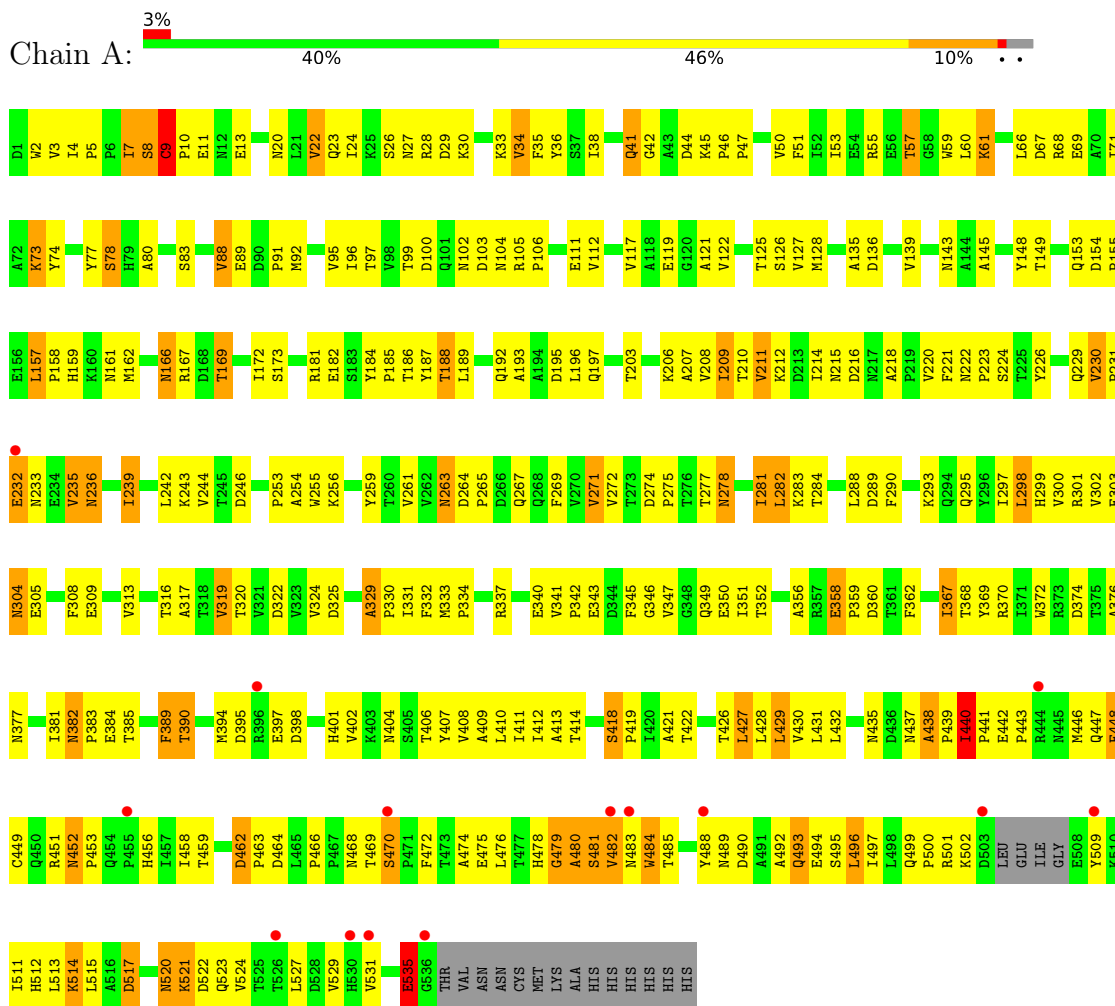
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total	O	0	0
			55	55		
5	B	80	Total	O	0	0
			80	80		

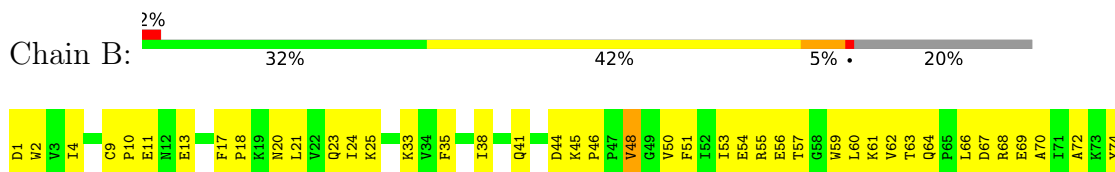
3 Residue-property plots

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: Cadherin-1



• Molecule 1: Cadherin-1



GLY	MET	I371	K372	E306	Q229	F163	Y77
	GLU	GLN	P307	E307	Q230	T164	
TYR	PHE	R373	F308	F308	P231	V165	
LYS	CYS	D374	E309	E309	E232	M166	Y95
ILE	GLN				V235		T97
HIS	ARG	W378	L312	L312			V98
LEU	ASN	L379	V313	V313	R238	G170	T99
LYS	PRO	Q380	E380	E380	I239	V171	D100
LEU	GLN	E381	S315	S315	T239		Q101
ALA	PRO	N382	T316	T316	A240	L175	
ASP	HIS	N383	A317	A317	T241	T176	
ASN	ILE	P384			L242	S177	R105
GLN	ILE	T385	T320	T320	L243		P106
ASN	THR	G386	V321	V321	V244	D180	E107
LYS	ILE	A387	D322	D322	T245	R181	F108
ASP	LEU	L388	V323	V323	D246	E182	
GLN	D462	F389	V324	V324	D247	S183	E111
VAL	P463	R390	D325	D325	D248	Y184	F112
THR		T391	V326	V326	A249	P185	F113
THR	P466	A392	N327	N327	F250	T186	E114
LEU	P467	E393	E328	E328	N251	Y187	G115
ASP	ASN	M394	A329	A329	T252	T188	S116
VAL	THR	R396	P330	P330	P253	L189	V117
HIS	SER	I331	D395	D395	A254	V190	A118
VAL	PRO	E397	F332	F332	W255	Q192	E119
CYS	PHE	D398			K256	G192	G120
ASP	THR		R337	R337		A193	A121
CYS	ALA	T406	R338	R338	T260	A194	V122
GLU	GLU		V339	V339	V261	D195	P123
GLY	THR	L410	E340	E340	V262	L196	G124
THR	LEU	I411	V341	V341	N263	Q197	T125
VAL	HIS	I412	P342	P342	G198	S126	V126
ASN	GLY	A413	E343	E343	V271	F199	V127
ASN	ALA	T414	D344	D344		G200	M128
CYS	SER	D415	F345	F345	D274	L201	K129
MET	VAL	D416	G346	G346		S202	
LYS	ASN	G417	V347	V347	T277	T203	A132
ALA	TRP	S418	G348	G348	N278		
HIS	THR	P419	Q349	Q349	D279	K206	D136
HIS	ILE	I420	E350	E350	G280	A207	D137
HIS	GLU	A421	T351	T351	I281	E208	D138
HIS	TYR	T422	T352	T352	L282	V139	
HIS	ASN		S353	S353	T210		
ASP	ASP	L429	Y354	Y354	G287	T210	
ALA	ALA	V430	T355	T355	V211	A144	A145
ALA	ALA	L431	A356	A356	K212	I146	
GLN	GLN	D432	R357	R357	D213	A147	
GLU	GLU	D433	E358	E358	T214	Y148	
SER	SER	V434	P359	P359	D216	T149	
LEU	LEU	ASN	D360	D360	N217	I150	
ILE	ILE	ASP	T361	T361	A218	V151	
LEU	LEU	ASN	F362	F362	P219	S152	
GLN	GLN	ALA	L298	L298	V220	Q153	
PRO	PRO	PRO	D364	D364	F221	D154	
ARG	ARG	ILE	Q365	Q365	N222		
PRO	PRO	PRO	K366	K366	R301	P223	
ASP	ASP	GLU	T367	T367	V302		
LEU	LEU	PRO	T368	T368	E303		L157
GLU	GLU	ASN	Y369	Y369	N304	Y226	P158
ILE	ILE	ASN	R370	R370	E305	Q227	R159
						G228	M162

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.14Å 79.70Å 176.00Å 90.00° 98.56° 90.00°	Depositor
Resolution (Å)	19.92 – 3.40 19.92 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.92-3.40) 99.3 (19.92-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.230 , 0.293 0.229 , 0.287	Depositor DCC
R_{free} test set	1254 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7871	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% 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: MN, CA, MAN

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	0.57	0/4200	1.08	30/5755 (0.5%)
1	B	0.60	4/3469 (0.1%)	1.03	19/4752 (0.4%)
All	All	0.58	4/7669 (0.1%)	1.06	49/10507 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	HIS	ND1-CE1	6.83	1.39	1.32
1	B	159	HIS	CG-ND1	-5.69	1.31	1.38
1	B	159	HIS	CE1-NE2	-5.42	1.27	1.32
1	B	419	PRO	N-CD	5.10	1.54	1.47

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	ALA	N-CA-CB	-10.48	93.98	111.17
1	A	492	ALA	N-CA-C	10.10	125.59	112.26
1	A	232	GLU	N-CA-C	9.77	126.02	112.45
1	A	233	ASN	N-CA-C	9.43	124.71	112.26
1	A	470	SER	N-CA-C	9.02	124.97	113.25
1	B	419	PRO	CB-CA-C	8.88	126.21	111.56
1	A	451	ARG	N-CA-C	8.68	124.20	111.96
1	B	419	PRO	N-CA-C	-8.67	94.62	112.47
1	A	329	ALA	CA-C-N	8.35	128.38	119.78
1	A	329	ALA	C-N-CA	8.35	128.38	119.78
1	A	452	ASN	N-CA-C	-8.13	91.18	108.73
1	A	462	ASP	CA-C-N	7.34	127.20	119.05
1	A	462	ASP	C-N-CA	7.34	127.20	119.05
1	A	452	ASN	N-CA-CB	7.15	124.47	110.61
1	A	313	VAL	CA-C-N	7.06	127.03	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	VAL	C-N-CA	7.06	127.03	119.76
1	A	438	ALA	CA-C-N	6.72	126.70	119.78
1	A	438	ALA	C-N-CA	6.72	126.70	119.78
1	B	4	ILE	CA-C-N	6.66	124.52	119.66
1	B	4	ILE	C-N-CA	6.66	124.52	119.66
1	A	236	ASN	N-CA-C	6.46	124.55	110.80
1	B	415	ASP	N-CA-C	6.36	120.43	110.32
1	B	364	ASP	N-CA-C	6.33	120.63	112.41
1	A	440	ILE	CA-C-N	6.12	126.03	119.85
1	A	440	ILE	C-N-CA	6.12	126.03	119.85
1	A	479	GLY	N-CA-C	6.00	127.40	113.18
1	B	184	TYR	CA-C-N	5.95	127.28	119.84
1	B	184	TYR	C-N-CA	5.95	127.28	119.84
1	A	235	VAL	CB-CA-C	-5.77	101.65	110.95
1	B	416	ASP	N-CA-C	5.57	122.66	110.80
1	A	493	GLN	N-CA-C	5.55	119.23	111.74
1	A	233	ASN	N-CA-CB	-5.54	102.08	111.17
1	B	313	VAL	CA-C-N	5.49	125.40	119.85
1	B	313	VAL	C-N-CA	5.49	125.40	119.85
1	A	382	ASN	CA-C-N	5.46	126.66	119.84
1	A	382	ASN	C-N-CA	5.46	126.66	119.84
1	B	365	GLN	N-CA-C	5.44	118.93	110.17
1	A	220	VAL	N-CA-C	5.43	115.72	108.11
1	B	208	VAL	N-CA-C	5.41	115.64	107.80
1	B	218	ALA	CA-C-N	5.34	125.10	119.76
1	B	218	ALA	C-N-CA	5.34	125.10	119.76
1	B	127	VAL	CB-CA-C	-5.25	105.60	111.80
1	A	535	GLU	N-CA-C	-5.20	107.00	113.55
1	A	9	CYS	CA-C-N	5.18	126.31	119.84
1	A	9	CYS	C-N-CA	5.18	126.31	119.84
1	B	231	PRO	N-CA-C	-5.17	101.82	112.47
1	B	232	GLU	N-CA-C	5.07	118.23	111.75
1	B	159	HIS	CG-CD2-NE2	-5.04	102.17	107.20
1	A	448	PHE	N-CA-C	5.00	117.50	110.14

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	4113	0	3949	357	0
1	B	3399	0	3284	274	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	99	0	90	1	0
4	B	99	0	90	4	0
5	A	55	0	0	1	0
5	B	80	0	0	0	0
All	All	7871	0	7413	621	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 41.

All (621) 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:483:ASN:CG	1:A:502:LYS:HB2	1.46	1.37
1:A:483:ASN:OD1	1:A:502:LYS:HB2	1.23	1.31
1:B:418:SER:HB2	1:B:419:PRO:CD	1.61	1.30
1:A:483:ASN:OD1	1:A:502:LYS:CB	1.81	1.29
1:B:418:SER:HB2	1:B:419:PRO:HD2	1.23	1.15
1:B:418:SER:CB	1:B:419:PRO:HD3	1.76	1.15
1:A:483:ASN:ND2	1:A:502:LYS:HB2	1.60	1.13
1:B:232:GLU:O	1:B:288:LEU:O	1.65	1.11
1:B:314:PRO:HB2	4:B:804:MAN:O6	1.52	1.08
1:B:186:THR:HG22	1:B:210:THR:HG22	1.34	1.04
1:B:418:SER:CB	1:B:419:PRO:CD	2.24	1.03
1:A:483:ASN:CG	1:A:502:LYS:CB	2.28	1.02
1:A:222:ASN:HB3	1:A:223:PRO:HD3	1.39	1.02
1:A:483:ASN:ND2	1:A:502:LYS:CB	2.23	1.01
1:A:483:ASN:HD21	1:A:502:LYS:CB	1.74	0.99
1:B:186:THR:CG2	1:B:210:THR:HG22	1.94	0.97
1:A:27:ASN:HD21	1:B:1:ASP:N	1.60	0.97
1:A:28:ARG:HD3	1:A:88:VAL:HG13	1.47	0.97
1:B:414:THR:OG1	1:B:422:THR:HG23	1.64	0.97
1:A:483:ASN:HA	1:A:501:ARG:HB3	1.44	0.97
1:A:490:ASP:CB	1:A:494:GLU:HG2	1.96	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ASN:OD1	1:A:468:ASN:HB3	1.69	0.93
1:A:36:TYR:O	1:A:55:ARG:HD2	1.68	0.92
1:B:358:GLU:OE2	1:B:365:GLN:OE1	1.88	0.92
1:A:340:GLU:HA	1:A:430:VAL:HG13	1.52	0.91
1:A:414:THR:HG22	1:A:422:THR:CG2	1.99	0.91
1:A:442:GLU:HB2	1:A:459:THR:HB	1.51	0.91
1:A:442:GLU:HB3	1:A:443:PRO:HD3	1.53	0.91
1:A:27:ASN:HD21	1:B:1:ASP:H2	1.03	0.91
1:B:418:SER:HB3	1:B:419:PRO:HD3	1.51	0.90
1:B:256:LYS:HB2	1:B:305:GLU:OE2	1.73	0.89
1:A:483:ASN:OD1	1:A:502:LYS:CG	2.19	0.88
1:A:484:TRP:CZ2	1:A:511:ILE:HD11	2.08	0.88
1:A:452:ASN:HB3	1:A:535:GLU:O	1.75	0.87
1:A:483:ASN:CG	1:A:502:LYS:H	1.82	0.86
1:A:154:ASP:HB3	1:A:188:THR:HG22	1.55	0.86
1:A:483:ASN:CG	1:A:502:LYS:N	2.34	0.86
1:A:189:LEU:HB2	1:A:207:ALA:HB3	1.56	0.86
1:B:120:GLY:H	1:B:214:ILE:HD12	1.40	0.85
1:B:68:ARG:HD3	1:B:100:ASP:OD1	1.75	0.85
1:A:46:PRO:HA	1:A:47:PRO:C	2.02	0.84
1:A:509:TYR:CZ	1:A:529:VAL:HB	2.12	0.84
1:A:414:THR:HG22	1:A:422:THR:HG21	1.58	0.84
1:B:220:VAL:O	1:B:244:VAL:HA	1.79	0.83
1:A:301:ARG:HD3	4:A:804:MAN:H3	1.60	0.83
1:B:221:PHE:CZ	1:B:302:VAL:HG13	2.13	0.83
1:A:232:GLU:O	1:A:288:LEU:O	1.97	0.82
1:B:119:GLU:HG3	1:B:181:ARG:H	1.42	0.82
1:B:406:THR:HG22	1:B:430:VAL:HG22	1.61	0.81
1:A:360:ASP:HB3	1:A:362:PHE:CE2	2.15	0.81
1:A:119:GLU:HG3	1:A:181:ARG:H	1.46	0.80
1:B:137:ASP:HB2	1:B:139:VAL:HG12	1.64	0.80
1:B:263:ASN:H	1:B:263:ASN:HD22	1.26	0.80
1:B:378:TRP:CE3	1:B:394:MET:HG2	2.17	0.80
1:A:478:HIS:HB2	1:A:512:HIS:HB2	1.64	0.80
1:A:3:VAL:HG22	1:A:4:ILE:H	1.47	0.79
1:A:480:ALA:O	1:A:484:TRP:HB2	1.81	0.79
1:A:414:THR:HA	1:A:422:THR:HG22	1.65	0.79
1:B:21:LEU:HD12	1:B:60:LEU:HD22	1.65	0.78
1:A:232:GLU:CD	1:A:290:PHE:H	1.91	0.78
1:A:483:ASN:ND2	1:A:502:LYS:CA	2.45	0.78
1:B:152:SER:HB3	1:B:190:VAL:HG12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASN:HA	1:A:501:ARG:CB	2.14	0.77
1:B:277:THR:O	1:B:278:ASN:ND2	2.17	0.77
1:A:41[B]:GLN:CD	1:A:41[B]:GLN:H	1.91	0.77
1:A:480:ALA:C	1:A:484:TRP:HB2	2.10	0.77
1:B:72:ALA:HA	1:B:98:VAL:HG13	1.67	0.77
1:B:314:PRO:CB	4:B:804:MAN:O6	2.33	0.77
1:A:112:VAL:HG22	1:A:206:LYS:HB2	1.65	0.77
1:A:27:ASN:ND2	1:B:1:ASP:N	2.32	0.76
1:A:340:GLU:HB3	1:A:432:LEU:HD11	1.66	0.76
1:A:347:VAL:O	1:A:390:THR:HB	1.85	0.76
1:A:483:ASN:OD1	1:A:502:LYS:HG3	1.86	0.76
1:A:489:ASN:HB2	1:A:497:ILE:HG13	1.66	0.76
1:B:232:GLU:O	1:B:288:LEU:C	2.29	0.75
1:A:484:TRP:HA	1:A:484:TRP:CE3	2.22	0.74
1:B:263:ASN:HD21	1:B:298:LEU:HB2	1.52	0.74
1:A:446:MET:C	1:A:529:VAL:HG13	2.13	0.74
1:B:194:ALA:HB3	1:B:198:GLY:HA2	1.68	0.74
1:B:113:PHE:O	1:B:207:ALA:HA	1.88	0.74
1:B:351:ILE:HD12	1:B:388:ILE:HG22	1.69	0.74
1:B:215:ASN:O	1:B:309:GLU:HG3	1.87	0.74
1:A:483:ASN:O	1:A:484:TRP:CE3	2.40	0.74
1:B:242:LEU:HD12	1:B:280:GLY:HA3	1.70	0.73
1:A:474:ALA:HB2	1:A:515:LEU:HD23	1.70	0.73
1:B:195:ASP:OD1	1:B:201:LEU:HB2	1.88	0.73
1:A:483:ASN:ND2	1:A:502:LYS:C	2.46	0.73
1:A:239:ILE:HD11	1:A:282:LEU:HD13	1.71	0.72
1:A:414:THR:HG22	1:A:422:THR:HG22	1.70	0.72
1:A:443:PRO:HD2	1:A:458:ILE:HG23	1.69	0.72
1:A:263:ASN:N	1:A:263:ASN:HD22	1.83	0.72
1:B:263:ASN:H	1:B:263:ASN:ND2	1.88	0.72
1:A:483:ASN:CG	1:A:502:LYS:CA	2.63	0.72
1:A:462:ASP:HB3	1:A:469:THR:HG23	1.72	0.71
1:A:111:GLU:CD	1:A:111:GLU:H	1.99	0.71
1:A:480:ALA:HA	1:A:484:TRP:CD1	2.26	0.70
1:A:224:SER:O	1:A:317:ALA:HB1	1.91	0.70
1:B:217:ASN:HB2	1:B:248:ASP:OD1	1.91	0.70
1:B:111:GLU:CD	1:B:111:GLU:H	2.00	0.70
1:A:390:THR:HG23	1:A:394:MET:HE3	1.73	0.70
1:B:185:PRO:HA	1:B:211:VAL:HG13	1.72	0.70
1:A:117:VAL:HB	1:A:127:VAL:HG13	1.73	0.70
1:A:341:VAL:HG13	1:A:342:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:CD1	1:B:280:GLY:HA3	2.22	0.69
1:A:230:VAL:CG1	1:A:239:ILE:HG22	2.23	0.69
1:A:484:TRP:HA	1:A:484:TRP:HE3	1.54	0.69
1:B:117:VAL:O	1:B:212:LYS:HG2	1.93	0.69
1:B:176:THR:HG22	1:B:177:SER:H	1.57	0.69
1:A:155:PRO:HD2	1:A:187:TYR:CE1	2.28	0.69
1:A:372:TRP:HB2	1:A:412:ILE:HG23	1.74	0.69
1:B:72:ALA:HA	1:B:98:VAL:CG1	2.23	0.68
1:B:145:ALA:O	1:B:195:ASP:HA	1.92	0.68
1:B:186:THR:HG22	1:B:210:THR:CG2	2.18	0.68
1:A:476:LEU:HD22	1:A:511:ILE:HG22	1.74	0.68
1:A:442:GLU:CB	1:A:459:THR:HB	2.23	0.68
1:A:274:ASP:CG	1:A:277:THR:HG22	2.18	0.68
1:B:138:ASP:HB3	1:B:144:ALA:HB3	1.74	0.67
1:B:166:ASN:C	1:B:166:ASN:HD22	2.02	0.67
1:B:232:GLU:C	1:B:288:LEU:O	2.37	0.67
1:A:127:VAL:HG23	1:A:173:SER:HA	1.75	0.67
1:A:264:ASP:N	1:A:265:PRO:HD3	2.10	0.67
1:B:263:ASN:HD22	1:B:263:ASN:N	1.89	0.67
1:A:483:ASN:HD21	1:A:502:LYS:C	2.04	0.66
1:B:114:GLU:HB3	1:B:208:VAL:HG23	1.77	0.66
1:A:57:THR:HB	1:A:59:TRP:CD1	2.31	0.65
1:A:214:ILE:HG12	1:A:309:GLU:HG3	1.78	0.65
1:A:3:VAL:HG22	1:A:4:ILE:N	2.12	0.65
1:A:74:TYR:HB2	1:A:96:ILE:HB	1.78	0.65
1:A:246:ASP:OD2	1:A:255:TRP:HA	1.95	0.65
1:A:446:MET:O	1:A:529:VAL:HG13	1.96	0.65
1:A:7:ILE:HD12	1:A:7:ILE:H	1.61	0.65
1:A:57:THR:HB	1:A:59:TRP:HD1	1.62	0.65
1:A:448:PHE:CE1	1:A:500:PRO:HD3	2.31	0.64
1:A:474:ALA:CB	1:A:515:LEU:HD23	2.27	0.64
1:B:152:SER:HB3	1:B:190:VAL:CG1	2.27	0.64
1:A:298:LEU:CD1	1:A:319:VAL:HG13	2.27	0.64
1:A:121:ALA:HB1	1:A:125:THR:HG21	1.79	0.64
1:A:480:ALA:HA	1:A:484:TRP:HB2	1.79	0.64
1:A:239:ILE:HG12	1:A:282:LEU:HB3	1.80	0.64
1:B:290:PHE:CD2	1:B:325:ASP:CA	2.80	0.64
1:B:290:PHE:CE2	1:B:325:ASP:N	2.67	0.63
1:A:480:ALA:CA	1:A:484:TRP:HB2	2.28	0.63
1:A:459:THR:HA	1:A:495:SER:HB3	1.81	0.63
1:B:290:PHE:CD2	1:B:325:ASP:N	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PRO:HA	1:A:211:VAL:HG23	1.79	0.63
1:B:263:ASN:ND2	1:B:298:LEU:HB2	2.13	0.63
1:A:10:PRO:HA	1:A:99:THR:OG1	1.99	0.63
1:A:236:ASN:HA	1:A:284:THR:H	1.63	0.63
1:A:119:GLU:HB2	1:A:212:LYS:O	1.99	0.63
1:B:342:PRO:HB3	1:B:434:VAL:HG21	1.81	0.63
1:A:458:ILE:O	1:A:495:SER:HB2	1.99	0.62
1:A:489:ASN:CG	1:A:497:ILE:HD11	2.23	0.62
1:A:231:PRO:HA	1:A:324:VAL:HB	1.80	0.62
1:B:148:TYR:HA	1:B:192:GLN:O	2.00	0.62
1:A:78:SER:O	1:A:91:PRO:HA	2.00	0.62
1:A:329:ALA:HA	1:A:421:ALA:HB1	1.82	0.62
1:B:10:PRO:HA	1:B:99:THR:OG1	2.00	0.61
1:B:358:GLU:CD	1:B:365:GLN:OE1	2.43	0.61
1:A:483:ASN:OD1	1:A:502:LYS:N	2.32	0.61
1:A:483:ASN:HD21	1:A:502:LYS:CA	2.12	0.61
1:B:369:TYR:O	1:B:383:PRO:HA	1.99	0.61
1:B:11:GLU:HG3	1:B:68:ARG:H	1.64	0.61
1:B:395:ASP:HB3	1:B:398:ASP:HB2	1.83	0.61
1:A:159:HIS:HB3	5:A:586:HOH:O	2.00	0.61
1:A:230:VAL:HG11	1:A:239:ILE:HG22	1.83	0.61
1:B:290:PHE:CE2	1:B:325:ASP:HB2	2.36	0.61
1:A:38:ILE:HA	1:A:77:TYR:O	2.01	0.60
1:A:480:ALA:HA	1:A:484:TRP:CB	2.30	0.60
1:A:143:ASN:HD22	1:A:196:LEU:HD21	1.64	0.60
1:A:474:ALA:HA	1:A:514:LYS:O	2.01	0.60
1:B:290:PHE:HE1	1:B:294:GLN:HG3	1.66	0.60
1:A:119:GLU:OE1	1:A:214:ILE:HG22	2.01	0.60
1:A:343:GLU:OE1	1:A:395:ASP:OD1	2.20	0.60
1:B:108:PHE:HA	1:B:132:ALA:HA	1.84	0.60
1:A:73:LYS:HD2	1:A:95:VAL:HG13	1.83	0.60
1:A:374:ASP:HB2	1:A:407:TYR:OH	2.01	0.60
1:A:221:PHE:CE2	1:A:302:VAL:HG12	2.37	0.60
1:A:448:PHE:HE1	1:A:500:PRO:HD3	1.67	0.60
1:A:122:VAL:HG23	1:A:125:THR:HB	1.82	0.60
1:A:298:LEU:HD12	1:A:319:VAL:O	2.02	0.60
1:A:480:ALA:HA	1:A:484:TRP:HD1	1.67	0.60
1:A:223:PRO:CD	1:A:243:LYS:HB2	2.32	0.60
1:B:344:ASP:OD1	1:B:434:VAL:HG11	2.02	0.60
1:A:483:ASN:OD1	1:A:502:LYS:CA	2.50	0.60
1:A:119:GLU:OE2	1:A:182:GLU:OE2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ALA:O	1:A:195:ASP:HA	2.03	0.59
1:A:105:ARG:HD3	1:A:203:THR:HG22	1.84	0.59
1:A:222:ASN:HB3	1:A:223:PRO:CD	2.23	0.59
1:A:345:PHE:CE2	1:A:349:GLN:HB2	2.37	0.59
1:B:249:ALA:O	1:B:255:TRP:HB2	2.03	0.59
1:B:337:ARG:HB2	1:B:354:TYR:CE1	2.37	0.59
1:A:429:LEU:HD21	1:A:431:LEU:HD21	1.84	0.59
1:B:378:TRP:HA	1:B:392:ALA:HB3	1.84	0.59
1:B:226:TYR:CE1	1:B:242:LEU:HA	2.37	0.59
1:B:241:THR:HA	1:B:280:GLY:O	2.03	0.59
1:B:100:ASP:OD2	1:B:136:ASP:HB3	2.02	0.59
1:A:340:GLU:HA	1:A:430:VAL:CG1	2.31	0.58
1:B:218:ALA:HB2	1:B:308:PHE:HE2	1.68	0.58
1:A:376:ALA:HB2	1:A:401:HIS:CD2	2.39	0.58
1:B:362:PHE:C	1:B:364:ASP:H	2.09	0.58
1:A:382:ASN:ND2	1:A:385:THR:H	2.01	0.58
1:B:68:ARG:NH1	1:B:100:ASP:OD1	2.36	0.58
1:B:288:LEU:HD22	1:B:296:TYR:CE2	2.38	0.58
1:B:361:THR:HG22	1:B:361:THR:O	2.03	0.58
1:A:381:ILE:O	1:A:383:PRO:HD3	2.03	0.58
1:A:511:ILE:O	1:A:527:LEU:HD12	2.03	0.57
1:B:68:ARG:NH1	1:B:69:GLU:OE2	2.37	0.57
1:B:235:VAL:HG22	1:B:287:GLY:N	2.19	0.57
1:B:344:ASP:OD1	1:B:434:VAL:CG1	2.52	0.57
1:A:513:LEU:O	1:A:523:GLN:HA	2.04	0.57
1:B:330:PRO:HA	1:B:359:PRO:CD	2.35	0.57
1:A:440:ILE:HG22	1:A:441:PRO:HD2	1.87	0.57
1:B:325:ASP:CG	1:B:362:PHE:HE1	2.13	0.57
1:B:112:VAL:HG22	1:B:206:LYS:HB2	1.87	0.57
1:B:246:ASP:OD2	1:B:304:ASN:ND2	2.35	0.57
1:A:409:ALA:HB3	1:A:427:LEU:HB3	1.86	0.56
1:A:186:THR:HG22	1:A:210:THR:HG22	1.88	0.56
1:A:297:ILE:HG12	1:A:320:THR:HG23	1.87	0.56
1:B:158:PRO:HG2	1:B:162:MET:HE1	1.87	0.56
1:B:348:GLY:N	1:B:390:THR:O	2.38	0.56
1:A:264:ASP:CG	1:A:264:ASP:O	2.46	0.56
1:A:402:VAL:HG12	1:A:404:ASN:O	2.06	0.56
1:A:472:PHE:HD2	1:A:493:GLN:O	1.88	0.56
1:B:290:PHE:CE1	1:B:294:GLN:HG3	2.40	0.56
1:B:412:ILE:HG23	1:B:422:THR:HG22	1.87	0.56
1:A:254:ALA:C	1:A:304:ASN:OD1	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:HA	1:A:389:PHE:HA	1.87	0.56
1:B:301:ARG:HD3	4:B:804:MAN:H61	1.88	0.56
1:A:341:VAL:O	1:A:431:LEU:HA	2.04	0.56
1:A:360:ASP:HB3	1:A:362:PHE:HE2	1.69	0.56
1:A:484:TRP:CE2	1:A:511:ILE:CD1	2.89	0.56
1:B:290:PHE:CD1	1:B:290:PHE:C	2.83	0.56
1:A:71:ILE:HG21	1:A:74:TYR:CE2	2.41	0.56
1:A:509:TYR:OH	1:A:529:VAL:HB	2.06	0.56
1:B:215:ASN:HB2	1:B:254:ALA:CB	2.36	0.56
1:B:368:THR:CG2	1:B:414:THR:HB	2.36	0.56
1:A:218:ALA:HA	1:A:308:PHE:HE1	1.71	0.56
1:A:382:ASN:HD22	1:A:385:THR:H	1.52	0.56
1:B:290:PHE:CD2	1:B:325:ASP:HA	2.41	0.56
1:A:489:ASN:HB2	1:A:497:ILE:CG1	2.36	0.55
1:A:478:HIS:CB	1:A:512:HIS:HB2	2.35	0.55
1:A:236:ASN:N	1:A:284:THR:O	2.39	0.55
1:A:447:GLN:O	1:A:447:GLN:HG2	2.04	0.55
1:B:374:ASP:OD2	1:B:379:LEU:HB2	2.05	0.55
1:A:239:ILE:HD11	1:A:282:LEU:HD22	1.89	0.55
1:B:229:GLN:HA	1:B:322:ASP:O	2.06	0.55
1:A:298:LEU:HD13	1:A:319:VAL:HG13	1.89	0.55
1:A:157:LEU:HA	1:A:158:PRO:C	2.32	0.55
1:A:230:VAL:HG13	1:A:239:ILE:HG22	1.88	0.55
1:B:11:GLU:HG2	1:B:67:ASP:HA	1.88	0.55
1:B:122:VAL:HG23	1:B:125:THR:HB	1.89	0.55
1:A:418:SER:CB	1:A:419:PRO:HD3	2.37	0.55
1:A:274:ASP:O	1:A:278:ASN:N	2.34	0.55
1:A:370:ARG:HD2	1:A:412:ILE:HD11	1.89	0.55
1:B:299:HIS:CD2	4:B:805:MAN:H2	2.42	0.55
1:A:441:PRO:HD3	1:A:524:VAL:HG21	1.89	0.55
1:B:119:GLU:OE1	1:B:182:GLU:OE1	2.25	0.55
1:A:104:ASN:HB2	1:A:136:ASP:OD1	2.07	0.54
1:B:41:GLN:HG2	1:B:45:LYS:HB3	1.90	0.54
1:A:299:HIS:HB3	1:A:316:THR:HG21	1.88	0.54
1:A:341:VAL:HG13	1:A:345:PHE:CD1	2.42	0.54
1:A:229:GLN:HA	1:A:322:ASP:O	2.08	0.54
1:A:166:ASN:O	1:A:167:ARG:C	2.51	0.54
1:A:382:ASN:HD21	1:A:384:GLU:HB2	1.72	0.54
1:B:114:GLU:CB	1:B:208:VAL:HG23	2.38	0.54
1:A:332:PHE:HA	1:A:356:ALA:HA	1.89	0.54
1:A:488:TYR:HA	1:A:496:LEU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASN:ND2	1:B:1:ASP:H3	2.04	0.54
1:B:222:ASN:N	1:B:222:ASN:HD22	2.06	0.54
1:A:517:ASP:OD2	1:A:517:ASP:N	2.41	0.54
1:A:346:GLY:HA3	1:A:349:GLN:HG3	1.89	0.54
1:A:382:ASN:ND2	1:A:384:GLU:HB2	2.22	0.54
1:A:126:SER:HA	1:A:173:SER:HB3	1.89	0.53
1:A:157:LEU:HA	1:A:159:HIS:N	2.22	0.53
1:A:189:LEU:CD1	1:A:209:ILE:HD11	2.37	0.53
1:A:337:ARG:HD3	1:A:352:THR:HG21	1.90	0.53
1:B:159:HIS:CD2	1:B:162:MET:HE1	2.42	0.53
1:A:269:PHE:CD1	1:A:284:THR:HG22	2.42	0.53
1:A:269:PHE:HA	1:A:284:THR:HA	1.90	0.53
1:A:5:PRO:HG2	1:B:23:GLN:HG3	1.90	0.53
1:A:119:GLU:HG3	1:A:181:ARG:N	2.19	0.53
1:A:489:ASN:H	1:A:496:LEU:HA	1.74	0.53
1:A:329:ALA:CA	1:A:421:ALA:HB1	2.38	0.53
1:B:100:ASP:O	1:B:101:GLN:HG2	2.09	0.53
1:A:470:SER:O	1:A:472:PHE:N	2.41	0.53
1:B:209:ILE:N	1:B:209:ILE:HD12	2.24	0.53
1:B:21:LEU:HD12	1:B:60:LEU:CD2	2.36	0.53
1:B:239:ILE:HG21	1:B:321:VAL:HG22	1.89	0.53
1:A:47:PRO:HB2	1:A:50:VAL:HG21	1.90	0.52
1:B:17:PHE:CB	1:B:18:PRO:HA	2.40	0.52
1:B:114:GLU:C	1:B:128:MET:HE3	2.35	0.52
1:A:274:ASP:HB3	1:A:277:THR:CG2	2.39	0.52
1:B:223:PRO:O	1:B:226:TYR:CE2	2.62	0.52
1:A:47:PRO:HB2	1:A:50:VAL:CG2	2.39	0.52
1:B:274:ASP:O	1:B:278:ASN:N	2.41	0.52
1:A:369:TYR:O	1:A:383:PRO:HA	2.10	0.52
1:B:290:PHE:C	1:B:290:PHE:HD1	2.17	0.52
1:A:68:ARG:HD3	1:A:100:ASP:OD2	2.10	0.52
1:B:380:GLU:OE1	1:B:391:ARG:HG2	2.10	0.52
1:B:11:GLU:HB2	1:B:99:THR:O	2.10	0.52
1:B:153:GLN:NE2	1:B:159:HIS:O	2.43	0.52
1:A:44:ASP:OD1	1:A:45:LYS:N	2.42	0.52
1:A:478:HIS:CG	1:A:512:HIS:HB2	2.45	0.52
1:A:484:TRP:CZ2	1:A:511:ILE:CD1	2.89	0.52
1:A:511:ILE:HB	1:A:527:LEU:HD13	1.91	0.52
1:B:368:THR:HG23	1:B:368:THR:O	2.10	0.52
1:A:330:PRO:HG3	1:A:358:GLU:OE2	2.10	0.52
1:A:479:GLY:O	1:A:480:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:HIS:HA	1:B:317:ALA:O	2.10	0.52
1:A:36:TYR:O	1:A:55:ARG:CD	2.50	0.51
1:A:337:ARG:HG3	1:A:337:ARG:HH11	1.75	0.51
1:A:480:ALA:O	1:A:481:SER:C	2.52	0.51
1:B:244:VAL:HG11	1:B:302:VAL:HG11	1.92	0.51
1:A:345:PHE:CD2	1:A:349:GLN:HB2	2.46	0.51
1:B:119:GLU:HB2	1:B:212:LYS:O	2.10	0.51
1:B:238:ARG:NH1	1:B:281:ILE:HD12	2.25	0.51
1:A:439:PRO:HB2	1:A:515:LEU:HB2	1.92	0.51
1:A:480:ALA:O	1:A:482:VAL:N	2.44	0.51
1:B:17:PHE:HB3	1:B:18:PRO:HA	1.91	0.51
1:B:232:GLU:HB2	1:B:288:LEU:O	2.10	0.51
1:A:41[A]:GLN:HA	1:A:45:LYS:O	2.10	0.51
1:A:128:MET:CE	1:A:207:ALA:HB1	2.41	0.51
1:B:345:PHE:HZ	1:B:350:GLU:O	1.94	0.51
1:A:476:LEU:HD22	1:A:511:ILE:CG2	2.39	0.51
1:A:51:PHE:CZ	1:A:66:LEU:HD11	2.46	0.51
1:A:166:ASN:C	1:A:166:ASN:HD22	2.19	0.51
1:B:122:VAL:O	1:B:123:PRO:C	2.52	0.51
1:A:232:GLU:HG3	1:A:289:ASP:HA	1.91	0.51
1:A:442:GLU:N	1:A:459:THR:O	2.44	0.51
1:B:145:ALA:HB1	1:B:197:GLN:HG3	1.92	0.51
1:B:327:ASN:ND2	1:B:415:ASP:OD1	2.43	0.51
1:A:186:THR:HA	1:A:210:THR:HA	1.92	0.50
1:A:376:ALA:HB2	1:A:401:HIS:NE2	2.25	0.50
1:B:119:GLU:OE1	1:B:216:ASP:OD2	2.30	0.50
1:A:11:GLU:OE1	1:A:103:ASP:OD1	2.29	0.50
1:A:226:TYR:HB2	1:A:319:VAL:HB	1.93	0.50
1:A:232:GLU:CG	1:A:289:ASP:HA	2.41	0.50
1:B:23:GLN:HB3	1:B:59:TRP:CD2	2.46	0.50
1:B:414:THR:OG1	1:B:422:THR:CG2	2.50	0.50
1:B:181:ARG:HD2	1:B:213:ASP:HA	1.94	0.50
1:A:256:LYS:O	1:A:304:ASN:ND2	2.45	0.50
1:A:223:PRO:HD2	1:A:243:LYS:HB2	1.94	0.50
1:B:325:ASP:C	1:B:325:ASP:OD2	2.54	0.50
1:A:215:ASN:ND2	1:A:308:PHE:HA	2.27	0.50
1:A:333:MET:HA	1:A:333:MET:HE2	1.93	0.49
1:B:371:ILE:HG13	1:B:410:LEU:O	2.12	0.49
1:A:236:ASN:HB2	1:A:283:LYS:HD3	1.93	0.49
1:B:151:VAL:HG23	1:B:190:VAL:HG13	1.94	0.49
1:B:176:THR:HG22	1:B:177:SER:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:VAL:O	1:B:323:VAL:HA	2.12	0.49
1:B:411:ILE:HG22	1:B:412:ILE:N	2.28	0.49
1:B:466:PRO:HA	1:B:467:PRO:C	2.37	0.49
1:A:242:LEU:HD12	1:A:271:VAL:HG21	1.95	0.49
1:B:327:ASN:OD1	1:B:415:ASP:OD1	2.31	0.49
1:A:35:PHE:HE2	1:A:83:SER:HB3	1.78	0.49
1:B:214:ILE:O	1:B:216:ASP:N	2.45	0.49
1:B:341:VAL:O	1:B:431:LEU:HA	2.12	0.49
1:B:352:THR:HG22	1:B:353:SER:N	2.27	0.49
1:B:373:ARG:HB3	1:B:410:LEU:H	1.78	0.49
1:A:22:VAL:HG12	1:A:23:GLN:H	1.77	0.49
1:A:67:ASP:OD2	1:A:67:ASP:C	2.55	0.49
1:A:277:THR:O	1:A:278:ASN:ND2	2.32	0.49
1:A:26:SER:OG	1:A:89:GLU:OE1	2.23	0.49
1:A:438:ALA:HB2	1:A:520:ASN:ND2	2.28	0.49
1:B:9:CYS:SG	1:B:13:GLU:OE2	2.71	0.49
1:B:220:VAL:O	1:B:244:VAL:CA	2.56	0.49
1:A:468:ASN:O	1:A:517:ASP:OD1	2.31	0.49
1:A:489:ASN:ND2	1:A:497:ILE:HD11	2.28	0.49
1:B:120:GLY:N	1:B:214:ILE:HD12	2.20	0.49
1:A:346:GLY:CA	1:A:349:GLN:HG3	2.42	0.48
1:A:484:TRP:CE2	1:A:511:ILE:HD11	2.47	0.48
1:B:271:VAL:HA	1:B:281:ILE:O	2.13	0.48
1:A:224:SER:O	1:A:317:ALA:CB	2.60	0.48
1:A:350:GLU:HA	1:A:389:PHE:HB3	1.96	0.48
1:A:521:LYS:HD3	1:A:521:LYS:N	2.28	0.48
1:A:3:VAL:CG2	1:A:4:ILE:H	2.22	0.48
1:A:437:ASN:HB2	1:A:464:ASP:OD2	2.13	0.48
1:B:358:GLU:HA	1:B:358:GLU:OE1	2.11	0.48
1:B:24:ILE:HD11	1:B:53:ILE:CD1	2.44	0.48
1:B:67:ASP:O	1:B:70:ALA:HB3	2.14	0.48
1:A:214:ILE:HG23	1:A:216:ASP:HB3	1.96	0.48
1:A:264:ASP:OD2	1:A:267:GLN:HA	2.13	0.48
1:A:409:ALA:O	1:A:410:LEU:HD23	2.14	0.48
1:B:215:ASN:HB2	1:B:254:ALA:HB1	1.95	0.48
1:B:221:PHE:HA	1:B:243:LYS:O	2.13	0.48
1:A:20:ASN:HA	1:A:61:LYS:HB3	1.95	0.48
1:A:223:PRO:HD2	1:A:226:TYR:OH	2.14	0.48
1:A:298:LEU:HD12	1:A:298:LEU:H	1.78	0.48
1:A:481:SER:O	1:A:483:ASN:N	2.46	0.48
1:A:111:GLU:CD	1:A:111:GLU:N	2.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:CB	1:A:125:THR:HG21	2.45	0.47
1:A:432:LEU:H	1:A:432:LEU:HD12	1.79	0.47
1:A:484:TRP:CE2	1:A:511:ILE:HD13	2.49	0.47
1:A:290:PHE:CD1	1:A:290:PHE:C	2.92	0.47
1:A:330:PRO:HA	1:A:359:PRO:HD3	1.96	0.47
1:B:38:ILE:HA	1:B:77:TYR:O	2.14	0.47
1:B:255:TRP:C	1:B:304:ASN:ND2	2.71	0.47
1:B:395:ASP:OD2	1:B:397:GLU:HB2	2.14	0.47
1:A:253:PRO:C	1:A:255:TRP:H	2.22	0.47
1:B:150:ILE:HG21	1:B:189:LEU:HD22	1.94	0.47
1:B:300:VAL:CG2	1:B:317:ALA:HB3	2.44	0.47
1:A:166:ASN:HB3	1:A:169:THR:HB	1.97	0.47
1:A:239:ILE:CD1	1:A:282:LEU:HD22	2.45	0.47
1:A:453:PRO:CB	1:A:500:PRO:HG2	2.45	0.47
1:A:474:ALA:HB2	1:A:515:LEU:CD2	2.43	0.47
1:B:263:ASN:OD1	1:B:298:LEU:HA	2.14	0.47
1:B:290:PHE:CD2	1:B:325:ASP:HB2	2.49	0.47
1:A:8:SER:HA	1:A:97:THR:O	2.15	0.47
1:A:184:TYR:O	1:A:211:VAL:HG21	2.15	0.47
1:B:62:VAL:HG21	1:B:66:LEU:HD11	1.97	0.47
1:A:80:ALA:HB3	1:A:89:GLU:HB2	1.96	0.47
1:A:148:TYR:HA	1:A:192:GLN:O	2.15	0.47
1:A:411:ILE:N	1:A:411:ILE:HD12	2.30	0.47
1:B:303:GLU:HA	1:B:308:PHE:HE1	1.80	0.47
1:A:53:ILE:HG23	1:A:55:ARG:HH11	1.80	0.47
1:B:53:ILE:HA	1:B:59:TRP:O	2.14	0.47
1:A:53:ILE:HA	1:A:59:TRP:O	2.15	0.47
1:A:345:PHE:CE2	1:A:349:GLN:CB	2.98	0.47
1:B:111:GLU:CD	1:B:111:GLU:N	2.73	0.47
1:A:475:GLU:O	1:A:513:LEU:HD12	2.14	0.46
1:A:509:TYR:CE2	1:A:511:ILE:HD11	2.49	0.46
1:B:114:GLU:HB3	1:B:208:VAL:CG2	2.43	0.46
1:B:187:TYR:N	1:B:209:ILE:O	2.39	0.46
1:B:312:LEU:N	1:B:312:LEU:HD12	2.30	0.46
1:A:128:MET:HE3	1:A:172:ILE:HD12	1.96	0.46
1:A:232:GLU:HG3	1:A:290:PHE:N	2.30	0.46
1:B:122:VAL:O	1:B:125:THR:HB	2.16	0.46
1:B:339:VAL:HG23	1:B:429:LEU:HD12	1.97	0.46
1:B:341:VAL:HG21	1:B:429:LEU:HD11	1.97	0.46
1:B:148:TYR:CD2	1:B:170:GLY:HA2	2.51	0.46
1:B:414:THR:CG2	1:B:420:ILE:HG23	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG11	1:A:302:VAL:HG11	1.96	0.46
1:B:20:ASN:HA	1:B:61:LYS:HG2	1.96	0.46
1:B:119:GLU:HA	1:B:211:VAL:HG23	1.98	0.46
1:B:380:GLU:HB3	1:B:389:PHE:CE1	2.51	0.46
1:B:108:PHE:HE1	1:B:203:THR:O	1.99	0.46
1:B:231:PRO:HA	1:B:324:VAL:HG23	1.97	0.46
1:B:290:PHE:HE2	1:B:325:ASP:H	1.62	0.46
1:B:332:PHE:HD1	1:B:355:THR:O	1.99	0.46
1:A:24:ILE:HD12	1:B:2:TRP:CH2	2.51	0.46
1:A:192:GLN:HG2	1:A:193:ALA:N	2.31	0.46
1:B:304:ASN:O	1:B:305:GLU:C	2.59	0.46
1:B:46:PRO:HA	1:B:48:VAL:N	2.31	0.46
1:B:158:PRO:HG2	1:B:162:MET:CE	2.44	0.46
1:A:3:VAL:HG13	1:B:25:LYS:HD3	1.97	0.46
1:A:41[B]:GLN:H	1:A:41[B]:GLN:NE2	2.13	0.46
1:A:153:GLN:HE22	1:A:162:MET:HG2	1.81	0.46
1:A:236:ASN:HA	1:A:284:THR:O	2.16	0.45
1:A:350:GLU:HB2	1:A:389:PHE:HD2	1.81	0.45
1:A:29:ASP:HA	1:A:34:VAL:HG22	1.97	0.45
1:A:274:ASP:HB3	1:A:277:THR:HG22	1.98	0.45
1:B:217:ASN:HB2	1:B:248:ASP:CG	2.41	0.45
1:A:485:THR:HG22	1:A:499:GLN:O	2.17	0.45
1:B:261:VAL:HG12	1:B:300:VAL:HG12	1.98	0.45
1:A:263:ASN:HD22	1:A:263:ASN:H	1.63	0.45
1:B:11:GLU:OE1	1:B:67:ASP:OD2	2.35	0.45
1:B:44:ASP:CG	1:B:45:LYS:HD2	2.42	0.45
1:B:219:PRO:O	1:B:302:VAL:HG21	2.17	0.45
1:A:102:ASN:HA	1:A:136:ASP:OD2	2.16	0.45
1:A:374:ASP:OD1	1:A:377:ASN:HA	2.16	0.45
1:A:449:CYS:HB3	1:A:453:PRO:HA	1.97	0.45
1:B:145:ALA:HB3	1:B:197:GLN:H	1.80	0.45
1:B:157:LEU:HA	1:B:158:PRO:C	2.42	0.45
1:A:67:ASP:OD2	1:A:69:GLU:N	2.50	0.44
1:B:119:GLU:HB3	1:B:214:ILE:HB	1.99	0.44
1:B:24:ILE:HD11	1:B:53:ILE:HD11	1.98	0.44
1:B:347:VAL:HG12	1:B:392:ALA:O	2.18	0.44
1:A:45:LYS:O	1:A:47:PRO:O	2.35	0.44
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.35	0.44
1:A:480:ALA:HA	1:A:484:TRP:CG	2.53	0.44
1:B:11:GLU:CG	1:B:67:ASP:HA	2.46	0.44
1:B:129:LYS:HD3	1:B:171:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:THR:CG2	1:B:430:VAL:HG22	2.38	0.44
1:A:30:LYS:HD2	1:A:30:LYS:HA	1.84	0.44
1:A:38:ILE:HG23	1:A:53:ILE:HG21	1.99	0.44
1:A:155:PRO:HD2	1:A:187:TYR:CD1	2.53	0.44
1:A:188:THR:OG1	1:A:208:VAL:HG22	2.18	0.44
1:A:253:PRO:HB3	1:A:305:GLU:HG2	1.99	0.44
1:A:143:ASN:ND2	1:A:196:LEU:HD21	2.31	0.44
1:A:447:GLN:N	1:A:529:VAL:HG13	2.32	0.44
1:B:11:GLU:CG	1:B:68:ARG:H	2.28	0.44
1:B:332:PHE:CD1	1:B:355:THR:O	2.71	0.44
1:B:414:THR:HA	1:B:422:THR:HA	1.99	0.44
1:B:150:ILE:HG13	1:B:165:VAL:HG12	2.00	0.44
1:B:166:ASN:HD22	1:B:167:ARG:N	2.14	0.44
1:B:180:ASP:HB3	1:B:183:SER:HB3	2.00	0.44
1:B:214:ILE:O	1:B:214:ILE:HG22	2.18	0.44
1:B:232:GLU:O	1:B:288:LEU:N	2.51	0.44
1:A:274:ASP:CB	1:A:277:THR:HG22	2.48	0.44
1:A:331:ILE:CD1	1:A:359:PRO:HG3	2.48	0.44
1:A:358:GLU:HA	1:A:359:PRO:HD3	1.81	0.44
1:A:263:ASN:OD1	1:A:298:LEU:HA	2.18	0.44
1:A:278:ASN:O	1:A:278:ASN:CG	2.61	0.44
1:A:472:PHE:H	1:A:493:GLN:CB	2.30	0.44
1:B:246:ASP:HB3	1:B:255:TRP:CD1	2.53	0.44
1:B:60:LEU:HD23	1:B:61:LYS:N	2.33	0.43
1:B:105:ARG:HB3	1:B:201:LEU:HD13	2.00	0.43
1:B:357:ARG:O	1:B:359:PRO:HD3	2.17	0.43
1:A:102:ASN:HB2	1:A:143:ASN:ND2	2.34	0.43
1:B:18:PRO:HB3	1:B:63:THR:HA	1.98	0.43
1:B:337:ARG:HA	1:B:337:ARG:HD2	1.88	0.43
1:B:379:LEU:N	1:B:379:LEU:HD12	2.32	0.43
1:A:456:HIS:O	1:A:497:ILE:HA	2.18	0.43
1:B:368:THR:HG23	1:B:414:THR:HB	1.99	0.43
1:A:2:TRP:CZ3	1:B:24:ILE:HD12	2.53	0.43
1:A:89:GLU:OE2	1:B:1:ASP:HA	2.18	0.43
1:A:89:GLU:HG2	1:B:2:TRP:CD1	2.53	0.43
1:A:221:PHE:HA	1:A:243:LYS:O	2.19	0.43
1:A:264:ASP:N	1:A:265:PRO:CD	2.78	0.43
1:B:50:VAL:HG22	1:B:64:GLN:NE2	2.33	0.43
1:B:253:PRO:HB2	1:B:306:GLU:HB2	2.01	0.43
1:A:341:VAL:HG21	1:A:351:ILE:HG23	2.00	0.43
1:B:337:ARG:HH22	1:B:352:THR:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41[B]:GLN:HA	1:A:45:LYS:O	2.18	0.43
1:A:483:ASN:HD21	1:A:502:LYS:HB3	1.74	0.43
1:A:106:PRO:O	1:A:203:THR:HG21	2.19	0.43
1:A:196:LEU:O	1:A:197:GLN:HB2	2.19	0.43
1:A:395:ASP:HB3	1:A:398:ASP:HB2	2.01	0.43
1:B:159:HIS:CD2	1:B:162:MET:CE	3.02	0.43
1:B:162:MET:HB3	1:B:163:PHE:CD2	2.54	0.43
1:B:240:ALA:O	1:B:282:LEU:HB2	2.18	0.43
1:B:462:ASP:HA	1:B:463:PRO:HD3	1.79	0.43
1:A:77:TYR:HA	1:A:92:MET:O	2.18	0.43
1:A:186:THR:CG2	1:A:210:THR:HG22	2.49	0.43
1:A:290:PHE:CG	1:A:325:ASP:HB2	2.54	0.43
1:A:333:MET:HA	1:A:334:PRO:HA	1.85	0.43
1:B:63:THR:OG1	1:B:64:GLN:HG2	2.19	0.43
1:A:42:GLY:HA2	1:A:47:PRO:O	2.19	0.43
1:A:290:PHE:CD2	1:A:325:ASP:HB2	2.54	0.43
1:B:218:ALA:HA	1:B:219:PRO:HD3	1.77	0.43
1:B:290:PHE:HD2	1:B:325:ASP:N	2.16	0.43
1:A:148:TYR:N	1:A:167:ARG:O	2.51	0.42
1:A:154:ASP:HA	1:A:155:PRO:HA	1.71	0.42
1:A:370:ARG:HG3	1:A:412:ILE:HG12	2.01	0.42
1:A:439:PRO:HB2	1:A:515:LEU:CB	2.48	0.42
1:B:229:GLN:CA	1:B:322:ASP:O	2.66	0.42
1:B:239:ILE:HG21	1:B:321:VAL:CG2	2.48	0.42
1:B:327:ASN:HB3	1:B:419:PRO:HD2	2.00	0.42
1:B:120:GLY:H	1:B:214:ILE:CD1	2.22	0.42
1:A:438:ALA:HB1	1:A:522:ASP:HB2	2.01	0.42
1:B:152:SER:O	1:B:189:LEU:HD23	2.19	0.42
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.19	0.42
1:B:51:PHE:CE2	1:B:74:TYR:CD2	3.07	0.42
1:B:432:LEU:HA	1:B:432:LEU:HD12	1.77	0.42
1:A:104:ASN:ND2	1:A:135:ALA:HB3	2.35	0.42
1:A:341:VAL:CG1	1:A:345:PHE:CD1	3.02	0.42
1:B:150:ILE:CG2	1:B:189:LEU:HD22	2.50	0.42
1:A:332:PHE:CZ	1:A:411:ILE:HG22	2.55	0.42
1:B:55:ARG:H	1:B:55:ARG:HG3	1.52	0.42
1:A:51:PHE:HZ	1:A:66:LEU:HD11	1.83	0.42
1:A:71:ILE:HG21	1:A:74:TYR:CZ	2.55	0.42
1:A:272:VAL:HG23	1:A:281:ILE:HG13	2.01	0.42
1:B:215:ASN:CB	1:B:254:ALA:HB1	2.49	0.42
1:B:412:ILE:HG23	1:B:422:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:HB3	1:A:277:THR:HG23	2.01	0.42
1:B:232:GLU:HG3	1:B:326:VAL:HG22	2.01	0.42
1:B:242:LEU:HD12	1:B:280:GLY:CA	2.44	0.42
1:A:9:CYS:SG	1:A:13:GLU:OE1	2.76	0.42
1:A:329:ALA:HA	1:A:330:PRO:HD3	1.81	0.42
1:B:95:VAL:C	1:B:96:ILE:HD13	2.44	0.42
1:A:263:ASN:N	1:A:263:ASN:ND2	2.53	0.41
1:A:414:THR:CG2	1:A:422:THR:HG22	2.45	0.41
1:B:45:LYS:HD2	1:B:45:LYS:N	2.35	0.41
1:B:115:GLY:N	1:B:128:MET:HE3	2.34	0.41
1:B:282:LEU:HA	1:B:282:LEU:HD23	1.76	0.41
1:B:382:ASN:HB3	1:B:387:ALA:HB3	2.01	0.41
1:A:244:VAL:HG22	1:A:259:TYR:OH	2.20	0.41
1:B:242:LEU:HD11	1:B:280:GLY:HA3	1.98	0.41
1:B:382:ASN:N	1:B:387:ALA:O	2.43	0.41
1:A:128:MET:HE2	1:A:209:ILE:HG23	2.02	0.41
1:A:367:ILE:HG22	1:A:413:ALA:HB1	2.01	0.41
1:A:462:ASP:HA	1:A:463:PRO:HD3	1.70	0.41
1:B:33:LYS:HG3	1:B:35:PHE:CE1	2.55	0.41
1:B:215:ASN:HB2	1:B:254:ALA:HB2	2.02	0.41
1:B:221:PHE:CD2	1:B:244:VAL:HG12	2.55	0.41
1:A:7:ILE:HD12	1:A:7:ILE:N	2.32	0.41
1:A:38:ILE:HG12	1:A:53:ILE:HG22	2.03	0.41
1:A:111:GLU:HG2	1:A:112:VAL:N	2.35	0.41
1:A:189:LEU:HA	1:A:189:LEU:HD23	1.84	0.41
1:A:406:THR:HG22	1:A:407:TYR:O	2.21	0.41
1:B:196:LEU:HB2	1:B:200:GLY:N	2.36	0.41
1:A:33:LYS:O	1:A:83:SER:N	2.54	0.41
1:A:466:PRO:HA	1:A:468:ASN:N	2.35	0.41
1:A:476:LEU:HD23	1:A:513:LEU:HA	2.01	0.41
1:B:325:ASP:CG	1:B:362:PHE:CE1	2.97	0.41
1:B:362:PHE:C	1:B:364:ASP:N	2.72	0.41
1:B:66:LEU:HD12	1:B:66:LEU:H	1.85	0.41
1:B:164:THR:HG23	1:B:175:LEU:HD22	2.03	0.41
1:B:185:PRO:O	1:B:210:THR:HA	2.20	0.41
1:B:301:ARG:HA	1:B:315:SER:O	2.21	0.41
1:B:373:ARG:HB3	1:B:410:LEU:HB2	2.01	0.41
1:B:390:THR:HG22	1:B:392:ALA:O	2.21	0.41
1:B:411:ILE:CG2	1:B:412:ILE:N	2.83	0.41
1:A:408:VAL:HG22	1:A:428:LEU:HD23	2.03	0.41
1:A:488:TYR:N	1:A:488:TYR:CD2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:O	1:B:288:LEU:CA	2.69	0.41
1:A:295:GLN:OE1	1:A:322:ASP:OD1	2.39	0.41
1:A:410:LEU:HD23	1:A:426:THR:HG23	2.01	0.41
1:A:442:GLU:HB3	1:A:443:PRO:CD	2.36	0.41
1:A:453:PRO:HB3	1:A:500:PRO:HG2	2.03	0.41
1:A:494:GLU:HG3	1:A:495:SER:N	2.36	0.41
1:A:515:LEU:O	1:A:521:LYS:HA	2.21	0.41
1:B:232:GLU:HG2	1:B:324:VAL:O	2.21	0.41
1:B:415:ASP:OD2	1:B:416:ASP:N	2.51	0.41
1:A:29:ASP:HA	1:A:34:VAL:CG2	2.51	0.41
1:A:372:TRP:HB2	1:A:412:ILE:CG2	2.47	0.41
1:A:441:PRO:CD	1:A:524:VAL:HG21	2.51	0.41
1:B:51:PHE:HE2	1:B:74:TYR:CG	2.37	0.41
1:B:105:ARG:HA	1:B:106:PRO:HD3	1.88	0.41
1:B:128:MET:CE	1:B:207:ALA:HB1	2.51	0.41
1:B:298:LEU:H	1:B:298:LEU:HD23	1.86	0.41
1:B:382:ASN:ND2	1:B:385:THR:H	2.19	0.41
1:B:152:SER:O	1:B:189:LEU:HA	2.20	0.40
1:B:373:ARG:HD3	1:B:410:LEU:HD13	2.02	0.40
1:A:414:THR:CA	1:A:422:THR:HG22	2.42	0.40
1:B:252:THR:O	1:B:255:TRP:N	2.49	0.40
1:A:274:ASP:O	1:A:275:PRO:C	2.64	0.40
1:A:51:PHE:CE2	1:A:96:ILE:HD13	2.56	0.40
1:A:281:ILE:H	1:A:281:ILE:HG12	1.72	0.40
1:A:418:SER:HB2	1:A:419:PRO:HD3	2.04	0.40
1:B:329:ALA:O	1:B:359:PRO:HG2	2.22	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	529/550 (96%)	454 (86%)	72 (14%)	3 (1%)	21	50
1	B	436/550 (79%)	387 (89%)	48 (11%)	1 (0%)	43	71
All	All	965/1100 (88%)	841 (87%)	120 (12%)	4 (0%)	30	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ALA
1	A	481	SER
1	A	482	VAL
1	B	419	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	458/482 (95%)	403 (88%)	55 (12%)	5	19
1	B	381/482 (79%)	344 (90%)	37 (10%)	8	28
All	All	839/964 (87%)	747 (89%)	92 (11%)	6	22

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	8	SER
1	A	9	CYS
1	A	22	VAL
1	A	34	VAL
1	A	41[A]	GLN
1	A	41[B]	GLN
1	A	57	THR
1	A	60	LEU
1	A	61	LYS
1	A	73	LYS
1	A	78	SER

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Mol	Chain	Res	Type
1	A	88	VAL
1	A	139	VAL
1	A	149	THR
1	A	157	LEU
1	A	161	ASN
1	A	166	ASN
1	A	169	THR
1	A	188	THR
1	A	209	ILE
1	A	211	VAL
1	A	230	VAL
1	A	235	VAL
1	A	239	ILE
1	A	261	VAL
1	A	263	ASN
1	A	271	VAL
1	A	278	ASN
1	A	281	ILE
1	A	282	LEU
1	A	293	LYS
1	A	298	LEU
1	A	300	VAL
1	A	303	GLU
1	A	304	ASN
1	A	319	VAL
1	A	358	GLU
1	A	367	ILE
1	A	368	THR
1	A	389	PHE
1	A	390	THR
1	A	397	GLU
1	A	418	SER
1	A	427	LEU
1	A	429	LEU
1	A	440	ILE
1	A	484	TRP
1	A	496	LEU
1	A	514	LYS
1	A	517	ASP
1	A	520	ASN
1	A	521	LYS
1	A	531	VAL

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Mol	Chain	Res	Type
1	A	535	GLU
1	B	48	VAL
1	B	56	GLU
1	B	98	VAL
1	B	122	VAL
1	B	146	ILE
1	B	154	ASP
1	B	159	HIS
1	B	162	MET
1	B	166	ASN
1	B	186	THR
1	B	188	THR
1	B	208	VAL
1	B	211	VAL
1	B	214	ILE
1	B	222	ASN
1	B	227	GLN
1	B	230	VAL
1	B	232	GLU
1	B	242	LEU
1	B	251	ASN
1	B	260	THR
1	B	263	ASN
1	B	278	ASN
1	B	282	LEU
1	B	290	PHE
1	B	312	LEU
1	B	320	THR
1	B	323	VAL
1	B	350	GLU
1	B	355	THR
1	B	363	MET
1	B	367	ILE
1	B	384	GLU
1	B	385	THR
1	B	390	THR
1	B	422	THR
1	B	433	ASP

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

Mol	Chain	Res	Type
1	A	12	ASN
1	A	20	ASN
1	A	27	ASN
1	A	64	GLN
1	A	84	ASN
1	A	104	ASN
1	A	143	ASN
1	A	161	ASN
1	A	166	ASN
1	A	217	ASN
1	A	233	ASN
1	A	263	ASN
1	A	299	HIS
1	A	382	ASN
1	A	450	GLN
1	A	489	ASN
1	A	512	HIS
1	A	520	ASN
1	B	64	GLN
1	B	143	ASN
1	B	166	ASN
1	B	197	GLN
1	B	217	ASN
1	B	222	ASN
1	B	227	GLN
1	B	263	ASN
1	B	299	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 26 are monoatomic - leaving 18 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
4	MAN	B	808	1	11,11,12	0.61	0	15,15,17	0.65	0
4	MAN	B	802	1	11,11,12	0.55	0	15,15,17	0.85	1 (6%)
4	MAN	A	807	1	11,11,12	0.56	0	15,15,17	1.03	2 (13%)
4	MAN	B	806	1	11,11,12	0.61	0	15,15,17	0.80	0
4	MAN	A	802	1	11,11,12	0.62	0	15,15,17	0.76	0
4	MAN	A	801	1	11,11,12	0.53	0	15,15,17	1.12	1 (6%)
4	MAN	A	809	1	11,11,12	0.56	0	15,15,17	0.86	1 (6%)
4	MAN	A	803	1	11,11,12	0.70	0	15,15,17	0.80	1 (6%)
4	MAN	A	808	1	11,11,12	0.55	0	15,15,17	0.90	1 (6%)
4	MAN	B	801	1	11,11,12	0.62	0	15,15,17	0.61	0
4	MAN	B	804	1	11,11,12	0.71	0	15,15,17	1.17	1 (6%)
4	MAN	B	805	1	11,11,12	0.59	0	15,15,17	0.65	0
4	MAN	A	805	1	11,11,12	0.58	0	15,15,17	0.68	0
4	MAN	B	807	1	11,11,12	0.64	0	15,15,17	0.72	0
4	MAN	A	806	1	11,11,12	0.55	0	15,15,17	0.81	1 (6%)
4	MAN	B	809	1	11,11,12	0.57	0	15,15,17	0.73	0
4	MAN	B	803	1	11,11,12	0.67	0	15,15,17	0.72	0
4	MAN	A	804	1	11,11,12	0.54	0	15,15,17	0.87	1 (6%)

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
4	MAN	B	808	1	-	0/2/19/22	0/1/1/1
4	MAN	B	802	1	-	2/2/19/22	0/1/1/1
4	MAN	A	807	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	806	1	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	802	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	801	1	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	A	801	1	-	2/2/19/22	0/1/1/1
4	MAN	B	805	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	803	1	-	2/2/19/22	0/1/1/1
4	MAN	A	808	1	-	0/2/19/22	0/1/1/1
4	MAN	B	804	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	809	1	-	2/2/19/22	0/1/1/1
4	MAN	A	805	1	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	B	807	1	-	2/2/19/22	0/1/1/1
4	MAN	A	806	1	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	B	809	1	-	2/2/19/22	0/1/1/1
4	MAN	B	803	1	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	A	804	1	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	MAN	C1-O5-C5	3.77	117.24	112.19
4	B	804	MAN	C1-C2-C3	3.27	114.41	109.64
4	A	808	MAN	C1-O5-C5	2.57	115.63	112.19
4	A	809	MAN	C1-O5-C5	2.52	115.57	112.19
4	B	802	MAN	C1-O5-C5	2.38	115.37	112.19
4	A	806	MAN	C1-O5-C5	2.35	115.34	112.19
4	A	807	MAN	C1-O5-C5	2.30	115.26	112.19
4	A	804	MAN	C1-O5-C5	2.27	115.23	112.19
4	A	807	MAN	C3-C4-C5	2.09	114.02	110.23
4	A	803	MAN	C1-C2-C3	2.08	112.67	109.64

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	802	MAN	C1
4	A	804	MAN	C1
4	A	805	MAN	C1
4	A	806	MAN	C1
4	A	807	MAN	C1
4	B	801	MAN	C1

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Mol	Chain	Res	Type	Atom
4	B	803	MAN	C1
4	B	804	MAN	C1
4	B	805	MAN	C1

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	MAN	O5-C5-C6-O6
4	B	807	MAN	O5-C5-C6-O6
4	A	806	MAN	C4-C5-C6-O6
4	A	805	MAN	C4-C5-C6-O6
4	B	806	MAN	O5-C5-C6-O6
4	B	807	MAN	C4-C5-C6-O6
4	B	802	MAN	C4-C5-C6-O6
4	A	805	MAN	O5-C5-C6-O6
4	B	809	MAN	C4-C5-C6-O6
4	A	801	MAN	O5-C5-C6-O6
4	B	802	MAN	O5-C5-C6-O6
4	B	809	MAN	O5-C5-C6-O6
4	B	803	MAN	C4-C5-C6-O6
4	B	803	MAN	O5-C5-C6-O6
4	B	806	MAN	C4-C5-C6-O6
4	A	801	MAN	C4-C5-C6-O6
4	B	801	MAN	C4-C5-C6-O6
4	A	809	MAN	C4-C5-C6-O6
4	A	803	MAN	C4-C5-C6-O6
4	B	801	MAN	O5-C5-C6-O6
4	A	809	MAN	O5-C5-C6-O6
4	A	803	MAN	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	804	MAN	3	0
4	B	805	MAN	1	0
4	A	804	MAN	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	532/550 (96%)	0.11	14 (2%) 57 42	17, 59, 123, 157	1 (0%)
1	B	440/550 (80%)	0.22	9 (2%) 65 49	32, 61, 112, 131	0
All	All	972/1100 (88%)	0.16	23 (2%) 59 45	17, 60, 116, 157	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	TYR	5.1
1	B	432	LEU	3.8
1	B	433	ASP	3.4
1	B	368	THR	3.0
1	A	531	VAL	2.9
1	B	412	ILE	2.9
1	B	420	ILE	2.9
1	A	455	PRO	2.7
1	B	419	PRO	2.7
1	A	483	ASN	2.7
1	A	488	TYR	2.6
1	A	536	GLY	2.3
1	B	413	ALA	2.3
1	A	482	VAL	2.3
1	A	232	GLU	2.3
1	A	470	SER	2.3
1	A	396	ARG	2.2
1	A	526	THR	2.2
1	B	309	GLU	2.2
1	A	503	ASP	2.2
1	A	444	ARG	2.1
1	A	530	HIS	2.1
1	B	394	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
4	MAN	B	808	11/12	0.48	0.13	114,123,126,127	0
4	MAN	B	804	11/12	0.49	0.25	91,100,120,132	0
4	MAN	B	807	11/12	0.55	0.19	106,117,122,129	0
4	MAN	B	806	11/12	0.57	0.13	99,109,124,129	0
2	CA	B	611	1/1	0.63	0.12	104,104,104,104	0
4	MAN	A	809	11/12	0.69	0.20	87,91,98,112	0
4	MAN	B	802	11/12	0.70	0.15	67,71,81,83	0
4	MAN	B	805	11/12	0.72	0.13	79,84,96,96	0
4	MAN	A	806	11/12	0.72	0.16	73,88,105,107	0
4	MAN	A	805	11/12	0.76	0.15	66,69,89,95	0
4	MAN	A	808	11/12	0.77	0.15	72,85,90,98	0
4	MAN	B	803	11/12	0.78	0.19	72,93,114,121	0
4	MAN	B	809	11/12	0.79	0.12	95,99,112,113	0
2	CA	B	609	1/1	0.80	0.09	105,105,105,105	0
4	MAN	A	802	11/12	0.80	0.18	59,63,79,91	0
4	MAN	A	803	11/12	0.82	0.11	50,69,77,78	0
2	CA	B	612	1/1	0.83	0.12	89,89,89,89	0
4	MAN	B	801	11/12	0.83	0.11	55,60,72,73	0
4	MAN	A	807	11/12	0.84	0.14	74,85,90,91	0
4	MAN	A	804	11/12	0.88	0.18	47,60,76,80	0
2	CA	B	610	1/1	0.90	0.09	93,93,93,93	0
2	CA	B	608	1/1	0.90	0.12	81,81,81,81	0
4	MAN	A	801	11/12	0.91	0.09	44,48,59,71	0
2	CA	B	605	1/1	0.93	0.07	38,38,38,38	0
2	CA	B	601	1/1	0.93	0.14	44,44,44,44	0
2	CA	B	604	1/1	0.93	0.09	37,37,37,37	0
2	CA	B	606	1/1	0.94	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	608	1/1	0.94	0.07	58,58,58,58	0
2	CA	A	605	1/1	0.94	0.07	31,31,31,31	0
2	CA	B	602	1/1	0.95	0.07	38,38,38,38	0
2	CA	A	610	1/1	0.95	0.10	74,74,74,74	0
2	CA	A	604	1/1	0.95	0.09	35,35,35,35	0
2	CA	A	607	1/1	0.96	0.08	72,72,72,72	0
3	MN	B	901	1/1	0.96	0.14	54,54,54,54	0
2	CA	A	601	1/1	0.96	0.18	41,41,41,41	0
2	CA	A	606	1/1	0.96	0.07	35,35,35,35	0
3	MN	A	901	1/1	0.97	0.14	59,59,59,59	0
2	CA	B	607	1/1	0.97	0.07	87,87,87,87	0
2	CA	A	611	1/1	0.97	0.06	81,81,81,81	0
2	CA	A	603	1/1	0.97	0.07	39,39,39,39	0
2	CA	B	603	1/1	0.98	0.05	38,38,38,38	0
2	CA	A	609	1/1	0.98	0.03	87,87,87,87	0
2	CA	A	612	1/1	0.98	0.09	74,74,74,74	0
2	CA	A	602	1/1	0.99	0.08	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.