



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:05 PM UTC

PDB ID : 1FWX / pdb_00001fwx
Title : CRYSTAL STRUCTURE OF NITROUS OXIDE REDUCTASE FROM P. DENITRIFICANS
Authors : Brown, K.; Djinovic-Carugo, K.; Haltia, T.; Cabrito, I.; Saraste, M.; Moura, J.J.; Moura, I.; Tegoni, M.; Cambillau, C.
Deposited on : 2000-09-25
Resolution : 1.60 Å(reported)

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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

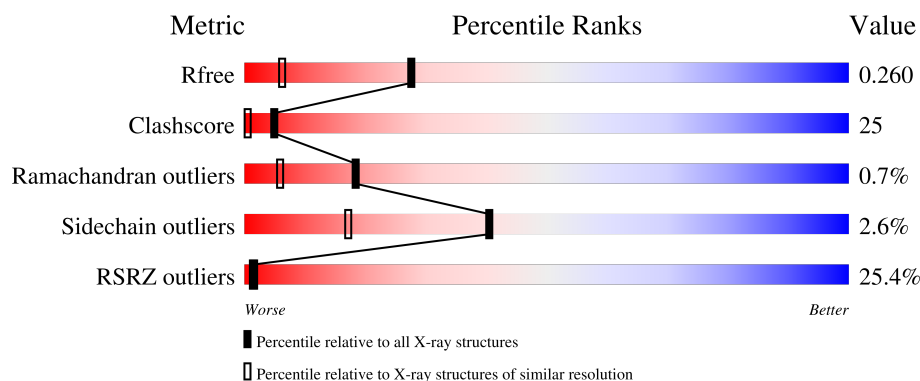
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	595	14% 69% 28% ..
1	B	595	9% 71% 24% ..
1	C	595	23% 65% 30% ..
1	D	595	55% 52% 42% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21176 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 NITROUS OXIDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4633	2913	796	892	32			
1	B	589	Total	C	N	O	S	0	0	0
			4619	2904	793	890	32			
1	C	590	Total	C	N	O	S	0	0	0
			4628	2910	795	891	32			
1	D	588	Total	C	N	O	S	0	0	0
			4611	2900	792	887	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	VAL	ALA	see remark 999	UNP Q51705
A	8	ALA	GLY	see remark 999	UNP Q51705
B	291	VAL	ALA	see remark 999	UNP Q51705
B	8	ALA	GLY	see remark 999	UNP Q51705
C	291	VAL	ALA	see remark 999	UNP Q51705
C	8	ALA	GLY	see remark 999	UNP Q51705
D	291	VAL	ALA	see remark 999	UNP Q51705
D	8	ALA	GLY	see remark 999	UNP Q51705

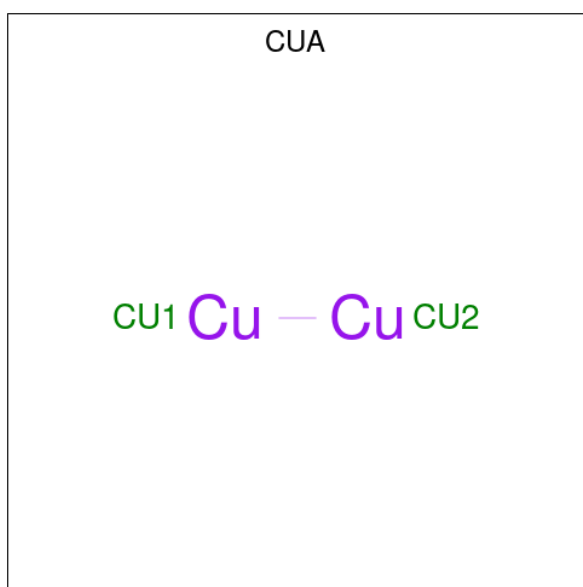
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

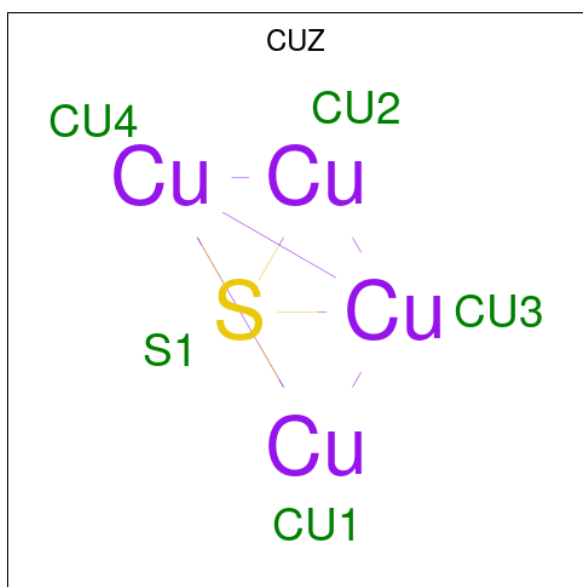
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0
3	C	3	Total 3	Ca 3	0	0
3	D	2	Total 2	Ca 2	0	0

- Molecule 4 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 2	Cu 2	0	0
4	B	1	Total 2	Cu 2	0	0
4	C	1	Total 2	Cu 2	0	0
4	D	1	Total 2	Cu 2	0	0

- Molecule 5 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (CCD ID: CUZ) (formula: Cu₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Cu	S	0	0
			5	4	1		
5	B	1	Total	Cu	S	0	0
			5	4	1		
5	C	1	Total	Cu	S	0	0
			5	4	1		
5	D	1	Total	Cu	S	0	0
			5	4	1		

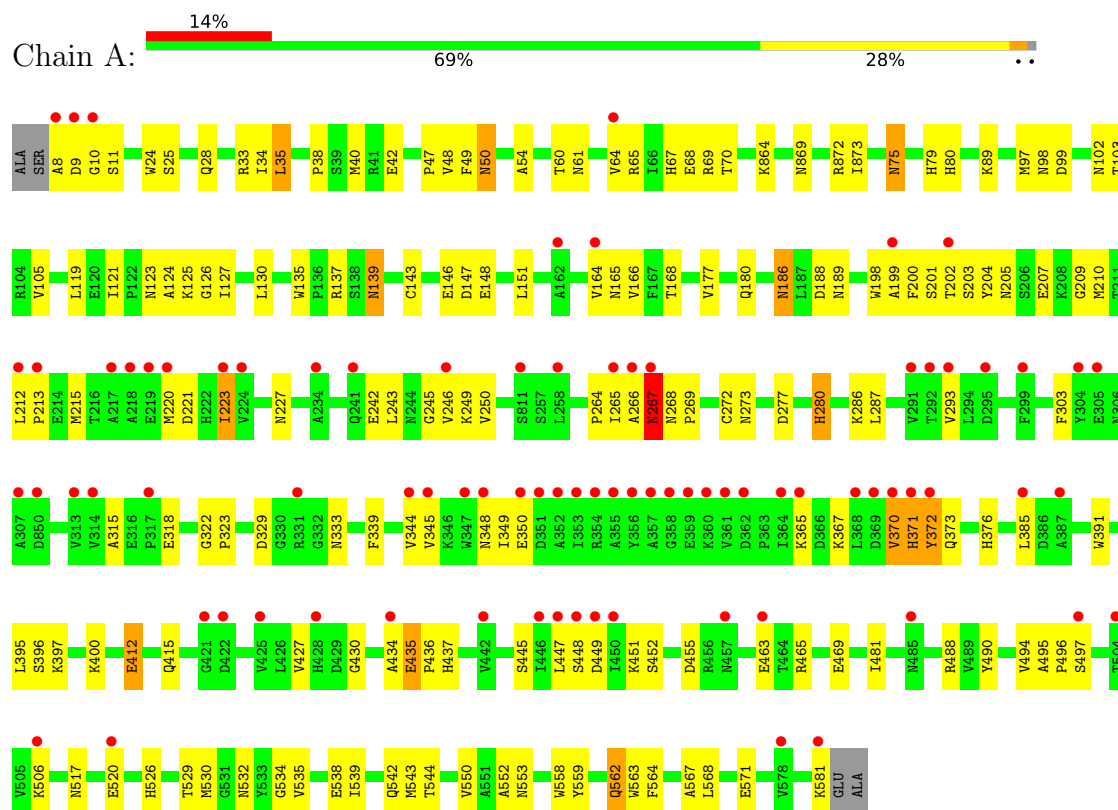
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	724	Total	O	0	0
			724	724		
6	B	750	Total	O	0	0
			750	750		
6	C	657	Total	O	0	0
			657	657		
6	D	511	Total	O	0	0
			511	511		

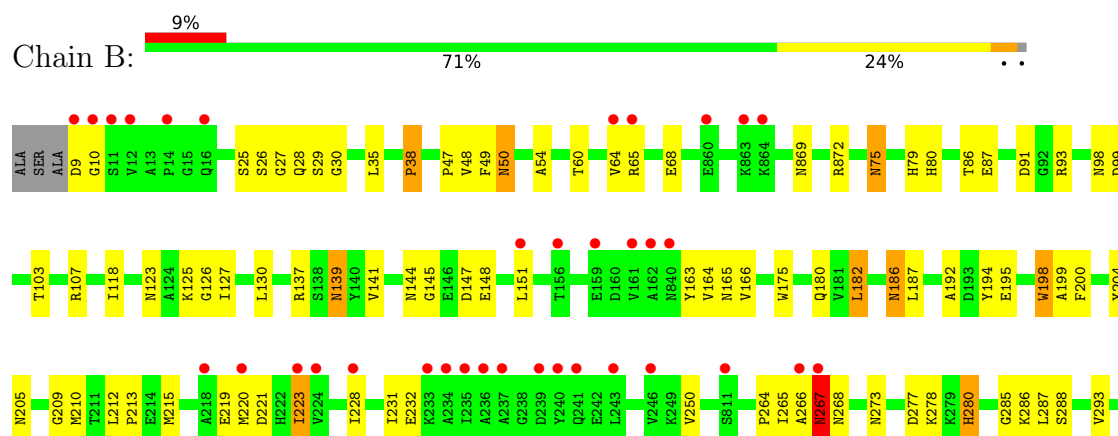
3 Residue-property plots

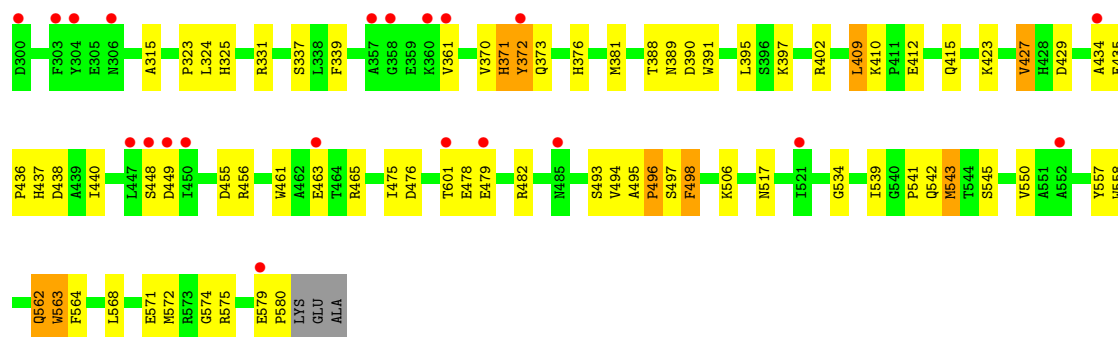
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

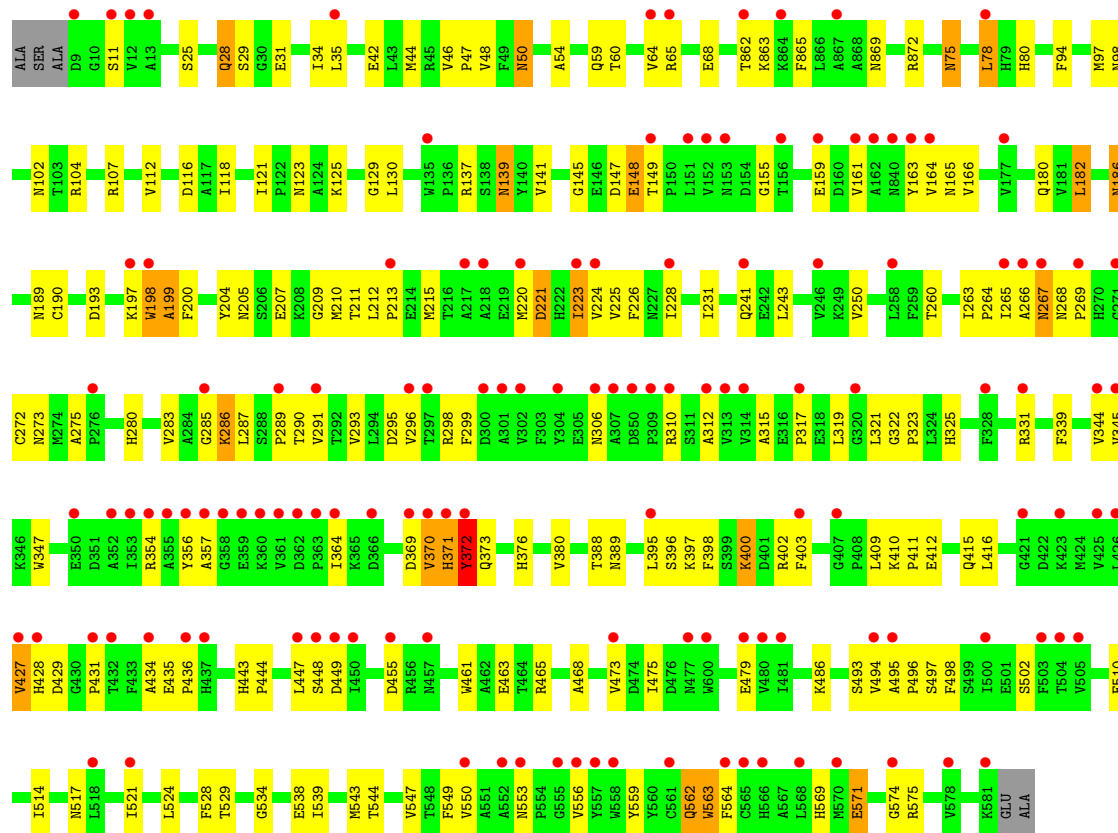


• Molecule 1: NITROUS OXIDE REDUCTASE

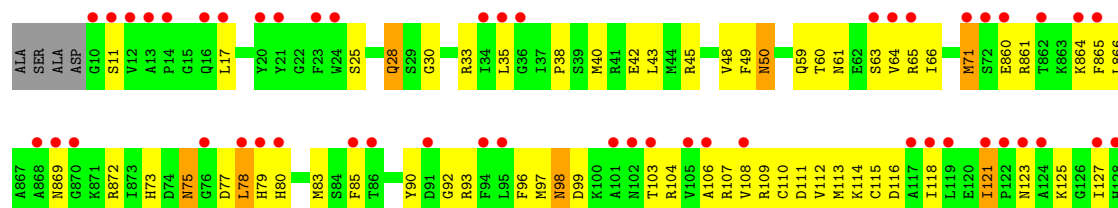




● Molecule 1: NITROUS OXIDE REDUCTASE



● Molecule 1: NITROUS OXIDE REDUCTASE



M517	D438	D369	P309	V251	D188	G129
L518	A439	V370	R310	D252	N189	L130
D519	I440	H371	S311	G253	C190	R131
E520	A441	Y372	A312	R254		P132
I521	V442	Q373	V313	K255	D193	K133
D522	H443	P374	V314	E256	Y194	K134
D523	P444	G375	A315	A810	E195	W135
L524	S445	H376	E316	S811	G196	F136
T525	I446	L377	P317	S257	K197	S137
H526	L447D	K378	E318	L258	W198	S138
G527	S448	T379	L319	F259	N139	N139
F528	D449	V380	G320	T260	F200	Y140
T529	I450	M381	L321	R261	S201	T141
M530	K451	G382	G322	V262	T202	F142
	S452	E383	P323	L263	S203	C143
G534	V453	T384	L324	P264	Y204	N144
V535	W454	L385	H325	L265	N205	G145
	D455	D386	T326	A266	S206	E146
E538	R456	A387	A327	N267	E207	D147
I539	N457	T388	F328	N268	K208	E148
G540	D458	R389	D329	P269	G209	T149
P541	P459	D390	G330	H270	M210	P150
Q542	M460	W391	R331	G271	T211	L151
M543	W461	L392	G332	C272	L212	V152
T544	A462	V393	N333	N273	P213	M153
	E463	C394	A334	M274	E214	D154
V547	T464	L395	Y335	A275	N215	G155
	R465	S396	T336	P276	K216	T156
V550	A466	K397	S337	D277	A217	M157
A551	Q467	F398	L338	K278	A218	M158
A552	A468	S399	F339	K279	E219	E159
P554	E469	K400	L340	H280	M220	D160
G555		D401	D341	L281	D221	V161
V556	V473	R402	S342	C282	H222	A162
Y557	D474		Q343	V283	I223	N840
	I475	P408	V344	A284	V224	Y163
		L409	V345	G285	V225	V164
		K410	K346	K286	F226	M165
T601	E478	P411	W347	L287	N227	V166
V560	E479	E412	N348	S288	L228	F167
C561	W480	W413	I349	P289	A229	T168
Q562		D414	E350	T290	E230	A169
W563	W485	Q415	D351	V291	T231	
F564		L416	A352	T292	E232	D171
		I417	R353	V293	K233	A172
		D418	L294	L294	A234	D173
M569	S492	I419	K354	D295	L235	K174
M570	S493	S420	A355	V296	A236	W175
E571	V494	G421	V356	T297	A237	E176
M572	A495	D421	A357	R298	G238	V177
D573	P496	K422	G358	K298	D239	A178
G574	S497	K423	E359	F299	D239	A178
	F498	M424	K360	D300	W179	
R575		W425	V361	A301	Q241	Q180
W576		L426	D362	V302	E242	Q180
L577	S502	V427	P363	F303	L243	V181
V578			I364	V304	N244	L182
E579	K506		L365	S305	G245	V183
P580	E507	A434	K366	E305	G246	S184
LYS	G508	E435	D366	N306	V246	G185
		P436	A367	A307	K249	M186
GLU	T516	H437	L369	N350	V250	L187

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.59Å 105.09Å 116.70Å 90.00° 110.69° 90.00°	Depositor
Resolution (Å)	29.83 – 1.60 29.83 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.4 (29.83-1.60) 89.5 (29.83-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.60Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.241 , 0.264 0.236 , 0.260	Depositor DCC
R_{free} test set	1331 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21176	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: CL, CUA, CA, CUZ

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	0.40	0/4744	1.03	27/6443 (0.4%)
1	B	0.42	1/4730 (0.0%)	1.04	29/6425 (0.5%)
1	C	0.39	0/4739	1.02	29/6436 (0.5%)
1	D	0.37	1/4722 (0.0%)	0.97	24/6414 (0.4%)
All	All	0.39	2/18935 (0.0%)	1.01	109/25718 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	543	MET	SD-CE	-6.17	1.64	1.79
1	D	71	MET	SD-CE	-5.91	1.64	1.79

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	GLU	N-CA-C	13.88	140.48	109.81
1	C	435	GLU	N-CA-C	13.07	138.70	109.81
1	A	435	GLU	N-CA-C	12.50	137.44	109.81
1	B	267	ASN	N-CA-C	9.90	131.88	110.80
1	C	267	ASN	N-CA-C	9.66	131.37	110.80
1	D	435	GLU	N-CA-C	9.31	130.39	109.81
1	A	10	GLY	N-CA-C	-8.99	102.75	115.43
1	D	371	HIS	N-CA-C	8.97	124.48	108.24
1	A	267	ASN	N-CA-C	8.76	129.46	110.80
1	C	449	ASP	N-CA-C	8.34	122.80	113.21
1	A	371	HIS	N-CA-C	8.33	124.23	107.41
1	C	371	HIS	N-CA-C	8.31	124.19	107.41
1	D	436	PRO	N-CA-C	-8.10	99.25	111.41
1	B	371	HIS	N-CA-C	8.10	123.28	107.57
1	D	450	ILE	N-CA-C	-8.08	98.18	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	SER	N-CA-C	-7.77	99.33	110.59
1	A	221	ASP	N-CA-C	-7.67	102.49	108.78
1	B	25	SER	N-CA-C	-7.52	100.83	110.53
1	B	427	VAL	N-CA-C	7.36	117.86	111.90
1	C	449	ASP	CB-CA-C	-7.35	97.71	110.72
1	D	25	SER	N-CA-C	-7.35	99.94	110.59
1	C	223	ILE	N-CA-C	-7.17	98.15	108.48
1	A	25	SER	N-CA-C	-7.06	101.42	110.53
1	C	436	PRO	N-CA-C	-6.97	100.04	111.68
1	A	497	SER	N-CA-C	6.85	119.59	109.24
1	A	280	HIS	N-CA-C	6.79	120.01	109.07
1	A	412	GLU	N-CA-C	-6.76	100.79	110.59
1	D	435	GLU	CA-C-N	-6.62	113.48	120.03
1	D	435	GLU	C-N-CA	-6.62	113.48	120.03
1	C	497	SER	N-CA-C	6.56	119.15	109.24
1	B	199	ALA	N-CA-C	-6.53	99.10	109.23
1	A	266	ALA	N-CA-C	6.52	119.67	109.96
1	A	436	PRO	N-CA-C	-6.42	101.81	111.57
1	B	141	VAL	N-CA-C	-6.35	98.48	107.75
1	D	266	ALA	N-CA-C	6.32	119.53	110.24
1	B	223	ILE	N-CA-C	-6.30	99.14	108.85
1	B	372	TYR	N-CA-C	6.29	124.20	110.80
1	B	449	ASP	N-CA-C	6.26	119.61	112.97
1	B	412	GLU	N-CA-C	-6.26	101.51	110.59
1	D	412	GLU	N-CA-C	-6.23	101.55	110.59
1	B	370	VAL	CA-C-N	-6.22	113.56	122.77
1	B	370	VAL	C-N-CA	-6.22	113.56	122.77
1	B	497	SER	N-CA-C	6.20	118.59	109.24
1	A	198	TRP	N-CA-C	6.12	118.26	109.14
1	C	199	ALA	N-CA-C	-6.07	99.47	108.99
1	A	223	ILE	N-CA-C	-6.04	99.78	108.48
1	B	198	TRP	N-CA-C	6.03	118.58	109.41
1	B	280	HIS	N-CA-C	6.03	119.07	109.24
1	D	872	ARG	N-CA-C	-5.97	106.13	113.41
1	D	146	GLU	N-CA-C	5.95	117.84	111.36
1	B	266	ALA	N-CA-C	5.91	118.77	109.96
1	A	199	ALA	N-CA-C	-5.88	99.76	108.99
1	C	139	ASN	N-CA-C	-5.87	105.01	111.82
1	D	198	TRP	N-CA-C	5.87	118.33	109.41
1	B	221	ASP	N-CA-C	-5.82	103.16	108.75
1	C	266	ALA	N-CA-C	5.78	123.12	110.80
1	B	498	PHE	N-CA-C	-5.75	102.01	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	ALA	CA-C-N	5.74	125.45	119.82
1	C	275	ALA	C-N-CA	5.74	125.45	119.82
1	B	273	ASN	N-CA-C	5.71	117.72	108.41
1	C	498	PHE	N-CA-C	-5.70	102.09	110.52
1	A	54	ALA	N-CA-C	5.66	117.26	111.14
1	A	370	VAL	CA-C-N	-5.64	114.38	123.23
1	A	370	VAL	C-N-CA	-5.64	114.38	123.23
1	D	121	ILE	N-CA-C	5.63	113.12	107.55
1	C	141	VAL	N-CA-C	-5.61	99.47	107.77
1	A	447	LEU	CB-CA-C	-5.60	104.17	111.40
1	C	356	TYR	N-CA-C	-5.58	105.20	111.28
1	B	391	TRP	N-CA-C	5.56	118.62	109.72
1	C	412	GLU	N-CA-C	-5.53	102.57	110.59
1	A	273	ASN	N-CA-C	5.50	117.38	108.41
1	C	198	TRP	N-CA-C	5.49	117.53	109.24
1	C	455	ASP	N-CA-C	-5.49	100.73	109.96
1	D	222	HIS	N-CA-C	5.49	116.57	107.73
1	C	370	VAL	CA-C-N	-5.47	114.64	123.23
1	C	370	VAL	C-N-CA	-5.47	114.64	123.23
1	C	273	ASN	N-CA-C	5.46	117.31	108.41
1	C	372	TYR	N-CA-C	5.41	122.32	110.80
1	C	68	GLU	N-CA-C	5.40	119.59	112.89
1	C	221	ASP	N-CA-C	-5.40	103.57	108.75
1	B	390	ASP	N-CA-C	5.39	119.80	111.56
1	A	68	GLU	N-CA-C	5.37	119.68	113.18
1	A	455	ASP	N-CA-C	-5.35	100.97	109.96
1	B	54	ALA	N-CA-C	5.35	116.92	111.14
1	D	372	TYR	N-CA-C	5.34	122.17	110.80
1	B	68	GLU	N-CA-C	5.33	119.50	112.89
1	C	145	GLY	N-CA-C	-5.32	100.58	113.18
1	A	103	THR	N-CA-C	5.30	117.64	111.02
1	A	391	TRP	N-CA-C	5.25	118.14	109.85
1	B	139	ASN	N-CA-C	-5.24	105.74	111.82
1	B	166	VAL	N-CA-C	5.21	115.41	108.11
1	B	436	PRO	N-CA-C	-5.21	103.09	111.38
1	A	139	ASN	N-CA-C	-5.20	105.69	111.36
1	D	498	PHE	N-CA-C	-5.19	102.07	110.32
1	B	455	ASP	N-CA-C	-5.18	101.26	109.96
1	C	54	ALA	N-CA-C	5.18	116.73	111.14
1	D	370	VAL	CA-C-N	-5.18	115.11	122.41
1	D	370	VAL	C-N-CA	-5.18	115.11	122.41
1	C	427	VAL	N-CA-C	5.17	116.46	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	391	TRP	N-CA-C	5.16	117.98	109.72
1	D	267	ASN	N-CA-C	5.16	121.78	110.80
1	D	497	SER	N-CA-C	5.15	117.02	109.24
1	D	273	ASN	N-CA-C	5.14	117.27	108.90
1	A	318	GLU	N-CA-C	-5.12	101.42	109.25
1	B	145	GLY	N-CA-C	-5.12	101.05	113.18
1	A	24	TRP	N-CA-C	5.10	118.12	109.76
1	D	139	ASN	N-CA-C	-5.05	105.96	111.82
1	A	372	TYR	N-CA-C	5.04	121.53	110.80
1	D	448	SER	N-CA-C	5.01	121.47	110.80

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	4633	0	4443	185	0
1	B	4619	0	4425	164	0
1	C	4628	0	4438	244	0
1	D	4611	0	4421	359	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	5	0	0	0	0
6	A	724	0	0	82	0
6	B	750	0	0	69	0
6	C	657	0	0	132	0
6	D	511	0	0	208	0
All	All	21176	0	17727	914	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 25.

All (914) 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:D:326:THR:HG22	1:D:336:THR:HG22	1.19	1.14
1:B:456:ARG:HA	6:B:6235:HOH:O	1.54	1.04
1:D:547:VAL:HA	6:D:8122:HOH:O	1.58	1.04
1:D:71:MET:SD	6:D:8077:HOH:O	2.18	1.02
1:C:215:MET:HG2	6:C:7335:HOH:O	1.59	1.01
1:D:540:GLY:HA2	6:D:8240:HOH:O	1.59	1.01
1:D:860:GLU:HG3	1:D:864:LYS:HE2	1.44	0.99
1:D:201:SER:HB3	6:D:8189:HOH:O	1.63	0.99
1:A:550:VAL:H	1:B:869:ASN:HD21	1.10	0.98
1:D:392:LEU:HB3	6:D:8101:HOH:O	1.62	0.97
1:D:336:THR:HG23	1:D:347:TRP:HE1	1.29	0.97
1:B:371:HIS:H	1:B:415:GLN:HE22	1.07	0.96
1:C:553:ASN:ND2	1:D:865:PHE:HB2	1.80	0.96
1:D:540:GLY:HA3	6:D:8169:HOH:O	1.65	0.95
1:D:541:PRO:HD3	6:D:8240:HOH:O	1.64	0.95
1:C:104:ARG:HA	6:C:6962:HOH:O	1.66	0.94
1:D:371:HIS:H	1:D:415:GLN:HE22	1.02	0.94
1:C:28:GLN:H	1:C:28:GLN:HE21	1.04	0.94
1:D:134:LYS:HB2	6:D:8275:HOH:O	1.67	0.93
1:D:502:SER:HA	6:D:7910:HOH:O	1.67	0.93
1:A:105:VAL:HG22	6:A:5276:HOH:O	1.68	0.92
1:D:578:VAL:HB	6:D:7861:HOH:O	1.70	0.92
1:A:371:HIS:H	1:A:415:GLN:HE22	1.02	0.92
1:D:416:LEU:HA	6:D:8178:HOH:O	1.68	0.92
1:C:291:VAL:HG21	6:C:7096:HOH:O	1.69	0.91
1:B:148:GLU:HG3	1:B:165:ASN:HD21	1.36	0.91
1:D:210:MET:HB3	6:D:8300:HOH:O	1.70	0.91
1:D:194:TYR:HA	6:D:8275:HOH:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:GLN:H	1:D:28:GLN:HE21	1.15	0.91
1:C:129:GLY:HA3	6:C:7014:HOH:O	1.69	0.90
1:C:121:ILE:HG12	6:C:6962:HOH:O	1.71	0.90
1:B:65:ARG:HD2	1:B:463:GLU:OE2	1.71	0.90
1:C:371:HIS:H	1:C:415:GLN:HE22	1.10	0.90
1:D:371:HIS:H	1:D:415:GLN:NE2	1.70	0.90
1:A:452:SER:HA	6:B:6426:HOH:O	1.70	0.89
1:A:137:ARG:HH11	1:A:139:ASN:ND2	1.70	0.89
1:C:250:VAL:HB	6:C:7063:HOH:O	1.72	0.89
1:A:371:HIS:H	1:A:415:GLN:NE2	1.71	0.88
1:C:31:GLU:HB3	6:C:7454:HOH:O	1.73	0.88
1:A:69:ARG:HB3	6:A:5290:HOH:O	1.74	0.88
1:A:188:ASP:HB3	6:A:5348:HOH:O	1.73	0.87
1:C:403:PHE:HA	6:C:7395:HOH:O	1.75	0.87
1:A:869:ASN:HD21	1:B:550:VAL:H	1.17	0.87
1:C:869:ASN:HD21	1:D:550:VAL:H	1.22	0.87
1:C:241:GLN:HG3	6:C:7063:HOH:O	1.75	0.86
1:B:381:MET:HB2	6:B:6223:HOH:O	1.76	0.85
1:D:577:LEU:HD11	6:D:7871:HOH:O	1.76	0.85
1:A:49:PHE:HB3	6:A:5395:HOH:O	1.77	0.84
1:B:50:ASN:HD22	1:B:50:ASN:H	1.25	0.84
1:B:388:THR:HG23	6:B:6223:HOH:O	1.76	0.84
1:D:371:HIS:N	1:D:415:GLN:HE22	1.76	0.83
1:C:296:VAL:HB	6:C:7268:HOH:O	1.77	0.83
1:C:220:MET:HB3	6:C:6998:HOH:O	1.77	0.83
1:D:267:ASN:HB3	1:D:287:LEU:HB2	1.59	0.83
1:C:161:VAL:HG23	6:C:7192:HOH:O	1.77	0.83
1:D:48:VAL:HG11	6:D:8262:HOH:O	1.77	0.83
1:D:137:ARG:HH11	1:D:139:ASN:ND2	1.77	0.82
1:C:371:HIS:H	1:C:415:GLN:NE2	1.77	0.82
1:C:272:CYS:HB2	6:C:7324:HOH:O	1.80	0.82
1:A:50:ASN:H	1:A:50:ASN:HD22	1.28	0.81
1:C:486:LYS:HE2	6:C:7391:HOH:O	1.79	0.81
1:C:207:GLU:HB2	6:C:7143:HOH:O	1.79	0.81
1:B:9:ASP:OD1	1:B:10:GLY:N	2.13	0.81
1:B:195:GLU:HA	6:B:6421:HOH:O	1.79	0.81
1:C:289:PRO:HB3	6:C:7383:HOH:O	1.79	0.81
1:C:225:VAL:HG12	6:C:7399:HOH:O	1.81	0.81
1:C:155:GLY:HA3	6:D:7911:HOH:O	1.79	0.81
1:C:228:ILE:HG13	6:C:7373:HOH:O	1.79	0.80
1:A:371:HIS:N	1:A:415:GLN:HE22	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:SER:OG	6:A:5439:HOH:O	1.99	0.80
1:D:346:LYS:HD2	6:D:8187:HOH:O	1.81	0.80
1:B:123:ASN:HD22	1:B:180:GLN:HE22	1.29	0.80
1:A:148:GLU:HG3	1:A:165:ASN:HD21	1.45	0.80
1:C:123:ASN:HD22	1:C:180:GLN:HE22	1.27	0.80
1:A:168:THR:HB	6:A:5258:HOH:O	1.81	0.80
1:C:78:LEU:HD13	1:C:97:MET:HB2	1.62	0.80
1:D:535:VAL:HG22	6:D:8251:HOH:O	1.82	0.80
1:C:189:ASN:HB2	6:C:7324:HOH:O	1.82	0.79
1:C:286:LYS:HB3	6:C:7413:HOH:O	1.83	0.79
1:D:296:VAL:HG13	6:D:7891:HOH:O	1.82	0.79
1:D:302:VAL:HG22	6:D:8026:HOH:O	1.81	0.79
1:C:321:LEU:HA	6:C:7383:HOH:O	1.82	0.78
1:D:419:ILE:HG23	6:D:8101:HOH:O	1.81	0.78
1:B:148:GLU:HB2	6:B:6532:HOH:O	1.82	0.78
1:A:143:CYS:SG	6:A:5258:HOH:O	2.41	0.78
1:B:371:HIS:H	1:B:415:GLN:NE2	1.81	0.78
1:D:294:LEU:HD12	6:D:8132:HOH:O	1.82	0.78
1:D:353:ILE:HD11	6:D:8029:HOH:O	1.84	0.78
1:D:557:TYR:HE2	6:D:7861:HOH:O	1.67	0.78
1:D:412:GLU:HG2	6:D:8066:HOH:O	1.84	0.77
1:A:177:VAL:HG11	1:A:246:VAL:HG21	1.67	0.77
1:D:71:MET:CG	6:D:7990:HOH:O	2.32	0.77
1:A:564:PHE:HE1	6:A:5572:HOH:O	1.68	0.77
1:C:410:LYS:HD3	6:C:7235:HOH:O	1.84	0.76
1:D:137:ARG:HH11	1:D:139:ASN:HD22	1.30	0.76
1:A:180:GLN:HB2	6:A:5552:HOH:O	1.85	0.76
1:C:107:ARG:HD2	1:C:116:ASP:OD2	1.83	0.76
1:D:377:LEU:HD22	6:D:8047:HOH:O	1.86	0.76
1:A:67:HIS:HB3	6:A:5517:HOH:O	1.85	0.76
1:D:310:ARG:HG2	6:D:8052:HOH:O	1.85	0.76
1:B:198:TRP:HA	1:B:228:ILE:HD13	1.68	0.76
1:D:223:ILE:HG23	1:D:265:ILE:HG13	1.66	0.76
1:A:488:ARG:HB2	6:A:5225:HOH:O	1.85	0.76
1:C:198:TRP:HB3	6:C:7338:HOH:O	1.85	0.75
1:C:228:ILE:HD13	6:C:6839:HOH:O	1.87	0.75
1:D:125:LYS:HG3	1:D:149:THR:HG21	1.68	0.75
1:D:220:MET:HB3	6:D:8039:HOH:O	1.85	0.75
1:D:225:VAL:HG12	6:D:8065:HOH:O	1.85	0.75
1:D:35:LEU:HD13	1:D:42:GLU:HA	1.68	0.75
1:B:267:ASN:HB3	1:B:287:LEU:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HH11	1:A:139:ASN:HD22	1.35	0.75
1:D:393:VAL:HA	6:D:8178:HOH:O	1.87	0.74
1:B:192:ALA:HA	6:B:6515:HOH:O	1.86	0.74
1:A:207:GLU:HB2	6:A:5455:HOH:O	1.87	0.74
1:C:550:VAL:H	1:D:869:ASN:HD21	1.35	0.74
1:C:243:LEU:HG	6:C:7063:HOH:O	1.87	0.74
1:C:50:ASN:H	1:C:50:ASN:HD22	1.32	0.74
1:D:115:CYS:SG	6:D:7943:HOH:O	2.46	0.74
1:D:271:GLY:HA2	6:D:7996:HOH:O	1.87	0.74
1:A:202:THR:HB	6:A:5348:HOH:O	1.85	0.74
1:A:245:GLY:HA2	6:A:5568:HOH:O	1.88	0.74
1:A:123:ASN:HD22	1:A:180:GLN:HE22	1.36	0.74
1:B:137:ARG:HH11	1:B:139:ASN:ND2	1.86	0.74
1:C:347:TRP:HB3	6:C:6950:HOH:O	1.87	0.74
1:D:417:ILE:HB	6:D:8101:HOH:O	1.86	0.73
1:C:369:ASP:HB3	6:C:7452:HOH:O	1.87	0.73
1:D:259:PHE:HA	6:D:8093:HOH:O	1.88	0.73
1:A:89:LYS:HE2	6:A:5385:HOH:O	1.89	0.73
1:C:148:GLU:HG3	6:C:7424:HOH:O	1.87	0.73
1:B:26:SER:OG	6:B:6545:HOH:O	2.07	0.73
1:B:475:ILE:HB	6:B:6389:HOH:O	1.88	0.73
1:D:106:ALA:HB1	6:D:7943:HOH:O	1.89	0.73
1:A:250:VAL:HG22	6:A:5552:HOH:O	1.89	0.72
1:D:93:ARG:HA	6:D:8164:HOH:O	1.89	0.72
1:D:516:THR:HB	6:D:8011:HOH:O	1.88	0.72
1:A:125:LYS:HE3	6:B:6544:HOH:O	1.88	0.72
1:C:223:ILE:HG23	1:C:265:ILE:HG13	1.71	0.72
1:B:498:PHE:HA	6:B:6478:HOH:O	1.89	0.72
1:C:148:GLU:CD	1:C:148:GLU:H	1.97	0.72
1:D:526:HIS:HB3	6:D:7895:HOH:O	1.89	0.72
1:D:465:ARG:HG2	1:D:475:ILE:HD11	1.72	0.72
1:A:272:CYS:HB2	6:A:5209:HOH:O	1.90	0.71
1:B:215:MET:HB2	6:B:6186:HOH:O	1.90	0.71
1:C:517:ASN:HB2	1:C:539:ILE:HG22	1.71	0.71
1:D:326:THR:HG22	1:D:336:THR:CG2	2.10	0.71
1:D:114:LYS:N	6:D:8146:HOH:O	2.21	0.71
1:C:148:GLU:HG2	6:C:7031:HOH:O	1.90	0.71
1:C:263:ILE:HG22	6:C:7066:HOH:O	1.89	0.71
1:C:118:ILE:HD11	6:C:7072:HOH:O	1.89	0.71
1:B:30:GLY:N	6:B:6545:HOH:O	2.19	0.71
1:D:348:ASN:O	6:D:8250:HOH:O	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:TRP:HZ2	6:B:6235:HOH:O	1.74	0.70
1:C:575:ARG:HD2	6:D:8300:HOH:O	1.90	0.70
1:D:112:VAL:HG22	6:D:8304:HOH:O	1.91	0.70
1:C:149:THR:HA	6:C:7140:HOH:O	1.91	0.70
1:D:475:ILE:HA	6:D:8068:HOH:O	1.91	0.70
1:A:550:VAL:H	1:B:869:ASN:ND2	1.88	0.70
1:D:108:VAL:HG13	6:D:8146:HOH:O	1.91	0.70
1:A:212:LEU:HA	6:A:5452:HOH:O	1.91	0.70
1:A:265:ILE:HD11	6:A:5520:HOH:O	1.89	0.70
1:B:87:GLU:HG3	6:B:6455:HOH:O	1.91	0.70
1:B:465:ARG:NH2	1:B:476:ASP:OD2	2.23	0.70
1:C:371:HIS:N	1:C:415:GLN:HE22	1.87	0.70
1:B:285:GLY:O	6:B:6340:HOH:O	2.08	0.70
1:C:286:LYS:HA	6:C:7309:HOH:O	1.92	0.70
1:C:521:ILE:HG23	1:C:524:LEU:HB2	1.74	0.70
1:D:866:LEU:HD11	6:D:8087:HOH:O	1.92	0.69
1:A:11:SER:HA	6:A:5461:HOH:O	1.91	0.69
1:B:575:ARG:HD3	6:B:5931:HOH:O	1.91	0.69
1:D:575:ARG:N	6:D:7910:HOH:O	2.22	0.69
1:D:230:GLU:HB2	6:D:8093:HOH:O	1.93	0.69
1:B:539:ILE:HA	1:B:543:MET:HE2	1.75	0.69
1:D:491:MET:HB3	6:D:7982:HOH:O	1.93	0.69
1:A:869:ASN:ND2	1:B:550:VAL:H	1.89	0.69
1:C:285:GLY:HA2	6:C:7279:HOH:O	1.91	0.68
1:C:28:GLN:H	1:C:28:GLN:NE2	1.85	0.68
1:D:73:HIS:N	6:D:8087:HOH:O	2.26	0.68
1:D:336:THR:CG2	1:D:347:TRP:HE1	2.04	0.68
1:D:97:MET:HG3	6:D:8262:HOH:O	1.93	0.68
1:B:187:LEU:HD22	6:B:6516:HOH:O	1.94	0.68
1:B:231:ILE:HB	6:B:6166:HOH:O	1.94	0.68
2:D:4908:CL:CL	6:D:7996:HOH:O	2.49	0.67
1:D:572:MET:HB3	6:D:7995:HOH:O	1.93	0.67
1:C:339:PHE:CE1	1:C:373:GLN:HB3	2.29	0.67
1:D:535:VAL:HG12	6:D:8198:HOH:O	1.94	0.67
1:B:456:ARG:NH1	6:B:6235:HOH:O	2.28	0.67
1:C:212:LEU:HD11	1:D:568:LEU:HD13	1.76	0.67
1:A:202:THR:HG23	1:A:269:PRO:HG2	1.74	0.67
1:B:557:TYR:HA	6:B:6544:HOH:O	1.93	0.67
1:D:137:ARG:HB2	6:D:8246:HOH:O	1.95	0.67
1:A:70:THR:HG23	6:A:5290:HOH:O	1.94	0.67
1:A:348:ASN:HB2	1:A:365:LYS:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:VAL:HG13	6:C:7419:HOH:O	1.94	0.67
1:C:553:ASN:HD21	1:D:865:PHE:HB2	1.60	0.66
6:C:7165:HOH:O	1:D:149:THR:HB	1.94	0.66
1:C:547:VAL:HG22	6:C:7415:HOH:O	1.95	0.66
1:D:78:LEU:HD13	1:D:97:MET:HB2	1.75	0.66
1:D:402:ARG:HB3	6:D:8015:HOH:O	1.94	0.66
1:C:221:ASP:HB2	6:C:7427:HOH:O	1.96	0.66
1:D:109:ARG:HB3	6:D:8304:HOH:O	1.96	0.66
1:B:86:THR:HG23	6:B:6455:HOH:O	1.95	0.66
1:D:71:MET:HG2	6:D:7990:HOH:O	1.95	0.66
1:D:570:MET:HA	6:D:8201:HOH:O	1.96	0.66
1:D:61:ASN:N	6:D:8122:HOH:O	2.29	0.66
1:D:314:VAL:HG12	1:D:353:ILE:HG23	1.77	0.66
1:A:80:HIS:H	1:A:98:ASN:ND2	1.93	0.66
1:B:371:HIS:N	1:B:415:GLN:HE22	1.87	0.66
1:C:310:ARG:HG2	6:C:7066:HOH:O	1.94	0.66
1:D:351:ASP:HB2	6:D:8250:HOH:O	1.95	0.66
1:D:298:ARG:O	6:D:7928:HOH:O	2.13	0.65
1:B:456:ARG:NH2	6:B:6389:HOH:O	2.27	0.65
1:C:564:PHE:HB3	6:D:7946:HOH:O	1.94	0.65
1:D:372:TYR:N	1:D:372:TYR:CD1	2.63	0.65
1:B:27:GLY:O	6:B:6545:HOH:O	2.14	0.65
1:C:865:PHE:HB2	6:C:7377:HOH:O	1.96	0.65
1:C:199:ALA:N	6:C:7373:HOH:O	2.29	0.65
1:A:127:ILE:HD12	6:A:5318:HOH:O	1.97	0.65
1:A:552:ALA:N	6:A:5417:HOH:O	2.29	0.65
1:D:415:GLN:HB2	6:D:8274:HOH:O	1.96	0.65
1:D:561:CYS:HB3	6:D:7995:HOH:O	1.95	0.65
1:A:61:ASN:ND2	6:A:5221:HOH:O	2.29	0.65
1:A:35:LEU:HD21	6:A:5511:HOH:O	1.97	0.65
1:C:50:ASN:CG	6:C:7454:HOH:O	2.38	0.65
1:D:365:LYS:HE3	6:D:7994:HOH:O	1.97	0.65
1:D:416:LEU:HD12	6:D:8178:HOH:O	1.96	0.65
1:A:246:VAL:HG23	6:A:4947:HOH:O	1.96	0.65
1:A:567:ALA:HA	6:A:5572:HOH:O	1.97	0.65
1:C:312:ALA:HB2	6:C:7114:HOH:O	1.97	0.65
1:C:475:ILE:HD11	6:C:7081:HOH:O	1.97	0.64
1:C:534:GLY:HA2	1:D:75:ASN:HD21	1.63	0.64
1:D:121:ILE:HD12	1:D:127:ILE:HD13	1.79	0.64
1:D:228:ILE:HG13	6:D:8221:HOH:O	1.97	0.64
1:C:372:TYR:HB3	1:C:398:PHE:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:LYS:HD3	6:D:7898:HOH:O	1.96	0.64
1:C:121:ILE:N	6:C:6962:HOH:O	2.30	0.64
1:C:354:ARG:O	1:C:357:ALA:HB3	1.97	0.64
1:D:50:ASN:HD22	1:D:50:ASN:H	1.46	0.64
1:A:534:GLY:HA2	1:B:75:ASN:HD21	1.63	0.64
1:B:440:ILE:HG22	6:B:6224:HOH:O	1.98	0.64
1:D:28:GLN:H	1:D:28:GLN:NE2	1.94	0.64
1:C:268:ASN:N	1:C:269:PRO:HD3	2.12	0.64
1:D:121:ILE:HB	1:D:127:ILE:HD11	1.80	0.64
1:B:50:ASN:H	1:B:50:ASN:ND2	1.95	0.64
1:C:226:PHE:O	6:C:7373:HOH:O	2.15	0.64
1:C:46:VAL:HG22	6:C:7326:HOH:O	1.97	0.63
1:D:557:TYR:HB3	6:D:7992:HOH:O	1.99	0.63
6:A:5596:HOH:O	1:B:574:GLY:HA2	1.99	0.63
1:C:265:ILE:N	6:C:6998:HOH:O	2.29	0.63
1:D:148:GLU:CD	1:D:148:GLU:H	2.06	0.63
1:D:335:TYR:HE2	6:D:8187:HOH:O	1.81	0.63
1:C:293:VAL:HB	1:C:315:ALA:HB3	1.81	0.63
1:B:493:SER:HA	6:B:6478:HOH:O	1.98	0.63
1:C:280:HIS:HB3	6:C:7419:HOH:O	1.97	0.63
1:D:265:ILE:N	6:D:8039:HOH:O	2.31	0.63
1:C:465:ARG:HB2	6:C:7081:HOH:O	1.99	0.63
1:A:50:ASN:H	1:A:50:ASN:ND2	1.96	0.63
1:D:447(D):LEU:O	1:D:450:ILE:HG13	1.98	0.63
1:D:397:LYS:HB3	6:D:7946:HOH:O	1.97	0.62
1:D:397:LYS:HD2	6:D:7946:HOH:O	1.99	0.62
1:A:137:ARG:NH1	1:A:139:ASN:HD22	1.98	0.62
1:D:542:GLN:HG2	6:D:7900:HOH:O	1.99	0.62
1:B:277:ASP:OD2	1:B:280:HIS:HD2	1.83	0.62
1:A:65:ARG:CZ	1:A:463:GLU:HG3	2.29	0.62
1:D:45:ARG:HG3	6:D:8305:HOH:O	1.99	0.62
1:D:526:HIS:HB2	6:D:8220:HOH:O	2.00	0.62
1:A:581:LYS:HE3	6:A:5178:HOH:O	1.98	0.62
1:D:325:HIS:HB2	6:D:8047:HOH:O	1.99	0.62
1:D:395:LEU:HG	6:D:7989:HOH:O	1.99	0.62
1:D:109:ARG:N	6:D:8146:HOH:O	2.33	0.62
1:A:535:VAL:HB	6:A:5306:HOH:O	1.99	0.62
1:B:339:PHE:CE1	1:B:373:GLN:HB3	2.35	0.62
1:C:65:ARG:HH11	1:C:463:GLU:HB2	1.65	0.62
1:A:75:ASN:HD21	1:B:534:GLY:HA2	1.64	0.61
1:A:143:CYS:O	6:A:5258:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:THR:HG22	1:B:479:GLU:H	1.64	0.61
1:D:543:MET:HE3	6:D:8169:HOH:O	1.99	0.61
1:A:242:GLU:HG2	6:A:5568:HOH:O	2.01	0.61
1:A:269:PRO:O	6:A:5609:HOH:O	2.16	0.61
1:A:212:LEU:HB3	1:A:213:PRO:HD3	1.83	0.61
1:A:215:MET:HB2	6:A:5452:HOH:O	1.99	0.61
1:A:33:ARG:HB3	6:A:5511:HOH:O	2.00	0.61
1:C:44:MET:HG3	6:C:7326:HOH:O	2.01	0.61
1:C:50:ASN:H	1:C:50:ASN:ND2	1.97	0.61
1:D:554:PRO:HB2	6:D:7911:HOH:O	1.99	0.61
1:D:263:ILE:HG22	6:D:8052:HOH:O	2.01	0.61
1:D:575:ARG:HB2	6:D:7871:HOH:O	2.01	0.61
1:C:112:VAL:HB	6:C:7106:HOH:O	2.00	0.61
1:C:211:THR:O	1:C:215:MET:HG3	2.01	0.61
1:A:530:MET:HB3	6:A:5306:HOH:O	2.01	0.61
1:A:201:SER:HB3	6:A:5168:HOH:O	2.00	0.61
1:B:437:HIS:HB3	6:B:6184:HOH:O	2.01	0.61
1:C:28:GLN:HE21	1:C:28:GLN:N	1.88	0.61
1:C:345:VAL:HG22	6:C:6950:HOH:O	2.00	0.61
1:C:564:PHE:N	1:D:435:GLU:OE2	2.34	0.61
1:D:302:VAL:HG23	6:D:7928:HOH:O	1.99	0.61
1:B:212:LEU:HD12	6:B:6186:HOH:O	2.00	0.60
1:D:65:ARG:HD2	1:D:463:GLU:OE2	2.02	0.60
1:A:130:LEU:HB3	6:A:5305:HOH:O	2.01	0.60
1:D:385:LEU:HD23	6:D:8292:HOH:O	2.01	0.60
1:A:168:THR:O	6:A:5258:HOH:O	2.17	0.60
1:B:465:ARG:HH22	1:B:476:ASP:CG	2.08	0.60
1:D:866:LEU:CD1	6:D:8087:HOH:O	2.49	0.60
1:C:869:ASN:ND2	1:D:550:VAL:H	1.98	0.60
1:D:40:MET:HE2	6:D:8000:HOH:O	2.01	0.60
1:C:94:PHE:CE2	1:C:107:ARG:HD3	2.36	0.60
1:D:80:HIS:H	1:D:98:ASN:ND2	1.99	0.60
1:C:29:SER:O	6:C:7454:HOH:O	2.16	0.60
1:B:80:HIS:H	1:B:98:ASN:ND2	2.00	0.60
1:B:232:GLU:HG3	6:B:6381:HOH:O	2.01	0.60
1:D:127:ILE:HG12	6:D:8234:HOH:O	2.01	0.60
1:D:465:ARG:HB3	6:D:8038:HOH:O	2.02	0.60
1:B:107:ARG:NH1	6:B:6506:HOH:O	2.34	0.60
1:B:123:ASN:HD22	1:B:180:GLN:NE2	1.99	0.60
1:A:339:PHE:CE1	1:A:373:GLN:HB3	2.37	0.59
1:B:493:SER:OG	1:B:517:ASN:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:HH11	1:C:139:ASN:ND2	2.00	0.59
1:D:393:VAL:HG22	6:D:8178:HOH:O	2.01	0.59
1:D:348:ASN:HB3	6:D:7994:HOH:O	2.01	0.59
1:A:8:ALA:O	1:A:9:ASP:HB2	2.02	0.59
1:C:575:ARG:CD	6:D:8300:HOH:O	2.47	0.59
1:D:502:SER:HB2	6:D:7871:HOH:O	2.01	0.59
1:A:202:THR:HG21	1:A:269:PRO:C	2.28	0.59
1:B:402:ARG:HD3	1:B:429:ASP:OD2	2.03	0.59
1:A:873:ILE:HG22	6:A:5517:HOH:O	2.01	0.59
1:A:267:ASN:HB3	1:A:287:LEU:HB2	1.85	0.59
1:D:63:SER:HB2	6:D:8013:HOH:O	2.03	0.59
1:C:286:LYS:HE2	6:C:7413:HOH:O	2.01	0.58
1:D:520:GLU:HA	6:D:7900:HOH:O	2.02	0.58
1:A:562:GLN:HE21	1:A:562:GLN:H	1.52	0.58
1:D:860:GLU:O	1:D:864:LYS:HG3	2.03	0.58
1:D:78:LEU:CD1	1:D:97:MET:HB2	2.33	0.58
1:D:233:LYS:HG3	1:D:234:ALA:N	2.19	0.58
1:D:440:ILE:HB	6:D:8141:HOH:O	2.03	0.58
1:C:260:THR:C	6:C:7250:HOH:O	2.46	0.58
1:B:517:ASN:HB2	1:B:539:ILE:HG22	1.86	0.58
6:C:7140:HOH:O	1:D:556:VAL:HG11	2.01	0.58
1:B:60:THR:O	1:B:64:VAL:HG23	2.04	0.58
1:B:209:GLY:O	1:B:210:MET:HE2	2.04	0.58
1:D:306:ASN:HB2	6:D:8116:HOH:O	2.03	0.58
1:D:345:VAL:HG22	1:D:367:LYS:HG2	1.84	0.58
1:C:75:ASN:HD21	1:D:534:GLY:HA2	1.69	0.58
1:C:267:ASN:HB3	1:C:287:LEU:HB2	1.85	0.58
1:D:116:ASP:HA	1:D:460:MET:HE1	1.85	0.58
1:D:861:ARG:HD2	6:D:8286:HOH:O	2.03	0.57
1:C:265:ILE:HG22	6:C:7279:HOH:O	2.04	0.57
1:D:374:PRO:HA	1:D:396:SER:HA	1.85	0.57
1:A:97:MET:HB2	6:A:5480:HOH:O	2.03	0.57
1:D:295:ASP:HB2	1:D:314:VAL:HG21	1.86	0.57
1:D:551:ALA:N	6:D:8167:HOH:O	2.37	0.57
1:D:562:GLN:H	1:D:562:GLN:HE21	1.52	0.57
1:B:212:LEU:HA	6:B:6186:HOH:O	2.04	0.57
1:C:125:LYS:HG3	1:C:149:THR:HG21	1.86	0.57
1:D:109:ARG:CB	6:D:8304:HOH:O	2.52	0.57
1:B:423:LYS:HE3	6:B:6094:HOH:O	2.04	0.57
1:D:575:ARG:CZ	6:D:7871:HOH:O	2.52	0.57
1:D:50:ASN:H	1:D:50:ASN:ND2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ILE:HB	6:C:7139:HOH:O	2.05	0.57
1:D:165:ASN:CG	1:D:186:ASN:HA	2.30	0.57
1:A:465:ARG:O	1:A:469:GLU:HG3	2.05	0.57
1:C:80:HIS:H	1:C:98:ASN:ND2	2.02	0.57
1:C:295:ASP:HB3	6:C:7097:HOH:O	2.04	0.57
1:D:400:LYS:N	6:D:7898:HOH:O	2.38	0.56
1:C:564:PHE:CD2	1:D:397:LYS:HE3	2.40	0.56
1:D:196:GLY:N	6:D:8194:HOH:O	2.38	0.56
1:D:293:VAL:HG11	6:D:8029:HOH:O	2.04	0.56
1:A:365:LYS:HB3	6:A:5288:HOH:O	2.05	0.56
1:C:11:SER:HA	6:C:7301:HOH:O	2.06	0.56
1:C:400:LYS:N	6:C:7235:HOH:O	2.37	0.56
1:D:344:VAL:HG23	1:D:370:VAL:CG1	2.35	0.56
1:B:26:SER:C	6:B:6545:HOH:O	2.47	0.56
1:B:228:ILE:N	1:B:228:ILE:HD12	2.21	0.56
1:A:189:ASN:HB2	6:A:5209:HOH:O	2.04	0.56
1:B:48:VAL:HG12	6:B:6156:HOH:O	2.05	0.56
1:D:109:ARG:N	6:D:7833:HOH:O	2.37	0.56
1:C:468:ALA:HB1	1:C:473:VAL:HG23	1.86	0.56
1:C:60:THR:O	1:C:64:VAL:HG23	2.06	0.56
1:D:96:PHE:HE2	6:D:8236:HOH:O	1.88	0.56
1:D:144:ASN:HD21	1:D:190:CYS:HB3	1.69	0.56
1:C:521:ILE:HG23	1:C:524:LEU:CB	2.36	0.56
1:D:322:GLY:HA3	1:D:340:LEU:HD13	1.88	0.56
1:B:164:VAL:HG12	6:B:6011:HOH:O	2.04	0.56
1:C:493:SER:OG	1:C:517:ASN:HA	2.06	0.56
1:D:555:GLY:N	6:D:7861:HOH:O	2.39	0.55
1:C:550:VAL:H	1:D:869:ASN:ND2	2.03	0.55
1:A:864:LYS:HG2	6:B:6327:HOH:O	2.06	0.55
1:A:349:ILE:HD13	6:A:5450:HOH:O	2.05	0.55
1:C:197:LYS:HG3	1:C:198:TRP:NE1	2.21	0.55
1:C:402:ARG:HA	6:C:7221:HOH:O	2.06	0.55
1:A:517:ASN:HB2	1:A:539:ILE:HG22	1.87	0.55
1:C:198:TRP:CD1	6:C:7268:HOH:O	2.58	0.55
1:C:215:MET:HE2	6:C:7054:HOH:O	2.05	0.55
1:C:290:THR:CG2	6:C:7417:HOH:O	2.54	0.55
1:A:445:SER:O	1:A:448:SER:OG	2.24	0.55
1:D:376:HIS:HB2	1:D:437:HIS:O	2.06	0.55
1:A:246:VAL:HG22	6:A:5552:HOH:O	2.07	0.55
1:C:137:ARG:HH11	1:C:139:ASN:HD22	1.55	0.55
1:C:402:ARG:HD2	1:C:429:ASP:OD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:THR:O	1:C:559:TYR:HA	2.06	0.55
1:D:393:VAL:HG13	6:D:8000:HOH:O	2.05	0.55
1:D:447(D):LEU:HD22	1:D:450:ILE:HD11	1.88	0.55
1:B:80:HIS:CD2	6:B:6184:HOH:O	2.60	0.55
1:C:268:ASN:HB2	6:C:7413:HOH:O	2.07	0.55
1:C:862:THR:HG23	6:C:7356:HOH:O	2.07	0.55
1:D:28:GLN:HE21	1:D:28:GLN:N	1.96	0.55
1:D:454:TRP:NE1	6:D:8169:HOH:O	2.38	0.55
1:A:146:GLU:HG3	6:A:5325:HOH:O	2.07	0.55
1:B:288:SER:CB	6:B:6340:HOH:O	2.54	0.54
1:C:148:GLU:HB3	1:C:165:ASN:HD21	1.70	0.54
1:A:80:HIS:H	1:A:98:ASN:HD21	1.55	0.54
1:A:80:HIS:HB2	6:A:5305:HOH:O	2.07	0.54
1:C:344:VAL:HG23	1:C:370:VAL:HG11	1.90	0.54
1:D:187:LEU:HG	6:D:8112:HOH:O	2.07	0.54
1:D:414:ASP:HB3	6:D:7989:HOH:O	2.06	0.54
1:A:35:LEU:HD22	1:A:42:GLU:HA	1.88	0.54
1:A:430:GLY:HA3	6:A:5223:HOH:O	2.08	0.54
6:C:7031:HOH:O	1:D:558:TRP:HZ2	1.90	0.54
1:C:317:PRO:C	6:C:7417:HOH:O	2.51	0.54
1:D:130:LEU:C	1:D:130:LEU:HD23	2.31	0.54
1:D:517:ASN:HB2	1:D:539:ILE:HG22	1.90	0.54
1:A:33:ARG:HD3	6:A:5511:HOH:O	2.06	0.54
1:C:130:LEU:HD23	1:C:130:LEU:C	2.33	0.54
1:A:42:GLU:HG3	6:A:5511:HOH:O	2.06	0.54
1:D:144:ASN:HB3	1:D:187:LEU:CB	2.38	0.54
1:B:438:ASP:HB2	6:B:6184:HOH:O	2.08	0.54
1:D:109:ARG:C	6:D:8304:HOH:O	2.51	0.54
1:A:280:HIS:HB2	6:A:5450:HOH:O	2.07	0.54
1:B:47:PRO:HA	1:B:50:ASN:HD21	1.72	0.54
1:C:465:ARG:NE	6:C:7081:HOH:O	2.40	0.53
1:D:547:VAL:HG21	6:D:8251:HOH:O	2.08	0.53
1:B:9:ASP:OD1	1:B:427:VAL:CG1	2.56	0.53
1:C:287:LEU:HD21	6:D:8008:HOH:O	2.07	0.53
1:D:78:LEU:C	1:D:78:LEU:HD12	2.33	0.53
1:D:137:ARG:NH1	1:D:139:ASN:HD22	2.02	0.53
1:D:526:HIS:ND1	1:D:572:MET:HE1	2.22	0.53
1:C:364:ILE:HA	6:C:6950:HOH:O	2.08	0.53
1:A:127:ILE:HG23	6:A:5318:HOH:O	2.09	0.53
1:A:558:TRP:HZ2	6:B:6532:HOH:O	1.91	0.53
1:D:65:ARG:HH11	1:D:463:GLU:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:HIS:H	1:D:98:ASN:HD21	1.56	0.53
1:D:133:GLN:OE1	1:D:139:ASN:HB2	2.08	0.53
1:B:410:LYS:NZ	6:B:6426:HOH:O	2.41	0.53
1:C:125:LYS:HD2	6:D:8206:HOH:O	2.07	0.53
1:D:344:VAL:HG23	1:D:370:VAL:HG13	1.90	0.53
1:D:539:ILE:HB	6:D:8220:HOH:O	2.08	0.53
1:B:137:ARG:HH11	1:B:139:ASN:HD22	1.55	0.53
1:D:121:ILE:HD12	1:D:127:ILE:CD1	2.37	0.53
1:D:369:ASP:HB3	6:D:8244:HOH:O	2.08	0.53
1:C:331:ARG:HG3	1:C:389:ASN:OD1	2.09	0.53
1:C:371:HIS:CE1	6:C:7452:HOH:O	2.62	0.53
1:C:473:VAL:HG12	1:C:479:GLU:OE1	2.09	0.53
1:C:521:ILE:CG2	1:C:524:LEU:HB2	2.38	0.53
1:D:299:PHE:C	6:D:7928:HOH:O	2.51	0.53
1:D:329:ASP:OD2	1:D:333:ASN:HB2	2.08	0.53
1:C:75:ASN:HD21	1:C:102:ASN:HD21	1.56	0.53
1:D:109:ARG:O	6:D:8146:HOH:O	2.18	0.53
1:D:202:THR:HG22	1:D:223:ILE:HG22	1.91	0.53
1:A:481:ILE:HB	6:A:5225:HOH:O	2.08	0.53
1:D:291:VAL:CG2	1:D:319:LEU:HD12	2.39	0.53
1:D:521:ILE:N	1:D:521:ILE:HD12	2.24	0.53
1:C:562:GLN:H	1:C:562:GLN:HE21	1.54	0.52
1:D:456:ARG:HG2	6:D:8261:HOH:O	2.08	0.52
1:C:215:MET:HA	6:C:7143:HOH:O	2.10	0.52
1:D:272:CYS:HB3	6:D:7947:HOH:O	2.09	0.52
1:D:397:LYS:HE2	6:D:8306:HOH:O	2.08	0.52
1:B:288:SER:HB3	6:B:6340:HOH:O	2.08	0.52
1:B:381:MET:HE3	6:B:6223:HOH:O	2.10	0.52
1:B:572:MET:HE3	6:B:6478:HOH:O	2.09	0.52
1:C:290:THR:HG22	6:C:7417:HOH:O	2.09	0.52
1:C:372:TYR:HB2	1:C:398:PHE:O	2.09	0.52
1:D:71:MET:HG3	6:D:8272:HOH:O	2.10	0.52
1:B:562:GLN:H	1:B:562:GLN:HE21	1.55	0.52
1:C:373:GLN:HE21	1:C:398:PHE:HD2	1.58	0.52
1:D:288:SER:HB2	6:D:7951:HOH:O	2.09	0.52
1:D:395:LEU:HD12	1:D:395:LEU:N	2.25	0.52
1:C:190:CYS:N	6:C:7014:HOH:O	2.43	0.52
1:D:288:SER:CB	6:D:7951:HOH:O	2.57	0.52
6:C:7106:HOH:O	1:D:408:PRO:HD2	2.09	0.52
1:D:316:GLU:N	1:D:317:PRO:HD3	2.24	0.52
1:A:202:THR:HG21	1:A:269:PRO:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ASN:CB	6:D:7996:HOH:O	2.57	0.52
1:D:412:GLU:HG3	1:D:435:GLU:HA	1.92	0.52
1:C:75:ASN:ND2	1:C:102:ASN:HD21	2.08	0.51
1:C:269:PRO:HD3	6:C:7427:HOH:O	2.10	0.51
1:C:286:LYS:HB2	6:C:7430:HOH:O	2.10	0.51
1:C:468:ALA:O	1:C:473:VAL:HG22	2.10	0.51
1:D:212:LEU:HB3	1:D:213:PRO:HD3	1.92	0.51
1:B:267:ASN:CB	6:B:6340:HOH:O	2.57	0.51
1:D:368:LEU:HD23	1:D:417:ILE:HD13	1.93	0.51
1:D:573:ARG:NH2	6:D:8057:HOH:O	2.43	0.51
1:B:331:ARG:HD3	1:B:389:ASN:OD1	2.11	0.51
1:C:321:LEU:HD23	6:C:7383:HOH:O	2.10	0.51
1:C:550:VAL:HG23	1:C:550:VAL:O	2.09	0.51
1:D:116:ASP:N	6:D:7833:HOH:O	2.42	0.51
1:D:326:THR:HB	6:D:8182:HOH:O	2.10	0.51
1:D:506:LYS:HE2	6:D:8100:HOH:O	2.10	0.51
6:C:7112:HOH:O	1:D:30:GLY:HA3	2.10	0.51
1:D:103:THR:HA	6:D:8217:HOH:O	2.10	0.51
1:D:241:GLN:HB2	6:D:8033:HOH:O	2.10	0.51
1:C:159:GLU:HA	6:C:7192:HOH:O	2.11	0.51
1:C:182:LEU:HD13	1:C:250:VAL:HG11	1.93	0.51
1:D:204:TYR:HA	1:D:268:ASN:HA	1.93	0.51
1:D:334:ALA:HB1	6:D:8182:HOH:O	2.09	0.51
1:A:186:ASN:ND2	1:A:205:ASN:H	2.09	0.51
1:B:79:HIS:H	1:B:98:ASN:HD21	1.56	0.51
1:B:175:TRP:N	6:B:6506:HOH:O	2.44	0.51
1:C:319:LEU:HB2	6:C:7134:HOH:O	2.11	0.51
1:C:550:VAL:HG22	1:D:869:ASN:CG	2.35	0.51
1:C:562:GLN:HB3	6:C:7425:HOH:O	2.10	0.51
1:D:127:ILE:HA	1:D:144:ASN:O	2.10	0.51
1:D:439:ALA:HB1	6:D:8173:HOH:O	2.10	0.51
1:A:385:LEU:HB2	6:A:5385:HOH:O	2.11	0.51
1:B:280:HIS:HE1	6:B:5864:HOH:O	1.92	0.51
1:C:287:LEU:HG	6:C:7413:HOH:O	2.11	0.51
1:D:340:LEU:HD12	1:D:340:LEU:N	2.26	0.51
1:D:363:PRO:CB	6:D:8250:HOH:O	2.59	0.51
1:D:380:VAL:HA	1:D:441:ALA:HB3	1.93	0.51
1:D:557:TYR:CE2	6:D:7861:HOH:O	2.52	0.51
1:C:372:TYR:CB	1:C:398:PHE:HB2	2.41	0.50
1:B:198:TRP:CA	1:B:228:ILE:HD13	2.40	0.50
1:D:554:PRO:C	6:D:7861:HOH:O	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ASN:HA	6:C:7427:HOH:O	2.11	0.50
1:C:538:GLU:HG3	6:C:7330:HOH:O	2.10	0.50
1:A:165:ASN:CG	1:A:186:ASN:HA	2.36	0.50
1:C:198:TRP:NE1	6:C:7268:HOH:O	2.43	0.50
1:A:223:ILE:HG23	1:A:265:ILE:HG13	1.93	0.50
6:A:5452:HOH:O	1:B:571:GLU:HB3	2.12	0.50
1:A:79:HIS:H	1:A:98:ASN:HD21	1.60	0.50
1:A:124:ALA:HB2	1:A:166:VAL:HB	1.94	0.50
1:B:80:HIS:H	1:B:98:ASN:HD21	1.59	0.50
1:B:163:TYR:HD1	6:B:6532:HOH:O	1.94	0.50
1:C:264:PRO:O	6:C:7066:HOH:O	2.18	0.50
1:D:85:PHE:HE2	6:D:8042:HOH:O	1.94	0.50
1:C:468:ALA:HB1	1:C:473:VAL:CG2	2.42	0.50
1:D:144:ASN:HB3	1:D:187:LEU:HB3	1.94	0.50
1:D:130:LEU:HB3	6:D:8134:HOH:O	2.12	0.50
1:D:601:THR:OG1	1:D:479:GLU:HG2	2.12	0.50
1:C:510:GLU:CD	6:C:7391:HOH:O	2.55	0.50
1:C:571:GLU:OE1	1:C:571:GLU:N	2.44	0.50
1:D:132:PRO:HA	6:D:7998:HOH:O	2.12	0.50
1:A:126:GLY:HA2	6:A:5264:HOH:O	2.12	0.49
1:A:558:TRP:CD1	1:B:147:ASP:HB3	2.47	0.49
1:C:47:PRO:HA	1:C:50:ASN:HD21	1.77	0.49
1:D:83:MET:HB3	1:D:90:TYR:CD1	2.47	0.49
1:D:469:GLU:N	6:D:8191:HOH:O	2.45	0.49
1:C:204:TYR:HA	1:C:268:ASN:HA	1.94	0.49
1:D:258:LEU:HG	6:D:8311:HOH:O	2.11	0.49
1:D:572:MET:HE2	6:D:7895:HOH:O	2.12	0.49
1:A:412:GLU:HG3	1:A:435:GLU:HA	1.93	0.49
1:C:461:TRP:CD1	6:C:7081:HOH:O	2.64	0.49
1:A:376:HIS:HB2	1:A:437:HIS:O	2.13	0.49
1:A:75:ASN:O	6:A:5395:HOH:O	2.20	0.49
1:A:202:THR:HG22	1:A:203:SER:N	2.28	0.49
1:A:535:VAL:N	6:A:5306:HOH:O	2.46	0.49
1:D:424:MET:HG2	6:D:8187:HOH:O	2.11	0.49
1:A:212:LEU:HD11	1:B:568:LEU:HD13	1.95	0.49
1:B:212:LEU:HB3	1:B:213:PRO:HD3	1.94	0.49
1:D:123:ASN:HD22	1:D:180:GLN:HE22	1.60	0.49
1:D:371:HIS:C	1:D:372:TYR:CG	2.90	0.49
1:B:65:ARG:NH1	1:B:463:GLU:HG3	2.27	0.49
1:D:322:GLY:N	1:D:323:PRO:HD3	2.28	0.49
1:A:8:ALA:HB2	6:A:5611:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:TYR:CD1	1:A:372:TYR:N	2.80	0.48
1:B:130:LEU:C	1:B:130:LEU:HD23	2.38	0.48
1:C:48:VAL:H	1:C:50:ASN:ND2	2.11	0.48
1:D:538:GLU:HB2	1:D:563:TRP:CH2	2.48	0.48
1:B:29:SER:N	6:B:6545:HOH:O	2.45	0.48
1:C:164:VAL:HG12	6:C:7050:HOH:O	2.13	0.48
1:C:322:GLY:N	1:C:323:PRO:HD3	2.28	0.48
1:A:562:GLN:HG3	1:B:28:GLN:HB3	1.94	0.48
1:C:64:VAL:HG11	1:C:872:ARG:NH2	2.28	0.48
1:C:197:LYS:HG3	1:C:198:TRP:CD1	2.48	0.48
1:C:298:ARG:NH1	6:C:7444:HOH:O	2.47	0.48
1:C:461:TRP:HD1	6:C:7081:HOH:O	1.97	0.48
1:D:180:GLN:HB2	1:D:250:VAL:HG22	1.94	0.48
1:D:267:ASN:CB	6:D:7951:HOH:O	2.62	0.48
1:D:307:ALA:CB	6:D:8026:HOH:O	2.62	0.48
1:D:352:ALA:N	6:D:8250:HOH:O	2.46	0.48
1:A:38:PRO:HD3	6:A:5296:HOH:O	2.14	0.48
1:D:111:ASP:OD1	6:D:8304:HOH:O	2.19	0.48
1:A:8:ALA:N	1:A:427:VAL:HG11	2.29	0.48
1:D:59:GLN:CD	6:D:8251:HOH:O	2.56	0.48
1:D:370:VAL:HG11	1:D:394:CYS:SG	2.54	0.48
1:D:562:GLN:HE21	1:D:562:GLN:N	2.12	0.48
1:A:562:GLN:HE21	1:A:562:GLN:N	2.11	0.48
1:C:166:VAL:HG22	1:C:182:LEU:HD12	1.95	0.48
1:C:298:ARG:HB2	6:C:7097:HOH:O	2.12	0.48
1:C:556:VAL:HB	6:C:7165:HOH:O	2.13	0.48
1:D:60:THR:O	1:D:64:VAL:HG23	2.14	0.48
1:D:61:ASN:ND2	6:D:8096:HOH:O	2.43	0.48
1:A:202:THR:HB	6:A:5209:HOH:O	2.13	0.48
1:C:310:ARG:CG	6:C:7066:HOH:O	2.57	0.48
6:C:7122:HOH:O	1:D:523:ASP:HA	2.14	0.48
1:D:33:ARG:HG2	6:D:8205:HOH:O	2.13	0.48
1:D:137:ARG:HD3	1:D:139:ASN:HD21	1.78	0.48
1:A:209:GLY:O	1:A:210:MET:HE2	2.14	0.48
1:B:91:ASP:CG	1:B:93:ARG:HD3	2.39	0.48
1:D:184:SER:OG	1:D:255:LYS:HG3	2.13	0.48
1:A:60:THR:O	1:A:64:VAL:HG23	2.14	0.48
1:C:299:PHE:HA	6:C:7114:HOH:O	2.14	0.48
1:C:550:VAL:HG22	1:D:869:ASN:ND2	2.29	0.48
1:C:223:ILE:O	1:C:223:ILE:HG13	2.14	0.47
1:D:182:LEU:HD13	1:D:250:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ASN:HB3	6:D:7996:HOH:O	2.14	0.47
1:C:80:HIS:H	1:C:98:ASN:HD21	1.61	0.47
1:C:209:GLY:C	6:C:7335:HOH:O	2.57	0.47
1:D:529:THR:O	1:D:559:TYR:HA	2.13	0.47
1:D:543:MET:HE2	6:D:8078:HOH:O	2.14	0.47
1:B:542:GLN:O	6:B:6235:HOH:O	2.20	0.47
1:A:121:ILE:CD1	6:A:5276:HOH:O	2.62	0.47
1:A:203:SER:C	6:A:5609:HOH:O	2.56	0.47
1:A:280:HIS:HE1	6:A:5045:HOH:O	1.97	0.47
1:D:259:PHE:HD1	6:D:8093:HOH:O	1.97	0.47
1:D:264:PRO:O	1:D:265:ILE:HD13	2.14	0.47
1:A:147:ASP:HB3	1:B:558:TRP:CD1	2.49	0.47
1:C:268:ASN:O	1:C:286:LYS:HE2	2.15	0.47
1:D:80:HIS:H	1:D:98:ASN:HD21	1.62	0.47
1:D:106:ALA:CB	6:D:7943:HOH:O	2.56	0.47
1:A:322:GLY:N	1:A:323:PRO:HD3	2.30	0.47
6:A:5448:HOH:O	1:B:324:LEU:HD11	2.15	0.47
1:D:103:THR:CA	6:D:8217:HOH:O	2.63	0.47
1:D:104:ARG:HD3	6:D:7977:HOH:O	2.14	0.47
1:D:274:MET:HE1	6:D:7891:HOH:O	2.13	0.47
1:C:298:ARG:HD2	6:C:7097:HOH:O	2.13	0.47
1:C:563:TRP:O	1:C:564:PHE:C	2.56	0.47
1:A:47:PRO:HA	1:A:50:ASN:HD21	1.79	0.47
1:A:64:VAL:HG11	1:A:872:ARG:NH2	2.29	0.47
1:A:148:GLU:CD	1:A:148:GLU:H	2.23	0.47
1:B:186:ASN:ND2	1:B:205:ASN:H	2.13	0.47
1:B:325:HIS:CE1	1:B:376:HIS:CE1	3.03	0.47
1:C:299:PHE:HD2	6:C:7114:HOH:O	1.98	0.47
1:D:106:ALA:HB3	6:D:8157:HOH:O	2.15	0.47
1:D:204:TYR:HB2	1:D:268:ASN:HB3	1.97	0.47
1:D:322:GLY:CA	1:D:340:LEU:HD13	2.45	0.47
1:A:538:GLU:OE2	1:B:409:LEU:HG	2.15	0.46
1:B:482:ARG:HB3	6:B:6274:HOH:O	2.15	0.46
1:C:198:TRP:HA	6:C:7373:HOH:O	2.13	0.46
1:D:11:SER:HA	6:D:8245:HOH:O	2.15	0.46
1:D:73:HIS:CG	6:D:8087:HOH:O	2.67	0.46
1:D:384:THR:HA	6:D:8042:HOH:O	2.14	0.46
1:D:397:LYS:HG2	6:D:8306:HOH:O	2.15	0.46
1:A:135:TRP:HB2	6:A:5261:HOH:O	2.16	0.46
1:B:461:TRP:CZ2	6:B:6235:HOH:O	2.55	0.46
1:B:601:THR:HG23	1:B:479:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:GLN:HE21	1:C:562:GLN:N	2.12	0.46
1:D:378:LYS:HD3	6:D:8252:HOH:O	2.16	0.46
1:A:571:GLU:HG2	6:B:6186:HOH:O	2.15	0.46
1:D:291:VAL:HG23	1:D:319:LEU:HD12	1.98	0.46
1:D:370:VAL:HG21	1:D:374:PRO:HG3	1.97	0.46
1:A:449:ASP:OD1	1:A:449:ASP:O	2.34	0.46
1:A:532:ASN:ND2	1:B:125:LYS:HD2	2.31	0.46
1:C:344:VAL:HG23	1:C:370:VAL:CG1	2.46	0.46
1:A:202:THR:CG2	1:A:203:SER:N	2.79	0.46
1:C:35:LEU:HD22	1:C:42:GLU:HA	1.97	0.46
1:C:94:PHE:CD2	1:C:107:ARG:HD3	2.50	0.46
1:D:165:ASN:ND2	1:D:186:ASN:HA	2.30	0.46
1:D:542:GLN:HB3	6:D:8261:HOH:O	2.15	0.46
1:B:219:GLU:HG3	6:B:6441:HOH:O	2.15	0.46
1:C:502:SER:HA	1:C:575:ARG:O	2.15	0.46
1:D:77:ASP:CG	1:D:79:HIS:HE2	2.24	0.46
1:B:461:TRP:CZ3	1:B:543:MET:HG3	2.50	0.46
1:C:209:GLY:CA	6:C:7335:HOH:O	2.64	0.46
1:B:223:ILE:HG23	1:B:265:ILE:HG13	1.98	0.46
1:D:317:PRO:CG	1:D:352:ALA:HB1	2.46	0.46
1:C:163:TYR:HD1	6:C:7031:HOH:O	1.98	0.46
1:C:226:PHE:C	6:C:7399:HOH:O	2.59	0.46
1:D:326:THR:CG2	1:D:336:THR:HG22	2.14	0.46
1:D:331:ARG:HD2	6:D:8238:HOH:O	2.16	0.46
1:D:385:LEU:HA	6:D:8292:HOH:O	2.15	0.46
1:B:495:ALA:HA	1:B:496:PRO:HA	1.79	0.45
1:B:541:PRO:O	1:B:542:GLN:HB2	2.16	0.45
1:D:103:THR:HG23	1:D:127:ILE:HG13	1.98	0.45
1:D:231:ILE:HG13	6:D:8093:HOH:O	2.16	0.45
1:D:250:VAL:HB	6:D:8033:HOH:O	2.16	0.45
1:A:164:VAL:HG12	6:A:5077:HOH:O	2.15	0.45
1:C:416:LEU:O	1:C:427:VAL:HG22	2.16	0.45
1:A:246:VAL:HG22	1:A:249:LYS:N	2.30	0.45
1:A:490:TYR:HE1	6:A:5225:HOH:O	1.98	0.45
1:D:527:GLY:HA2	1:D:539:ILE:HD12	1.98	0.45
1:A:130:LEU:C	1:A:130:LEU:HD23	2.41	0.45
1:B:64:VAL:HG11	1:B:872:ARG:CZ	2.46	0.45
6:C:7395:HOH:O	1:D:17:LEU:CD2	2.65	0.45
1:D:35:LEU:HD13	1:D:42:GLU:CA	2.44	0.45
1:D:186:ASN:ND2	1:D:205:ASN:H	2.13	0.45
1:B:562:GLN:HE21	1:B:562:GLN:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ASN:CG	6:C:7335:HOH:O	2.58	0.45
1:B:563:TRP:O	1:B:564:PHE:C	2.60	0.45
1:C:473:VAL:HB	6:C:7303:HOH:O	2.15	0.45
1:D:49:PHE:CE2	1:D:99:ASP:HB2	2.51	0.45
1:D:272:CYS:N	6:D:7996:HOH:O	2.49	0.45
1:D:293:VAL:HB	1:D:315:ALA:HB3	1.98	0.45
1:D:394:CYS:HB3	6:D:8274:HOH:O	2.15	0.45
1:D:601:THR:HG1	1:D:479:GLU:HG2	1.81	0.45
1:B:288:SER:N	6:B:6340:HOH:O	2.49	0.45
1:D:135:TRP:HB2	6:D:8211:HOH:O	2.16	0.45
1:A:372:TYR:O	1:A:396:SER:HB3	2.15	0.45
1:B:437:HIS:CB	6:B:6184:HOH:O	2.63	0.45
1:C:186:ASN:ND2	1:C:205:ASN:H	2.15	0.45
1:B:127:ILE:HA	1:B:144:ASN:O	2.17	0.45
1:C:306:ASN:HB2	6:C:7431:HOH:O	2.16	0.45
1:D:209:GLY:O	1:D:210:MET:HE2	2.17	0.45
1:D:287:LEU:HD23	6:D:8168:HOH:O	2.16	0.45
1:D:338:LEU:HD11	1:D:345:VAL:HG21	1.99	0.45
1:C:65:ARG:NH1	1:C:463:GLU:HB2	2.31	0.45
1:D:223:ILE:O	1:D:223:ILE:HG13	2.16	0.45
1:A:435:GLU:OE2	1:B:564:PHE:HB2	2.16	0.44
1:A:869:ASN:HD21	1:B:550:VAL:N	1.98	0.44
1:B:182:LEU:HD13	1:B:250:VAL:CG1	2.48	0.44
1:B:331:ARG:HD3	1:B:389:ASN:CG	2.42	0.44
1:C:431:PRO:HA	6:C:7400:HOH:O	2.16	0.44
1:D:231:ILE:O	1:D:235:ILE:HG12	2.17	0.44
1:A:400:LYS:HG2	6:B:6378:HOH:O	2.16	0.44
1:A:543:MET:HG2	1:A:544:THR:N	2.32	0.44
1:B:49:PHE:CE2	1:B:99:ASP:HB2	2.53	0.44
1:B:126:GLY:HA2	6:B:6442:HOH:O	2.16	0.44
1:C:494:VAL:O	1:C:495:ALA:C	2.60	0.44
1:D:276:PRO:HA	6:D:8292:HOH:O	2.17	0.44
1:D:351:ASP:HB2	6:D:7994:HOH:O	2.17	0.44
1:A:350:GLU:HG2	6:A:5155:HOH:O	2.17	0.44
1:A:568:LEU:HD13	1:B:212:LEU:HD11	2.00	0.44
1:B:278:LYS:HE2	6:B:6472:HOH:O	2.17	0.44
1:C:574:GLY:HA2	6:D:8248:HOH:O	2.18	0.44
1:A:345:VAL:HG22	1:A:367:LYS:HG2	2.00	0.44
1:C:380:VAL:HB	1:C:388:THR:OG1	2.17	0.44
1:D:129:GLY:HA3	1:D:189:ASN:HA	2.00	0.44
1:D:363:PRO:HA	6:D:7994:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:525:THR:HA	6:D:8240:HOH:O	2.17	0.44
1:B:98:ASN:H	1:B:98:ASN:HD22	1.63	0.44
1:B:204:TYR:HA	1:B:268:ASN:HA	2.00	0.44
1:C:534:GLY:HA2	1:D:75:ASN:ND2	2.32	0.44
1:D:417:ILE:HD11	6:D:8274:HOH:O	2.17	0.44
1:A:451:LYS:HE2	6:A:5629:HOH:O	2.18	0.44
1:A:532:ASN:ND2	1:B:125:LYS:CD	2.80	0.44
1:C:268:ASN:N	1:C:269:PRO:CD	2.80	0.44
1:B:198:TRP:HA	1:B:228:ILE:CD1	2.45	0.44
1:A:395:LEU:HD12	1:A:395:LEU:N	2.32	0.43
1:D:529:THR:HA	6:D:8198:HOH:O	2.16	0.43
1:C:322:GLY:C	6:C:7309:HOH:O	2.61	0.43
1:C:411:PRO:HB2	6:C:7400:HOH:O	2.17	0.43
1:D:118:ILE:HD12	6:D:8150:HOH:O	2.17	0.43
1:D:221:ASP:O	1:D:222:HIS:HB3	2.17	0.43
1:D:508:GLY:C	6:D:8167:HOH:O	2.61	0.43
1:A:227:ASN:HB2	1:A:303:PHE:CE2	2.53	0.43
1:B:93:ARG:HD2	6:B:6316:HOH:O	2.18	0.43
1:B:293:VAL:HB	1:B:315:ALA:HB3	2.00	0.43
1:C:369:ASP:CB	6:C:7452:HOH:O	2.55	0.43
1:C:372:TYR:CD1	1:C:372:TYR:N	2.82	0.43
1:D:281:LEU:N	6:D:7891:HOH:O	2.51	0.43
1:A:215:MET:HA	6:A:5455:HOH:O	2.17	0.43
1:B:165:ASN:CG	1:B:186:ASN:HA	2.43	0.43
1:C:372:TYR:O	1:C:396:SER:HB3	2.18	0.43
1:D:144:ASN:HB3	1:D:187:LEU:HB2	1.99	0.43
1:A:397:LYS:HE3	1:B:564:PHE:CD2	2.54	0.43
1:A:553:ASN:N	6:A:5417:HOH:O	2.51	0.43
1:A:69:ARG:NE	6:A:5290:HOH:O	2.52	0.43
1:A:177:VAL:CG1	1:A:246:VAL:HG21	2.42	0.43
1:A:293:VAL:HB	1:A:315:ALA:HB3	2.01	0.43
1:C:267:ASN:N	6:C:7427:HOH:O	2.51	0.43
1:D:49:PHE:CZ	1:D:99:ASP:HB2	2.54	0.43
1:D:186:ASN:ND2	1:D:186:ASN:C	2.76	0.43
1:D:436:PRO:HB3	6:D:8060:HOH:O	2.18	0.43
1:C:212:LEU:N	1:C:213:PRO:HD2	2.33	0.43
1:C:317:PRO:HD2	6:C:7086:HOH:O	2.17	0.43
1:A:28:GLN:HB3	1:B:562:GLN:HG3	2.00	0.43
1:B:506:LYS:HD2	6:B:6085:HOH:O	2.17	0.43
1:C:397:LYS:HD3	6:C:7350:HOH:O	2.18	0.43
1:B:118:ILE:HD11	6:B:6156:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:GLU:HA	1:B:580:PRO:HD3	1.93	0.43
1:D:498:PHE:HD2	6:D:7982:HOH:O	2.02	0.43
1:D:530:MET:HG3	6:D:8310:HOH:O	2.19	0.43
1:A:123:ASN:HD22	1:A:180:GLN:NE2	2.09	0.43
1:A:520:GLU:HG2	1:A:542:GLN:CD	2.44	0.43
1:C:123:ASN:HD22	1:C:180:GLN:NE2	2.04	0.43
1:D:390:ASP:OD1	1:D:391:TRP:N	2.49	0.43
1:D:424:MET:CG	6:D:8187:HOH:O	2.67	0.43
1:A:34:ILE:C	1:A:35:LEU:HD23	2.44	0.42
1:B:10:GLY:HA3	1:B:38:PRO:HB2	2.01	0.42
1:B:220:MET:HE2	1:B:264:PRO:C	2.43	0.42
1:C:395:LEU:HD12	1:C:395:LEU:N	2.34	0.42
1:C:549:PHE:HB3	6:C:7415:HOH:O	2.19	0.42
1:D:494:VAL:O	1:D:495:ALA:C	2.61	0.42
1:C:397:LYS:HE3	1:D:564:PHE:CD2	2.53	0.42
1:C:416:LEU:HB3	1:C:428:HIS:HB2	2.01	0.42
1:D:38:PRO:HB2	1:D:416:LEU:HD21	2.01	0.42
1:D:258:LEU:N	1:D:258:LEU:HD12	2.33	0.42
1:A:75:ASN:ND2	1:A:102:ASN:HD21	2.17	0.42
1:A:121:ILE:HD11	6:A:5276:HOH:O	2.18	0.42
1:A:277:ASP:OD2	1:A:280:HIS:HD2	2.03	0.42
1:C:225:VAL:HG13	6:C:7338:HOH:O	2.18	0.42
1:D:73:HIS:CD2	6:D:8087:HOH:O	2.72	0.42
1:B:601:THR:HG22	1:B:478:GLU:N	2.35	0.42
1:C:295:ASP:CG	6:C:7353:HOH:O	2.62	0.42
1:D:267:ASN:HB2	6:D:7951:HOH:O	2.18	0.42
1:A:371:HIS:C	1:A:372:TYR:CG	2.97	0.42
1:A:529:THR:O	1:A:559:TYR:HA	2.19	0.42
1:C:182:LEU:HD13	1:C:250:VAL:CG1	2.49	0.42
1:C:325:HIS:CE1	1:C:376:HIS:CE1	3.07	0.42
1:D:280:HIS:HE1	6:D:8021:HOH:O	2.02	0.42
1:D:543:MET:HG2	1:D:544:THR:N	2.33	0.42
1:A:243:LEU:O	1:A:246:VAL:HG12	2.19	0.42
1:A:344:VAL:HG23	1:A:370:VAL:HG11	2.00	0.42
1:B:64:VAL:HG11	1:B:872:ARG:NH2	2.35	0.42
1:C:193:ASP:OD2	1:C:197:LYS:HG2	2.20	0.42
1:D:226:PHE:C	6:D:8065:HOH:O	2.62	0.42
1:A:75:ASN:HD21	1:A:102:ASN:HD21	1.68	0.42
1:A:119:LEU:O	6:A:5276:HOH:O	2.22	0.42
1:A:223:ILE:O	1:A:223:ILE:HG13	2.20	0.42
1:A:448:SER:CB	6:A:5439:HOH:O	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASN:HD22	1:C:98:ASN:H	1.67	0.42
1:C:528:PHE:N	1:C:562:GLN:HE22	2.17	0.42
1:D:118:ILE:HG12	6:D:7943:HOH:O	2.18	0.42
1:D:288:SER:N	6:D:7951:HOH:O	2.52	0.42
1:D:479:GLU:HG2	1:D:479:GLU:H	1.62	0.42
1:D:541:PRO:O	1:D:542:GLN:HB2	2.19	0.42
1:B:395:LEU:N	1:B:395:LEU:HD12	2.35	0.42
1:C:34:ILE:C	1:C:35:LEU:HD23	2.44	0.42
1:D:110:CYS:O	1:D:113:MET:HE2	2.20	0.42
1:D:188:ASP:N	6:D:8189:HOH:O	2.51	0.42
1:D:469:GLU:CA	6:D:8191:HOH:O	2.67	0.42
1:A:526:HIS:CD2	6:A:5239:HOH:O	2.71	0.42
1:B:539:ILE:HG13	1:B:545:SER:OG	2.20	0.42
1:C:263:ILE:CG2	6:C:7066:HOH:O	2.58	0.42
1:D:108:VAL:HA	6:D:7833:HOH:O	2.20	0.42
1:D:538:GLU:HG2	1:D:539:ILE:N	2.34	0.42
1:B:198:TRP:C	6:B:6515:HOH:O	2.63	0.42
1:B:372:TYR:CD1	1:B:372:TYR:N	2.84	0.42
1:C:147:ASP:HB3	1:D:558:TRP:CD1	2.55	0.42
1:C:543:MET:HG2	1:C:544:THR:N	2.33	0.42
1:D:45:ARG:HG2	6:D:8205:HOH:O	2.20	0.42
1:A:67:HIS:C	6:A:5517:HOH:O	2.62	0.41
1:B:448:SER:CB	6:B:6256:HOH:O	2.68	0.41
1:B:456:ARG:HD2	6:B:6235:HOH:O	2.20	0.41
1:C:165:ASN:CG	1:C:186:ASN:HA	2.45	0.41
1:B:50:ASN:HD22	1:B:50:ASN:N	2.05	0.41
1:C:209:GLY:O	1:C:210:MET:HE2	2.19	0.41
6:C:7157:HOH:O	1:D:573:ARG:HD3	2.19	0.41
1:D:423:LYS:HE3	6:D:8216:HOH:O	2.19	0.41
1:C:223:ILE:HG21	1:C:283:VAL:HG21	2.01	0.41
1:D:339:PHE:CE1	1:D:373:GLN:HB3	2.55	0.41
1:A:65:ARG:NH1	1:A:463:GLU:HG3	2.34	0.41
1:A:75:ASN:ND2	1:B:534:GLY:HA2	2.33	0.41
1:A:143:CYS:N	6:A:5258:HOH:O	2.52	0.41
1:A:564:PHE:CD2	1:B:397:LYS:HE3	2.55	0.41
1:D:66:ILE:HD11	1:D:460:MET:HE1	2.02	0.41
1:A:204:TYR:HA	1:A:268:ASN:HA	2.03	0.41
1:B:65:ARG:HH12	1:B:463:GLU:H	1.67	0.41
1:B:228:ILE:CD1	1:B:228:ILE:H	2.33	0.41
1:C:180:GLN:HB2	1:C:250:VAL:HG22	2.01	0.41
1:C:569:HIS:HB3	6:C:7456:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:7377:HOH:O	1:D:553:ASN:CG	2.63	0.41
1:D:517:ASN:HB3	1:D:540:GLY:O	2.21	0.41
1:A:532:ASN:HD21	1:B:125:LYS:CD	2.32	0.41
1:B:494:VAL:O	1:B:495:ALA:C	2.63	0.41
1:B:48:VAL:H	1:B:50:ASN:ND2	2.18	0.41
1:B:601:THR:CG2	1:B:479:GLU:H	2.33	0.41
1:C:264:PRO:HB3	6:C:7152:HOH:O	2.20	0.41
1:C:371:HIS:C	1:C:372:TYR:CG	2.99	0.41
6:C:7371:HOH:O	1:D:103:THR:HB	2.20	0.41
1:D:860:GLU:CG	1:D:864:LYS:HE2	2.33	0.41
1:D:475:ILE:HG12	6:D:7920:HOH:O	2.21	0.41
1:A:264:PRO:O	1:A:265:ILE:HD13	2.21	0.41
1:B:148:GLU:H	1:B:148:GLU:CD	2.28	0.41
1:D:78:LEU:HD12	1:D:79:HIS:N	2.36	0.41
1:D:211:THR:O	1:D:215:MET:HG3	2.21	0.41
1:D:562:GLN:H	1:D:562:GLN:NE2	2.15	0.41
1:A:48:VAL:H	1:A:50:ASN:ND2	2.19	0.41
1:A:202:THR:CG2	1:A:269:PRO:HG2	2.47	0.41
1:A:220:MET:HE3	1:A:264:PRO:CB	2.51	0.41
1:A:494:VAL:O	1:A:495:ALA:C	2.64	0.41
1:A:562:GLN:H	1:A:562:GLN:NE2	2.19	0.41
1:B:49:PHE:CZ	1:B:99:ASP:HB2	2.56	0.41
1:B:228:ILE:N	1:B:228:ILE:CD1	2.83	0.41
1:B:228:ILE:HD12	1:B:228:ILE:H	1.84	0.41
1:B:438:ASP:N	6:B:6184:HOH:O	2.53	0.41
1:C:155:GLY:O	1:D:580:PRO:HD3	2.21	0.41
1:C:411:PRO:HB3	1:D:43:LEU:O	2.21	0.41
1:C:443:HIS:HA	1:C:444:PRO:HD3	1.94	0.41
1:C:521:ILE:CG2	1:C:524:LEU:CB	2.98	0.41
6:C:7395:HOH:O	1:D:17:LEU:HD22	2.20	0.41
1:D:134:LYS:HD3	6:D:8042:HOH:O	2.21	0.41
1:D:414:ASP:N	6:D:7979:HOH:O	2.53	0.41
1:A:506:LYS:HD2	6:A:5527:HOH:O	2.20	0.41
1:B:103:THR:HA	6:B:6442:HOH:O	2.20	0.41
1:C:514:ILE:N	1:C:514:ILE:HD12	2.36	0.41
1:D:83:MET:SD	1:D:92:GLY:HA2	2.60	0.41
1:A:49:PHE:CE2	1:A:99:ASP:HB2	2.56	0.40
1:A:329:ASP:OD2	1:A:333:ASN:HB2	2.21	0.40
1:B:194:TYR:O	6:B:6421:HOH:O	2.22	0.40
1:C:59:GLN:NE2	1:C:534:GLY:O	2.52	0.40
1:C:221:ASP:HB3	6:C:7337:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:PRO:N	6:C:7066:HOH:O	2.53	0.40
1:D:230:GLU:HA	1:D:233:LYS:HG2	2.03	0.40
1:D:371:HIS:CE1	6:D:8244:HOH:O	2.74	0.40
1:A:98:ASN:ND2	6:A:5480:HOH:O	2.53	0.40
1:B:228:ILE:HG23	6:B:6381:HOH:O	2.21	0.40
1:C:50:ASN:HD22	1:C:50:ASN:N	2.10	0.40
1:C:364:ILE:HG23	6:C:6950:HOH:O	2.20	0.40
1:D:107:ARG:HD2	6:D:8236:HOH:O	2.21	0.40
1:D:440:ILE:N	6:D:8173:HOH:O	2.52	0.40
1:A:186:ASN:HD21	1:A:204:TYR:H	1.68	0.40
1:A:371:HIS:HD2	1:A:415:GLN:OE1	2.03	0.40
1:B:65:ARG:HH11	1:B:463:GLU:HG3	1.87	0.40
1:B:323:PRO:HA	1:B:337:SER:O	2.22	0.40
1:D:343:GLN:HA	1:D:370:VAL:HG22	2.03	0.40
1:C:447:LEU:O	1:C:448:SER:C	2.63	0.40
1:C:538:GLU:HA	6:C:7330:HOH:O	2.21	0.40
1:D:185:GLY:HA3	1:D:206:SER:HA	2.04	0.40
1:D:307:ALA:C	6:D:8026:HOH:O	2.64	0.40
1:D:377:LEU:HA	1:D:393:VAL:O	2.21	0.40
1:D:410:LYS:HB3	6:D:7898:HOH:O	2.21	0.40
1:A:40:MET:HB3	6:A:5223:HOH:O	2.22	0.40
1:A:64:VAL:HG11	1:A:872:ARG:CZ	2.51	0.40
1:C:529:THR:HB	6:C:7425:HOH:O	2.22	0.40
1:D:103:THR:N	6:D:8217:HOH:O	2.50	0.40
1:D:150:PRO:HD3	1:D:163:TYR:CE2	2.57	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	589/595 (99%)	557 (95%)	29 (5%)	3 (0%)	24 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	587/595 (99%)	561 (96%)	23 (4%)	3 (0%)	24	10
1	C	588/595 (99%)	553 (94%)	31 (5%)	4 (1%)	18	6
1	D	586/595 (98%)	545 (93%)	35 (6%)	6 (1%)	12	3
All	All	2350/2380 (99%)	2216 (94%)	118 (5%)	16 (1%)	18	6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	B	434	ALA
1	D	267	ASN
1	A	434	ALA
1	B	267	ASN
1	B	286	LYS
1	C	286	LYS
1	C	434	ALA
1	D	286	LYS
1	A	286	LYS
1	C	372	TYR
1	D	189	ASN
1	D	372	TYR
1	D	434	ALA
1	C	400	LYS
1	D	184	SER

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	501/503 (100%)	492 (98%)	9 (2%)	51	28
1	B	500/503 (99%)	487 (97%)	13 (3%)	40	17
1	C	501/503 (100%)	486 (97%)	15 (3%)	36	13
1	D	499/503 (99%)	483 (97%)	16 (3%)	34	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2001/2012 (100%)	1948 (97%)	53 (3%)	40 17

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	50	ASN
1	A	75	ASN
1	A	151	LEU
1	A	186	ASN
1	A	200	PHE
1	A	496	PRO
1	A	562	GLN
1	A	563	TRP
1	B	35	LEU
1	B	38	PRO
1	B	50	ASN
1	B	75	ASN
1	B	151	LEU
1	B	182	LEU
1	B	186	ASN
1	B	200	PHE
1	B	361	VAL
1	B	409	LEU
1	B	496	PRO
1	B	562	GLN
1	B	563	TRP
1	C	28	GLN
1	C	50	ASN
1	C	863	LYS
1	C	75	ASN
1	C	78	LEU
1	C	148	GLU
1	C	182	LEU
1	C	186	ASN
1	C	200	PHE
1	C	224	VAL
1	C	409	LEU
1	C	496	PRO
1	C	562	GLN
1	C	563	TRP
1	C	571	GLU

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Mol	Chain	Res	Type
1	D	28	GLN
1	D	50	ASN
1	D	75	ASN
1	D	78	LEU
1	D	98	ASN
1	D	148	GLU
1	D	151	LEU
1	D	174	LYS
1	D	186	ASN
1	D	200	PHE
1	D	267	ASN
1	D	373	GLN
1	D	402	ARG
1	D	479	GLU
1	D	562	GLN
1	D	563	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	61	ASN
1	A	869	ASN
1	A	75	ASN
1	A	98	ASN
1	A	139	ASN
1	A	144	ASN
1	A	165	ASN
1	A	180	GLN
1	A	186	ASN
1	A	189	ASN
1	A	244	ASN
1	A	280	HIS
1	A	371	HIS
1	A	373	GLN
1	A	415	GLN
1	A	485	ASN
1	A	542	GLN
1	A	562	GLN
1	B	50	ASN
1	B	61	ASN
1	B	869	ASN

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Mol	Chain	Res	Type
1	B	75	ASN
1	B	98	ASN
1	B	139	ASN
1	B	144	ASN
1	B	840	ASN
1	B	165	ASN
1	B	180	GLN
1	B	186	ASN
1	B	241	GLN
1	B	244	ASN
1	B	280	HIS
1	B	306	ASN
1	B	371	HIS
1	B	415	GLN
1	B	428	HIS
1	B	485	ASN
1	B	562	GLN
1	C	28	GLN
1	C	50	ASN
1	C	61	ASN
1	C	869	ASN
1	C	75	ASN
1	C	98	ASN
1	C	123	ASN
1	C	139	ASN
1	C	165	ASN
1	C	180	GLN
1	C	186	ASN
1	C	189	ASN
1	C	244	ASN
1	C	280	HIS
1	C	371	HIS
1	C	373	GLN
1	C	415	GLN
1	C	477	ASN
1	C	562	GLN
1	D	28	GLN
1	D	50	ASN
1	D	61	ASN
1	D	869	ASN
1	D	75	ASN
1	D	98	ASN

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Mol	Chain	Res	Type
1	D	139	ASN
1	D	144	ASN
1	D	840	ASN
1	D	165	ASN
1	D	180	GLN
1	D	186	ASN
1	D	189	ASN
1	D	267	ASN
1	D	280	HIS
1	D	371	HIS
1	D	373	GLN
1	D	415	GLN
1	D	428	HIS
1	D	562	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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	CUA	B	4701	1	0,1,1	-	-	-		
5	CUZ	A	4801	1	0,9,9	-	-	-		
4	CUA	C	4701	1	0,1,1	-	-	-		
5	CUZ	B	5801	1	0,9,9	-	-	-		
4	CUA	D	4701	1	0,1,1	-	-	-		
4	CUA	A	4701	1	0,1,1	-	-	-		
5	CUZ	D	7801	1	0,9,9	-	-	-		
5	CUZ	C	6801	1	0,9,9	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	591/595 (99%)	0.98	83 (14%) 6 6	10, 18, 28, 39	0
1	B	589/595 (98%)	0.58	56 (9%) 14 14	10, 16, 25, 32	0
1	C	590/595 (99%)	1.37	134 (22%) 2 2	15, 23, 31, 42	0
1	D	588/595 (98%)	2.28	325 (55%) 0 0	17, 28, 38, 46	156 (26%)
All	All	2358/2380 (99%)	1.30	598 (25%) 1 1	10, 21, 33, 46	156 (6%)

All (598) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	ALA	7.4
1	C	357	ALA	6.8
1	D	449	ASP	6.5
1	B	434	ALA	6.4
1	A	434	ALA	6.2
1	D	301	ALA	6.1
1	D	266	ALA	6.0
1	D	357	ALA	6.0
1	D	850	ASP	5.9
1	D	372	TYR	5.9
1	A	267	ASN	5.8
1	D	450	ILE	5.5
1	D	185	GLY	5.4
1	D	162	ALA	5.4
1	D	330	GLY	5.4
1	B	266	ALA	5.4
1	D	299	PHE	5.4
1	D	364	ILE	5.3
1	D	262	TYR	5.3
1	D	302	VAL	5.3
1	D	259	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	213	PRO	5.2
1	A	9	ASP	5.1
1	D	152	VAL	5.1
1	C	361	VAL	5.0
1	D	238	GLY	5.0
1	D	156	THR	4.9
1	D	239	ASP	4.9
1	D	353	ILE	4.9
1	D	235	ILE	4.8
1	D	297	THR	4.8
1	B	9	ASP	4.7
1	D	233	LYS	4.7
1	D	189	ASN	4.7
1	D	300	ASP	4.7
1	A	352	ALA	4.7
1	D	361	VAL	4.7
1	D	282	CYS	4.7
1	C	266	ALA	4.7
1	A	353	ILE	4.6
1	D	178	ALA	4.6
1	A	8	ALA	4.5
1	D	350	GLU	4.5
1	B	372	TYR	4.5
1	C	269	PRO	4.5
1	D	135	TRP	4.5
1	D	258	LEU	4.5
1	D	218	ALA	4.5
1	D	446	ILE	4.5
1	D	275	ALA	4.5
1	B	10	GLY	4.4
1	A	355	ALA	4.4
1	D	315	ALA	4.4
1	D	159	GLU	4.4
1	D	309	PRO	4.4
1	D	387	ALA	4.4
1	C	434	ALA	4.4
1	D	271	GLY	4.4
1	D	349	ILE	4.4
1	A	354	ARG	4.3
1	D	229	ALA	4.3
1	D	334	ALA	4.3
1	C	9	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	356	TYR	4.2
1	A	64	VAL	4.2
1	D	296	VAL	4.2
1	A	360	LYS	4.1
1	D	303	PHE	4.1
1	C	370	VAL	4.1
1	D	314	VAL	4.1
1	C	352	ALA	4.1
1	D	236	ALA	4.1
1	D	447(D)	LEU	4.1
1	D	291	VAL	4.1
1	D	354	ARG	4.1
1	D	234	ALA	4.1
1	D	85	PHE	4.1
1	D	370	VAL	4.1
1	D	434	ALA	4.0
1	D	198	TRP	4.0
1	C	267	ASN	4.0
1	D	199	ALA	4.0
1	D	327	ALA	4.0
1	D	161	VAL	4.0
1	D	264	PRO	4.0
1	D	277	ASP	4.0
1	A	448	SER	4.0
1	D	223	ILE	3.9
1	D	840	ASN	3.9
1	D	371	HIS	3.9
1	D	306	ASN	3.9
1	D	172	ALA	3.9
1	D	184	SER	3.9
1	D	201	SER	3.9
1	C	301	ALA	3.9
1	D	289	PRO	3.9
1	C	448	SER	3.8
1	D	151	LEU	3.8
1	D	237	ALA	3.8
1	D	304	TYR	3.8
1	D	142	PHE	3.8
1	D	175	TRP	3.8
1	D	155	GLY	3.8
1	C	495	ALA	3.8
1	B	267	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	313	VAL	3.8
1	C	581	LYS	3.8
1	D	864	LYS	3.8
1	D	78	LEU	3.8
1	D	182	LEU	3.8
1	A	357	ALA	3.8
1	C	223	ILE	3.7
1	C	364	ILE	3.7
1	A	447	LEU	3.7
1	D	317	PRO	3.7
1	A	219	GLU	3.7
1	C	358	GLY	3.7
1	D	231	ILE	3.7
1	D	225	VAL	3.7
1	D	448	SER	3.7
1	A	217	ALA	3.7
1	D	352	ALA	3.7
1	C	360	LYS	3.7
1	D	212	LEU	3.7
1	D	355	ALA	3.7
1	D	163	TYR	3.7
1	D	356	TYR	3.7
1	C	355	ALA	3.6
1	D	187	LEU	3.6
1	D	205	ASN	3.6
1	D	865	PHE	3.6
1	D	136	PRO	3.6
1	D	453	VAL	3.6
1	D	130	LEU	3.6
1	D	267	ASN	3.6
1	A	371	HIS	3.6
1	C	428	HIS	3.6
1	A	364	ILE	3.6
1	D	157	ASN	3.5
1	D	265	ILE	3.5
1	D	466	ALA	3.5
1	C	372	TYR	3.5
1	D	268	ASN	3.5
1	B	552	ALA	3.5
1	D	91	ASP	3.5
1	B	16	GLN	3.5
1	D	240	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	188	ASP	3.5
1	A	581	LYS	3.5
1	C	447	LEU	3.5
1	A	370	VAL	3.5
1	C	306	ASN	3.5
1	D	141	VAL	3.5
1	D	250	VAL	3.5
1	D	288	SER	3.5
1	D	190	CYS	3.5
1	D	140	TYR	3.5
1	C	265	ILE	3.4
1	C	64	VAL	3.4
1	D	290	THR	3.4
1	D	150	PRO	3.4
1	D	117	ALA	3.4
1	A	258	LEU	3.4
1	D	251	VAL	3.4
1	D	149	THR	3.4
1	D	347	TRP	3.4
1	A	356	TYR	3.4
1	A	372	TYR	3.4
1	C	552	ALA	3.4
1	D	435	GLU	3.4
1	D	260	THR	3.4
1	D	179	TRP	3.4
1	B	236	ALA	3.3
1	D	219	GLU	3.3
1	D	153	ASN	3.3
1	D	227	ASN	3.3
1	D	244	ASN	3.3
1	D	254	ARG	3.3
1	C	313	VAL	3.3
1	C	561	CYS	3.3
1	D	202	THR	3.3
1	D	336	THR	3.3
1	C	78	LEU	3.3
1	C	350	GLU	3.3
1	D	344	VAL	3.3
1	B	360	LYS	3.3
1	A	313	VAL	3.3
1	B	228	ILE	3.2
1	D	440	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	437	HIS	3.2
1	C	473	VAL	3.2
1	D	257	SER	3.2
1	D	160	ASP	3.2
1	C	558	TRP	3.2
1	D	391	TRP	3.2
1	C	151	LEU	3.2
1	C	258	LEU	3.2
1	D	358	GLY	3.2
1	D	138	SER	3.2
1	A	361	VAL	3.2
1	D	457	ASN	3.2
1	D	17	LEU	3.2
1	D	868	ALA	3.2
1	D	468	ALA	3.2
1	D	181	VAL	3.2
1	B	159	GLU	3.2
1	C	297	THR	3.2
1	C	457	ASN	3.1
1	C	276	PRO	3.1
1	D	279	LYS	3.1
1	D	292	THR	3.1
1	A	345	VAL	3.1
1	B	485	ASN	3.1
1	D	241	GLN	3.1
1	C	300	ASP	3.1
1	A	450	ILE	3.1
1	D	281	LEU	3.1
1	D	164	VAL	3.1
1	D	170	VAL	3.1
1	D	133	GLN	3.1
1	D	228	ILE	3.1
1	A	218	ALA	3.1
1	B	162	ALA	3.1
1	D	811	SER	3.1
1	B	239	ASP	3.1
1	C	135	TRP	3.0
1	C	437	HIS	3.0
1	D	108	VAL	3.0
1	D	270	HIS	3.0
1	D	442	VAL	3.0
1	D	382	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	204	TYR	3.0
1	D	331	ARG	3.0
1	D	273	ASN	3.0
1	A	331	ARG	3.0
1	D	64	VAL	3.0
1	D	293	VAL	3.0
1	A	348	ASN	3.0
1	C	371	HIS	3.0
1	A	358	GLY	3.0
1	D	129	GLY	3.0
1	A	246	VAL	3.0
1	D	335	TYR	3.0
1	B	300	ASP	3.0
1	D	394	CYS	3.0
1	A	291	VAL	2.9
1	D	246	VAL	2.9
1	B	237	ALA	2.9
1	D	307	ALA	2.9
1	D	324	LEU	2.9
1	B	521	ILE	2.9
1	C	521	ILE	2.9
1	D	209	GLY	2.9
1	D	245	GLY	2.9
1	D	285	GLY	2.9
1	D	147	ASP	2.9
1	B	448	SER	2.9
1	D	217	ALA	2.9
1	B	306	ASN	2.9
1	D	139	ASN	2.9
1	C	426	LEU	2.9
1	D	243	LEU	2.9
1	D	377	LEU	2.9
1	D	253	GLY	2.9
1	D	444	PRO	2.9
1	B	241	GLN	2.9
1	A	497	SER	2.9
1	D	249	LYS	2.9
1	D	168	THR	2.9
1	C	550	VAL	2.9
1	A	347	TRP	2.9
1	C	162	ALA	2.8
1	D	345	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	449	ASP	2.8
1	C	213	PRO	2.8
1	A	223	ILE	2.8
1	D	388	THR	2.8
1	B	860	GLU	2.8
1	C	850	ASP	2.8
1	D	362	ASP	2.8
1	A	162	ALA	2.8
1	D	106	ALA	2.8
1	D	124	ALA	2.8
1	B	304	TYR	2.8
1	C	309	PRO	2.8
1	D	359	GLU	2.8
1	D	71	MET	2.8
1	D	167	PHE	2.8
1	A	224	VAL	2.8
1	B	64	VAL	2.8
1	C	436	PRO	2.8
1	D	148	GLU	2.8
1	D	194	TYR	2.8
1	B	151	LEU	2.8
1	D	232	GLU	2.8
1	D	143	CYS	2.8
1	D	118	ILE	2.8
1	D	220	MET	2.8
1	D	451	LYS	2.8
1	A	351	ASP	2.8
1	D	193	ASP	2.8
1	B	357	ALA	2.7
1	D	169	ALA	2.7
1	D	441	ALA	2.7
1	C	403	PHE	2.7
1	D	226	PHE	2.7
1	D	339	PHE	2.7
1	C	291	VAL	2.7
1	D	392	LEU	2.7
1	D	34	ILE	2.7
1	C	840	ASN	2.7
1	A	164	VAL	2.7
1	D	224	VAL	2.7
1	D	473	VAL	2.7
1	B	243	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	21	TYR	2.7
1	D	287	LEU	2.7
1	C	11	SER	2.7
1	D	86	THR	2.7
1	D	521	ILE	2.7
1	C	312	ALA	2.7
1	D	280	HIS	2.7
1	C	344	VAL	2.7
1	C	345	VAL	2.7
1	D	183	VAL	2.7
1	D	379	THR	2.7
1	D	385	LEU	2.7
1	D	332	GLY	2.7
1	D	263	ILE	2.7
1	D	366	ASP	2.7
1	D	369	ASP	2.7
1	A	292	THR	2.6
1	D	375	GLY	2.6
1	D	321	LEU	2.6
1	D	338	LEU	2.6
1	D	577	LEU	2.6
1	A	344	VAL	2.6
1	B	12	VAL	2.6
1	C	314	VAL	2.6
1	D	105	VAL	2.6
1	C	568	LEU	2.6
1	D	95	LEU	2.6
1	D	455	ASP	2.6
1	A	442	VAL	2.6
1	C	241	GLN	2.6
1	C	481	ILE	2.6
1	A	387	ALA	2.6
1	D	342	SER	2.6
1	D	363	PRO	2.6
1	D	374	PRO	2.6
1	B	840	ASN	2.6
1	C	553	ASN	2.6
1	B	579	GLU	2.6
1	C	518	LEU	2.6
1	D	376	HIS	2.6
1	A	293	VAL	2.6
1	B	246	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	425	VAL	2.6
1	A	811	SER	2.6
1	D	127	ILE	2.6
1	D	365	LYS	2.6
1	C	220	MET	2.6
1	D	165	ASN	2.6
1	A	213	PRO	2.6
1	D	76	GLY	2.5
1	C	423	LYS	2.5
1	D	294	LEU	2.5
1	B	240	TYR	2.5
1	D	144	ASN	2.5
1	D	186	ASN	2.5
1	D	261	ARG	2.5
1	D	479	GLU	2.5
1	D	13	ALA	2.5
1	D	284	ALA	2.5
1	D	462	ALA	2.5
1	C	421	GLY	2.5
1	C	432	THR	2.5
1	C	570	MET	2.5
1	B	479	GLU	2.5
1	C	354	ARG	2.5
1	A	317	PRO	2.5
1	C	161	VAL	2.5
1	C	555	GLY	2.5
1	C	149	THR	2.5
1	D	65	ARG	2.5
1	A	241	GLN	2.5
1	D	373	GLN	2.5
1	C	328	PHE	2.5
1	D	319	LEU	2.5
1	D	329	ASP	2.5
1	D	340	LEU	2.5
1	D	390	ASP	2.5
1	D	398	PHE	2.5
1	D	418	ASP	2.5
1	B	361	VAL	2.5
1	C	480	VAL	2.5
1	D	325	HIS	2.5
1	C	479	GLU	2.5
1	B	156	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	464	THR	2.5
1	D	389	ASN	2.4
1	D	465	ARG	2.4
1	B	11	SER	2.4
1	C	353	ILE	2.4
1	D	452	SER	2.4
1	D	485	ASN	2.4
1	C	362	ASP	2.4
1	B	233	LYS	2.4
1	D	208	LYS	2.4
1	D	122	PRO	2.4
1	D	810	ALA	2.4
1	D	311	SER	2.4
1	C	177	VAL	2.4
1	C	425	VAL	2.4
1	C	159	GLU	2.4
1	A	365	LYS	2.4
1	D	276	PRO	2.4
1	D	323	PRO	2.4
1	D	343	GLN	2.4
1	D	436	PRO	2.4
1	C	307	ALA	2.4
1	C	862	THR	2.4
1	D	862	THR	2.4
1	C	600	TRP	2.4
1	D	94	PHE	2.4
1	D	200	PHE	2.4
1	D	454	TRP	2.4
1	D	461	TRP	2.4
1	A	295	ASP	2.4
1	C	310	ARG	2.4
1	D	137	ARG	2.4
1	D	197	LYS	2.4
1	A	446	ILE	2.4
1	C	500	ILE	2.4
1	B	220	MET	2.4
1	C	477	ASN	2.3
1	D	870	GLY	2.3
1	D	269	PRO	2.3
1	A	520	GLU	2.3
1	A	422	ASP	2.3
1	C	218	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	35	LEU	2.3
1	D	368	LEU	2.3
1	C	450	ILE	2.3
1	B	224	VAL	2.3
1	C	152	VAL	2.3
1	A	485	ASN	2.3
1	C	153	ASN	2.3
1	C	407	GLY	2.3
1	D	10	GLY	2.3
1	A	350	GLU	2.3
1	C	359	GLU	2.3
1	A	506	LYS	2.3
1	D	174	LYS	2.3
1	D	360	LYS	2.3
1	D	506	LYS	2.3
1	C	565	CYS	2.3
1	C	867	ALA	2.3
1	D	158	MET	2.3
1	C	566	HIS	2.3
1	C	564	PHE	2.3
1	D	23	PHE	2.3
1	A	304	TYR	2.3
1	D	20	TYR	2.3
1	D	860	GLU	2.3
1	D	417	ILE	2.3
1	D	493	SER	2.3
1	D	283	VAL	2.3
1	D	427	VAL	2.3
1	B	449	ASP	2.3
1	C	369	ASP	2.3
1	C	431	PRO	2.3
1	D	216	THR	2.3
1	D	312	ALA	2.3
1	D	119	LEU	2.3
1	B	463	GLU	2.3
1	C	557	TYR	2.3
1	B	235	ILE	2.3
1	D	252	ASP	2.3
1	D	414	ASP	2.3
1	C	224	VAL	2.3
1	C	494	VAL	2.3
1	C	505	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	12	VAL	2.3
1	A	463	GLU	2.2
1	D	195	GLU	2.2
1	D	123	ASN	2.2
1	D	11	SER	2.2
1	D	72	SER	2.2
1	D	445	SER	2.2
1	A	369	ASP	2.2
1	C	449	ASP	2.2
1	D	351	ASP	2.2
1	A	421	GLY	2.2
1	B	303	PHE	2.2
1	A	425	VAL	2.2
1	C	302	VAL	2.2
1	D	177	VAL	2.2
1	D	480	VAL	2.2
1	C	317	PRO	2.2
1	A	202	THR	2.2
1	C	504	THR	2.2
1	C	217	ALA	2.2
1	D	206	SER	2.2
1	A	362	ASP	2.2
1	D	154	ASP	2.2
1	D	295	ASP	2.2
1	D	395	LEU	2.2
1	D	80	HIS	2.2
1	D	539	ILE	2.2
1	D	102	ASN	2.2
1	A	314	VAL	2.2
1	B	864	LYS	2.2
1	C	164	VAL	2.2
1	A	220	MET	2.2
1	A	305	GLU	2.2
1	A	359	GLU	2.2
1	A	212	LEU	2.2
1	C	320	GLY	2.2
1	D	79	HIS	2.2
1	A	265	ILE	2.2
1	B	223	ILE	2.2
1	B	450	ILE	2.2
1	C	228	ILE	2.2
1	C	156	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	363	PRO	2.2
1	A	578	VAL	2.1
1	C	296	VAL	2.1
1	D	166	VAL	2.1
1	A	307	ALA	2.1
1	C	65	ARG	2.1
1	C	35	LEU	2.1
1	C	198	TRP	2.1
1	D	24	TRP	2.1
1	C	503	PHE	2.1
1	D	601	THR	2.1
1	C	163	TYR	2.1
1	D	256	GLU	2.1
1	D	318	GLU	2.1
1	D	121	ILE	2.1
1	B	65	ARG	2.1
1	B	161	VAL	2.1
1	D	128	HIS	2.1
1	D	443	HIS	2.1
1	A	10	GLY	2.1
1	D	215	MET	2.1
1	C	455	ASP	2.1
1	D	63	SER	2.1
1	D	242	GLU	2.1
1	D	341	ASP	2.1
1	D	103	THR	2.1
1	D	211	THR	2.1
1	C	289	PRO	2.1
1	A	299	PHE	2.1
1	A	234	ALA	2.1
1	B	863	LYS	2.1
1	B	234	ALA	2.1
1	C	13	ALA	2.1
1	C	197	LYS	2.1
1	C	556	VAL	2.1
1	A	850	ASP	2.1
1	D	16	GLN	2.1
1	B	811	SER	2.1
1	A	385	LEU	2.1
1	B	447	LEU	2.1
1	B	601	THR	2.1
1	D	459	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	222	HIS	2.1
1	C	304	TYR	2.1
1	B	358	GLY	2.0
1	C	271	GLY	2.0
1	C	285	GLY	2.0
1	D	36	GLY	2.0
1	D	421	GLY	2.0
1	D	869	ASN	2.0
1	D	348	ASN	2.0
1	D	424	MET	2.0
1	C	12	VAL	2.0
1	C	331	ARG	2.0
1	C	427	VAL	2.0
1	C	578	VAL	2.0
1	A	368	LEU	2.0
1	C	395	LEU	2.0
1	A	428	HIS	2.0
1	A	504	THR	2.0
1	B	14	PRO	2.0
1	C	864	LYS	2.0
1	D	14	PRO	2.0
1	A	457	ASN	2.0
1	C	574	GLY	2.0
1	D	145	GLY	2.0
1	D	467	GLN	2.0
1	A	199	ALA	2.0
1	B	218	ALA	2.0
1	C	366	ASP	2.0
1	D	101	ALA	2.0
1	D	519	ASP	2.0
1	C	246	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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(Å ²)	Q<0.9
3	CA	C	4910	1/1	0.73	0.18	66,66,66,66	0
3	CA	A	4904	1/1	0.74	0.24	74,74,74,74	0
3	CA	D	4903	1/1	0.82	0.17	36,36,36,36	0
3	CA	B	4909	1/1	0.85	0.12	67,67,67,67	0
5	CUZ	D	7801	5/5	0.92	0.15	31,31,32,32	0
2	CL	D	4908	1/1	0.93	0.15	32,32,32,32	0
4	CUA	C	4701	2/2	0.95	0.09	24,24,24,25	0
3	CA	D	4904	1/1	0.97	0.10	25,25,25,25	0
2	CL	A	4901	1/1	0.97	0.05	17,17,17,17	0
5	CUZ	A	4801	5/5	0.97	0.09	18,19,19,20	0
5	CUZ	C	6801	5/5	0.97	0.12	21,21,21,22	0
3	CA	A	4903	1/1	0.97	0.05	21,21,21,21	0
4	CUA	D	4701	2/2	0.98	0.10	17,17,17,18	0
3	CA	A	4905	1/1	0.98	0.04	17,17,17,17	0
4	CUA	B	4701	2/2	0.98	0.05	17,17,17,17	0
2	CL	C	4907	1/1	0.98	0.06	18,18,18,18	0
3	CA	C	4905	1/1	0.99	0.12	22,22,22,22	0
3	CA	B	4905	1/1	0.99	0.04	14,14,14,14	0
3	CA	C	4903	1/1	0.99	0.10	17,17,17,17	0
5	CUZ	B	5801	5/5	0.99	0.07	14,15,15,15	0
4	CUA	A	4701	2/2	0.99	0.04	10,10,10,10	0
2	CL	B	4906	1/1	0.99	0.03	12,12,12,12	0
3	CA	B	4903	1/1	1.00	0.06	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.