



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:46 PM UTC

PDB ID : 1RWQ / pdb_00001rwq
Title : Human Dipeptidyl peptidase IV in complex with 5-aminomethyl-6-(2,4-dichloro-phenyl)-2-(3,5-dimethoxy-phenyl)-pyrimidin-4-ylamine
Authors : Hennig, M.; Thoma, R.; Stihle, M.
Deposited on : 2003-12-17
Resolution : 2.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

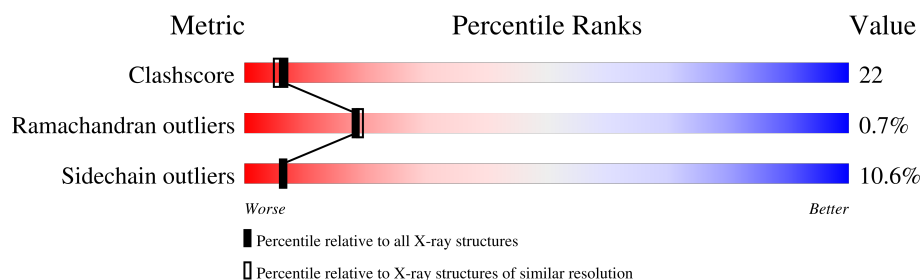
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	
1	B	728	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12190 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 Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



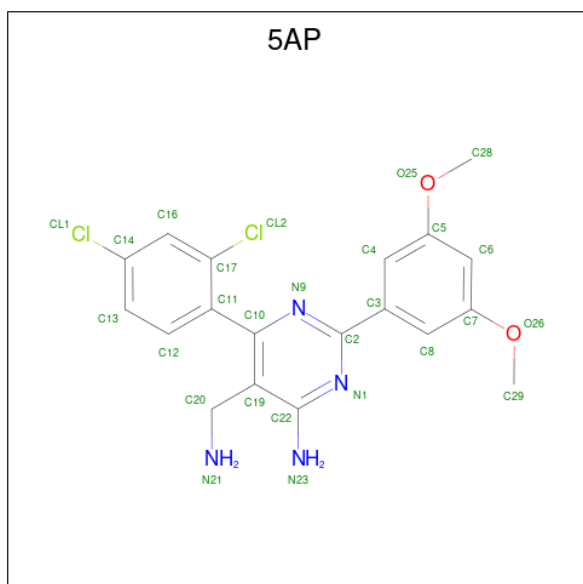
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 5-(AMINOMETHYL)-6-(2,4-DICHLOROPHENYL)-2-(3,5-DIMETHOXYPHENYL)PYRIMIDIN-4-AMINE (CCD ID: 5AP) (formula: C₁₉H₁₈Cl₂N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			27	19	2	4	2	0
3	B	1	Total	C	Cl	N	O	0
			27	19	2	4	2	0

- Molecule 4 is water.

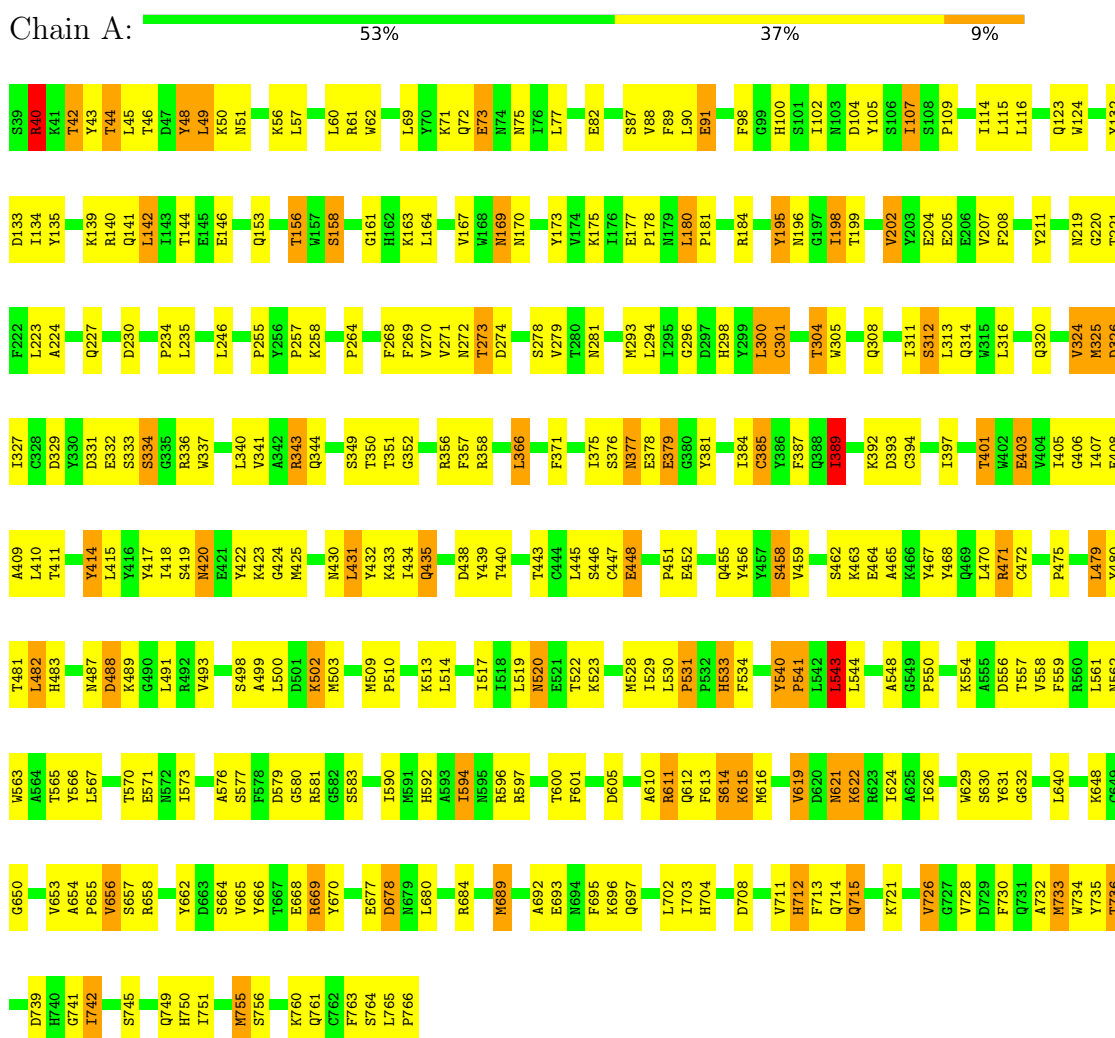
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	51	Total	O	0	0
			51	51		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: Dipeptidyl peptidase IV



- Molecule 1: Dipeptidyl peptidase IV



I719	S637	V558	K466	E379	L294	D200	T114	S39
V726	M638	V639	Y467	H383	I295	W201	L115	R40
Q731	L640	N562	Q469	Y386	H298	V202	E117	K41
A732	G643	V563	L470	F387	Y299	E206	Y120	Y43
H733	S644	A564	R471	F387	L300	V207	K122	T44
W734	G645	T565	C472	Q388	V303	F208	Y120	L45
Y735	V646	Y566	P478	I389	A306	Y211	K121	T46
T736	L567	L567	L479	K392	A306	Y211	Q123	
D737	R648	S569	Y480	D393	T307	L214	W124	L49
	C649	T570	T481	C394	Q308	W215	H126	K50
G741	G650	I574	L482	I397	E309	W216	S127	N51
I742	A652	V575	H483	T398	R310	S217	S127	T52
H750	V653	A576	S484	T398	I311	P218	Y132	Y53
I751	A654		S485		S312	N219		R54
Y752			V486		G220	N219		
T753	S657	G580		W402	L313	G220	D136	L60
H757	R658	R581	R492	E403	Q314	T221	L137	
F758	V659	V493	V404	V404	I319	F222	N138	T63
I759	E660	G584	L494	I405	L223	K139	K139	S64
		Y585		L410	Q320	A224	R140	D65
			L500		N321		Q141	H66
					Y322	Q227	L142	E67
	D663	I590		Y414			T143	T68
	S664	N591	V507	L415	M325	T236	T144	L69
	V665	H592	Q508	Y416	D326	E237	E145	K70
	Y666	A593	M509	I327			E146	T71
		I594	P510	N420	S242	S242	N150	Q72
R669		N595	S511	E421	D243	D243		E73
Y670		R596	K512	Y422	D331	E244		H74
M671		R597	K513	K423	E332	S245	V155	N75
		L598	L514		S333	L246	T156	
T675		G599		G428		Q247	W157	V78
P676		T600	I517	R429	W337	Y248	S158	
E677		F601	I518	N430	N338		P159	
D678		E602	L519	L431	C339		R253	E82
N679		V603	N520	Y432	L340			
L680		E604	E521	K433	S341	Y256	G161	N85
D681		D605	T522	I434	A342	P257	H162	S86
H682		Q606	K523	K435	R343	N257	K163	S87
		L607		L436		N263	V88	
	R684		Y526		E347	N263	I172	F39
		F613	Q527	K441	M348	P264	L90	L30
	E693	S614	E528	V442	S349	T265	K175	E91
	K696	M616	I529	T143	T350	K267	I176	N92
				C444	T351		E177	S93
							P178	T94
							N179	F95
	E699	V619	H533	S446	V354	V270	L180	D96
		D620	F534			V271		
	I703	N621	D635	E452	P362	N272	P181	
						T273		N103
	N710	T624	L542	Y456	H363		T188	D104
V711	L643	A625	L543		F364	S277	G189	S105
H712	I636		L544	V459	T365	S278	K190	Y106
F713			D545	S460	K374	V279	E191	I107
Q714		S630	V546	F461	I374	T280	D192	S108
Q715				S462	I375		I193	P109
S716		G633	G549	K463	S376	Q286	Y195	D110
A717				E464	N377		G111	
				A465	F379		N196	S112
								F113

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.68Å 69.14Å 422.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	84.3 (15.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.239 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12190	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 5AP

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	1.24	17/6135 (0.3%)	1.42	51/8344 (0.6%)
1	B	1.29	19/6135 (0.3%)	1.47	66/8344 (0.8%)
All	All	1.27	36/12270 (0.3%)	1.45	117/16688 (0.7%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	719	ILE	CA-CB	-10.09	1.42	1.54
1	B	630	SER	CA-C	-8.26	1.46	1.53
1	A	733	MET	SD-CE	7.58	1.98	1.79
1	A	207	VAL	C-O	-7.16	1.15	1.24
1	A	678	ASP	CA-C	7.08	1.55	1.52
1	B	172	ILE	CA-CB	-7.01	1.45	1.54
1	B	270	VAL	CA-CB	-6.96	1.45	1.54
1	B	429	ARG	NE-CZ	6.91	1.40	1.33
1	B	626	ILE	CA-CB	-6.83	1.44	1.54
1	A	624	ILE	CA-CB	-6.79	1.46	1.54
1	A	755	MET	SD-CE	-6.70	1.62	1.79
1	B	529	ILE	CA-CB	-6.42	1.46	1.54
1	B	638	MET	SD-CE	-6.38	1.63	1.79
1	A	257	PRO	C-O	-6.33	1.19	1.24
1	B	224	ALA	CA-CB	-6.30	1.43	1.53
1	B	624	ILE	CA-CB	-6.02	1.46	1.54
1	A	325	MET	SD-CE	-5.97	1.64	1.79
1	A	403	GLU	CA-C	-5.94	1.45	1.52
1	A	610	ALA	CA-CB	-5.94	1.43	1.53
1	B	751	ILE	CA-CB	-5.92	1.47	1.54
1	B	322	TYR	CA-C	-5.79	1.46	1.52
1	A	459	VAL	CA-C	-5.73	1.45	1.52
1	A	576	ALA	CA-CB	-5.67	1.43	1.53
1	B	678	ASP	CA-C	-5.59	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	689	MET	SD-CE	5.49	1.93	1.79
1	A	419	SER	CA-C	-5.44	1.46	1.52
1	B	654	ALA	C-O	-5.29	1.21	1.23
1	A	543	LEU	N-CA	-5.27	1.39	1.46
1	A	563	TRP	CA-C	-5.25	1.45	1.52
1	B	442	VAL	CA-CB	-5.25	1.48	1.54
1	B	257	PRO	C-O	-5.19	1.19	1.24
1	B	256	TYR	CA-C	-5.18	1.46	1.52
1	B	410	LEU	C-O	-5.16	1.18	1.23
1	A	425	MET	SD-CE	-5.10	1.66	1.79
1	A	389	ILE	CA-CB	-5.02	1.48	1.54
1	B	757	HIS	CA-C	-5.00	1.46	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ILE	N-CA-C	11.97	122.83	110.62
1	A	301	CYS	N-CA-C	8.66	123.97	113.41
1	A	590	ILE	N-CA-C	-8.61	104.41	111.81
1	A	133	ASP	N-CA-C	-8.34	96.33	109.50
1	B	389	ILE	N-CA-C	8.12	119.88	110.62
1	B	206	GLU	CA-C-N	-8.03	114.97	123.08
1	B	206	GLU	C-N-CA	-8.03	114.97	123.08
1	A	600	THR	CA-C-O	8.02	124.34	119.77
1	A	520	ASN	N-CA-C	-8.00	93.77	110.80
1	B	141	GLN	N-CA-C	7.97	122.23	108.76
1	A	220	GLY	N-CA-C	-7.89	104.31	115.43
1	A	656	VAL	N-CA-C	-7.74	98.87	109.55
1	B	630	SER	CB-CA-C	-7.68	107.72	116.63
1	A	139	LYS	N-CA-C	-7.50	97.95	109.65
1	B	220	GLY	N-CA-C	-7.47	103.58	115.08
1	A	301	CYS	CA-CB-SG	-7.46	97.23	114.40
1	A	304	THR	N-CA-C	7.37	122.51	107.69
1	B	354	VAL	CB-CA-C	-7.32	99.92	110.83
1	B	267	LYS	N-CA-C	-7.27	98.36	109.41
1	B	468	TYR	N-CA-C	7.25	121.15	108.75
1	A	366	LEU	N-CA-C	7.20	120.04	111.33
1	B	75	ASN	N-CA-C	-7.09	98.13	109.76
1	A	692	ALA	N-CA-C	6.99	119.74	111.71
1	A	493	VAL	N-CA-C	-6.86	98.28	109.12
1	B	257	PRO	CB-CA-C	-6.79	106.16	111.87
1	B	156	THR	N-CA-C	6.79	119.45	108.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	THR	N-CA-C	-6.70	105.64	113.88
1	A	40	ARG	N-CA-C	6.58	124.81	110.80
1	B	584	GLY	N-CA-C	6.49	123.15	112.89
1	B	85	ASN	N-CA-C	6.47	119.15	110.35
1	A	533	HIS	N-CA-C	-6.46	105.35	113.23
1	B	379	GLU	N-CA-C	-6.45	105.16	113.16
1	B	113	PHE	N-CA-C	6.42	118.94	109.24
1	B	633	GLY	N-CA-C	-6.41	104.25	113.86
1	B	590	ILE	N-CA-C	-6.40	104.80	111.58
1	A	556	ASP	N-CA-C	6.39	116.71	108.34
1	A	102	ILE	N-CA-C	6.37	117.97	108.23
1	B	96	ASP	N-CA-C	-6.30	104.65	112.72
1	B	485	SER	N-CA-C	6.30	119.13	111.82
1	B	67	GLU	N-CA-C	6.27	119.41	109.50
1	A	468	TYR	N-CA-C	6.22	118.76	108.99
1	B	200	ASP	N-CA-C	-6.21	100.15	109.96
1	A	712	HIS	N-CA-C	6.17	119.18	110.23
1	B	606	GLN	N-CA-C	-6.17	104.10	111.69
1	B	111	GLY	N-CA-C	6.15	127.76	113.18
1	A	77	LEU	CA-C-N	-6.15	115.57	123.19
1	A	77	LEU	C-N-CA	-6.15	115.57	123.19
1	B	319	ILE	N-CA-C	-6.14	98.15	107.73
1	B	512	LYS	N-CA-C	6.10	118.47	108.52
1	A	414	TYR	N-CA-C	6.05	118.61	109.23
1	A	258	LYS	N-CA-C	-6.01	102.78	110.53
1	B	311	ILE	CB-CA-C	-5.99	102.63	111.19
1	B	757	HIS	N-CA-C	-5.92	104.83	111.28
1	B	139	LYS	N-CA-C	-5.92	100.31	109.24
1	A	711	VAL	N-CA-C	-5.88	98.67	107.37
1	B	207	VAL	CB-CA-C	-5.88	105.85	111.44
1	B	478	PRO	CA-C-O	-5.87	114.72	121.36
1	A	156	THR	OG1-CB-CG2	-5.83	97.65	109.30
1	A	619	VAL	N-CA-C	5.82	116.38	107.77
1	A	142	LEU	N-CA-C	-5.82	102.15	110.59
1	A	140	ARG	N-CA-C	-5.80	103.47	110.44
1	B	137	LEU	N-CA-C	5.80	117.41	111.14
1	A	611	ARG	N-CA-C	-5.75	104.70	110.97
1	B	155	VAL	CB-CA-C	-5.75	100.41	110.71
1	A	531	PRO	O-C-N	5.75	123.85	121.15
1	B	264	PRO	N-CA-C	-5.73	102.46	111.34
1	B	338	ASN	N-CA-C	5.73	118.29	109.07
1	A	550	PRO	CB-CA-C	-5.68	104.42	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	THR	N-CA-C	5.64	119.17	110.42
1	B	222	PHE	N-CA-C	5.64	118.14	109.07
1	B	542	LEU	N-CA-C	5.63	118.07	108.90
1	B	127	SER	N-CA-C	5.62	118.80	110.48
1	B	42	THR	N-CA-CB	-5.62	101.88	110.42
1	B	364	PHE	N-CA-C	5.61	119.06	110.20
1	B	493	VAL	N-CA-C	-5.60	100.37	108.71
1	B	188	THR	N-CA-C	5.59	120.09	113.28
1	B	263	ASN	N-CA-C	5.57	117.97	110.29
1	B	664	SER	N-CA-C	5.56	117.78	111.11
1	A	202	VAL	CB-CA-C	-5.56	103.10	112.16
1	B	492	ARG	CB-CA-C	-5.54	100.31	111.17
1	B	64	SER	N-CA-C	-5.53	100.60	108.23
1	B	521	GLU	N-CA-CB	-5.51	108.59	114.10
1	A	622	LYS	N-CA-C	-5.51	106.60	113.38
1	B	264	PRO	CA-C-O	-5.51	115.06	121.95
1	B	678	ASP	N-CA-C	5.50	116.87	108.30
1	B	150	ASN	N-CA-C	-5.49	103.45	110.53
1	B	202	VAL	CB-CA-C	-5.48	103.38	112.26
1	B	558	VAL	N-CA-C	5.48	117.78	109.12
1	A	73	GLU	N-CA-C	-5.48	99.13	110.80
1	A	541	PRO	N-CA-C	-5.47	103.20	111.41
1	A	665	VAL	N-CA-C	5.46	116.19	110.62
1	A	268	PHE	N-CA-C	5.43	117.27	108.41
1	A	451	PRO	N-CA-C	5.43	120.98	113.98
1	A	401	THR	OG1-CB-CG2	-5.41	98.49	109.30
1	B	710	ASN	CA-C-N	-5.39	116.26	122.95
1	B	710	ASN	C-N-CA	-5.39	116.26	122.95
1	B	244	GLU	CB-CA-C	-5.39	98.11	110.18
1	B	110	ASP	CA-C-N	5.36	131.91	121.41
1	B	110	ASP	C-N-CA	5.36	131.91	121.41
1	B	645	GLY	N-CA-C	-5.35	107.93	115.32
1	A	405	ILE	N-CA-C	-5.35	105.91	111.58
1	A	448	GLU	CA-C-N	-5.32	113.52	120.44
1	A	448	GLU	C-N-CA	-5.32	113.52	120.44
1	A	498	SER	N-CA-C	-5.31	105.66	111.82
1	B	574	ILE	N-CA-C	-5.25	100.19	108.23
1	A	548	ALA	N-CA-C	5.25	118.95	112.24
1	A	597	ARG	N-CA-C	5.21	118.75	111.30
1	A	458	SER	N-CA-C	-5.16	101.85	109.18
1	B	665	VAL	N-CA-C	5.15	115.87	110.62
1	A	324	VAL	CB-CA-C	-5.11	103.06	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	562	ASN	N-CA-C	5.10	114.97	108.24
1	A	465	ALA	N-CA-C	5.09	119.44	113.23
1	B	543	LEU	CA-C-N	-5.05	116.05	122.77
1	B	543	LEU	C-N-CA	-5.05	116.05	122.77
1	B	753	THR	N-CA-C	-5.05	105.67	111.07
1	A	48	TYR	N-CA-C	-5.04	105.43	111.03
1	B	211	TYR	N-CA-C	-5.01	105.92	112.23

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	5963	0	5681	258	0
1	B	5963	0	5683	253	0
2	A	56	0	52	2	0
2	B	56	0	52	9	0
3	A	27	0	18	5	0
3	B	27	0	18	0	0
4	A	47	0	0	5	0
4	B	51	0	0	0	0
All	All	12190	0	11504	510	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (510) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:HD21	2:B:793:NAG:C1	1.45	1.28
1:B:600:THR:CG2	1:B:601:PHE:H	1.59	1.15
1:B:267:LYS:HD2	1:B:286:GLN:HE22	1.06	1.12
1:B:92:ASN:HD22	2:B:797:NAG:C1	1.65	1.08
1:B:600:THR:HG22	1:B:601:PHE:H	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLN:OE1	1:A:669:ARG:HG2	1.61	0.99
1:B:520:ASN:O	1:B:521:GLU:HB2	1.59	0.99
1:B:377:ASN:C	1:B:377:ASN:HD22	1.72	0.95
1:B:146:GLU:O	1:B:175:LYS:NZ	2.01	0.93
1:B:87:SER:OG	2:B:794:NAG:O7	1.87	0.93
1:A:614:SER:O	1:A:615:LYS:C	2.11	0.93
1:B:163:LYS:HZ3	1:B:273:THR:CG2	1.83	0.92
1:B:150:ASN:HD21	2:B:793:NAG:C2	1.83	0.91
1:A:221:THR:O	1:A:273:THR:HB	1.70	0.90
1:B:221:THR:O	1:B:273:THR:HB	1.71	0.89
1:A:735:TYR:OH	1:A:750:HIS:HD2	1.54	0.89
1:B:163:LYS:NZ	1:B:273:THR:CG2	2.35	0.89
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.53	0.89
1:B:267:LYS:HD2	1:B:286:GLN:NE2	1.88	0.88
1:A:745:SER:O	1:A:749:GLN:HG3	1.73	0.88
1:B:600:THR:CG2	1:B:601:PHE:N	2.27	0.88
1:B:236:ILE:HD12	1:B:712:HIS:CD2	2.09	0.87
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.04	0.87
1:A:621:ASN:C	1:A:621:ASN:HD22	1.82	0.87
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.06	0.84
1:A:463:LYS:O	1:A:464:GLU:HB2	1.75	0.84
1:A:471:ARG:O	1:A:471:ARG:HG3	1.76	0.84
1:B:600:THR:HG23	1:B:601:PHE:N	1.93	0.84
1:A:73:GLU:N	4:A:912:HOH:O	2.12	0.83
1:A:375:ILE:HG22	1:A:376:SER:O	1.77	0.83
1:B:549:GLY:O	1:B:552:SER:OG	1.96	0.83
1:B:163:LYS:HZ2	1:B:273:THR:HG21	1.45	0.82
1:B:110:ASP:OD2	1:B:161:GLY:N	2.14	0.81
1:B:657:SER:H	1:B:715:GLN:NE2	1.78	0.81
1:B:653:VAL:HG22	1:B:703:ILE:HD12	1.61	0.81
1:A:487:ASN:O	1:A:489:LYS:N	2.14	0.81
1:B:277:SER:HB3	1:B:280:THR:HB	1.62	0.80
1:B:600:THR:HG23	1:B:601:PHE:H	1.44	0.80
1:A:654:ALA:N	1:A:655:PRO:CD	2.45	0.80
1:B:680:LEU:HD22	1:B:684:ARG:CD	2.12	0.79
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.65	0.78
1:A:44:THR:HG22	1:A:46:THR:H	1.47	0.78
1:A:680:LEU:HD11	1:A:684:ARG:HD3	1.64	0.77
1:B:163:LYS:NZ	1:B:273:THR:HG21	1.99	0.77
1:A:43:TYR:CD2	1:A:565:THR:HG22	2.20	0.76
1:B:143:ILE:HD13	1:B:179:ASN:HA	1.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:GLU:H	1:B:420:ASN:HD21	1.32	0.76
1:B:63:ILE:HD13	1:B:69:LEU:HG	1.68	0.76
1:A:163:LYS:HZ2	1:A:273:THR:CG2	1.97	0.76
1:B:680:LEU:HD22	1:B:684:ARG:HD2	1.66	0.76
1:A:403:GLU:H	1:A:420:ASN:HD21	1.32	0.76
1:A:104:ASP:OD1	1:A:105:TYR:N	2.19	0.75
1:B:109:PRO:HD2	1:B:161:GLY:O	1.87	0.75
1:B:110:ASP:CG	1:B:161:GLY:H	1.94	0.75
1:A:499:ALA:O	1:A:502:LYS:HG3	1.87	0.74
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.87	0.73
1:B:163:LYS:HZ3	1:B:273:THR:HG22	1.52	0.73
1:A:219:ASN:HB2	1:A:308:GLN:OE1	1.88	0.73
1:A:613:PHE:O	1:A:616:MET:HB2	1.89	0.73
1:B:41:LYS:NZ	1:B:42:THR:O	2.21	0.73
1:B:322:TYR:HE1	1:B:348:MET:HE2	1.54	0.72
1:B:46:THR:HG23	1:B:50:LYS:HD2	1.71	0.72
1:B:155:VAL:HG12	1:B:156:THR:N	2.05	0.72
1:A:561:LEU:O	4:A:925:HOH:O	2.08	0.71
1:A:392:LYS:HD2	1:A:393:ASP:OD2	1.90	0.71
1:A:293:MET:HE2	1:A:324:VAL:HG23	1.72	0.71
1:A:430:ASN:OD1	1:A:446:SER:OG	2.09	0.71
1:B:351:THR:HG22	1:B:592:HIS:ND1	2.05	0.70
1:A:726:VAL:HG12	1:A:728:VAL:CG2	2.21	0.70
1:A:415:LEU:HD23	1:A:415:LEU:C	2.17	0.70
1:B:415:LEU:C	1:B:415:LEU:HD23	2.16	0.70
1:B:377:ASN:ND2	1:B:379:GLU:H	1.90	0.70
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.74	0.70
1:A:562:ASN:O	1:A:565:THR:HB	1.92	0.69
1:B:42:THR:HG23	1:B:570:THR:OG1	1.91	0.69
1:B:236:ILE:HD12	1:B:712:HIS:CG	2.28	0.69
1:A:680:LEU:HD11	1:A:684:ARG:CD	2.23	0.69
1:A:82:GLU:HB2	1:A:467:TYR:OH	1.94	0.68
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.75	0.68
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.76	0.68
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.76	0.67
1:A:736:THR:HG21	1:B:717:ALA:O	1.94	0.67
1:A:693:GLU:O	1:A:696:LYS:HG2	1.94	0.67
1:B:143:ILE:CD1	1:B:145:GLU:O	2.43	0.67
1:A:163:LYS:NZ	1:A:273:THR:CG2	2.57	0.67
1:A:163:LYS:HZ2	1:A:273:THR:HG22	1.57	0.66
1:B:435:GLN:NE2	1:B:441:LYS:HD2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:SER:OG	1:B:325:MET:HE3	1.95	0.66
1:B:742:ILE:O	1:B:742:ILE:HG22	1.96	0.66
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.77	0.65
1:B:435:GLN:HE22	1:B:441:LYS:HD2	1.62	0.65
1:A:105:TYR:CD1	1:A:105:TYR:C	2.73	0.65
1:A:482:LEU:HD13	1:A:491:LEU:HD12	1.76	0.65
1:B:143:ILE:HG13	1:B:143:ILE:O	1.96	0.65
1:B:377:ASN:C	1:B:377:ASN:ND2	2.45	0.65
1:A:219:ASN:CB	1:A:308:GLN:OE1	2.45	0.65
1:B:75:ASN:OD1	1:B:92:ASN:HB3	1.96	0.64
1:B:107:ILE:HG13	1:B:114:ILE:HG13	1.79	0.64
1:B:107:ILE:CG1	1:B:114:ILE:HD12	2.27	0.64
1:A:499:ALA:O	1:A:502:LYS:CG	2.46	0.64
1:A:123:GLN:HG2	1:A:124:TRP:H	1.63	0.64
1:A:72:GLN:O	1:A:73:GLU:HB2	1.97	0.64
1:A:320:GLN:OE1	1:A:669:ARG:CG	2.43	0.64
1:B:594:ILE:HD11	1:B:602:GLU:H	1.62	0.63
1:A:657:SER:H	1:A:715:GLN:NE2	1.96	0.63
1:A:123:GLN:HG2	1:A:124:TRP:N	2.13	0.63
1:B:332:GLU:HG2	1:B:333:SER:N	2.13	0.63
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.30	0.62
2:A:793:NAG:H83	2:A:793:NAG:H3	1.79	0.62
1:B:651:ILE:HD11	1:B:759:ILE:HD12	1.79	0.62
1:B:293:MET:O	1:B:298:HIS:HD2	1.82	0.62
1:B:471:ARG:O	1:B:471:ARG:HG2	1.99	0.62
1:A:594:ILE:HD11	1:A:601:PHE:HB2	1.77	0.62
1:B:150:ASN:ND2	2:B:793:NAG:C2	2.58	0.62
1:B:107:ILE:HG12	1:B:114:ILE:HD12	1.80	0.62
1:B:105:TYR:CD1	1:B:105:TYR:C	2.78	0.62
1:B:322:TYR:CE1	1:B:348:MET:HE2	2.33	0.62
1:A:272:ASN:C	1:A:272:ASN:OD1	2.42	0.62
1:B:620:ASP:OD1	1:B:620:ASP:O	2.18	0.62
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.82	0.61
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.81	0.61
1:B:223:LEU:C	1:B:223:LEU:HD22	2.26	0.61
1:A:180:LEU:HD12	1:A:181:PRO:HD3	1.81	0.61
1:A:417:TYR:CE1	1:A:434:ILE:HD11	2.36	0.61
1:B:120:TYR:OH	1:B:122:LYS:HB2	2.01	0.61
1:A:422:TYR:O	1:A:424:GLY:N	2.34	0.60
1:B:520:ASN:O	1:B:521:GLU:CB	2.40	0.60
1:B:620:ASP:OD1	1:B:620:ASP:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:MET:HE1	1:B:682:HIS:ND1	2.16	0.60
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.81	0.60
1:A:123:GLN:HG2	1:A:124:TRP:CG	2.37	0.60
1:A:654:ALA:N	1:A:655:PRO:HD2	2.16	0.60
1:A:463:LYS:O	1:A:464:GLU:CB	2.47	0.60
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.02	0.60
1:A:611:ARG:O	1:A:612:GLN:C	2.44	0.60
1:A:123:GLN:HG2	1:A:124:TRP:CD1	2.37	0.60
1:A:300:LEU:C	1:A:300:LEU:CD2	2.75	0.60
1:A:471:ARG:O	1:A:471:ARG:CG	2.48	0.60
1:B:42:THR:CG2	1:B:570:THR:OG1	2.49	0.60
1:A:455:GLN:HB2	1:A:475:PRO:HD3	1.84	0.59
1:B:69:LEU:HD23	1:B:78:VAL:HG22	1.85	0.59
1:B:414:TYR:CD1	1:B:433:LYS:HE2	2.38	0.59
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.83	0.59
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.37	0.59
1:A:293:MET:CE	1:A:324:VAL:HG23	2.33	0.59
1:A:351:THR:OG1	1:A:592:HIS:CD2	2.55	0.59
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.55	0.59
1:B:143:ILE:HD11	1:B:145:GLU:O	2.03	0.59
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.38	0.58
1:B:545:ASP:C	1:B:545:ASP:OD1	2.46	0.58
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.37	0.58
1:B:46:THR:HG23	1:B:50:LYS:CD	2.33	0.58
1:B:347:GLU:OE2	1:B:373:LYS:NZ	2.25	0.58
1:A:377:ASN:C	1:A:377:ASN:HD22	2.11	0.58
1:B:741:GLY:O	1:B:742:ILE:C	2.47	0.58
1:A:69:LEU:HD13	1:A:107:ILE:CD1	2.33	0.58
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.85	0.58
1:A:105:TYR:CD1	1:A:105:TYR:O	2.57	0.58
1:A:89:PHE:CE2	1:A:107:ILE:HD13	2.38	0.58
1:A:340:LEU:HB3	1:A:343:ARG:HD2	1.86	0.58
1:A:312:SER:O	1:A:313:LEU:HD23	2.04	0.57
1:A:431:LEU:HD22	1:A:432:TYR:N	2.20	0.57
1:B:120:TYR:CD1	1:B:120:TYR:C	2.83	0.57
1:B:651:ILE:HD11	1:B:759:ILE:CD1	2.34	0.57
1:B:217:SER:HB2	1:B:222:PHE:HB2	1.87	0.57
1:B:277:SER:CB	1:B:280:THR:HB	2.33	0.57
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.85	0.56
1:B:320:GLN:OE1	1:B:669:ARG:CD	2.53	0.56
1:B:562:ASN:C	1:B:562:ASN:HD22	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:SER:H	1:B:715:GLN:HE21	1.51	0.56
1:B:46:THR:CG2	1:B:50:LYS:CD	2.83	0.56
1:B:518:ILE:HA	1:B:522:THR:O	2.06	0.56
1:A:533:HIS:O	1:A:534:PHE:C	2.48	0.56
1:A:331:ASP:OD2	1:A:334:SER:HB3	2.06	0.56
1:A:69:LEU:HD11	1:A:107:ILE:HD12	1.88	0.56
1:A:594:ILE:HG23	1:A:594:ILE:O	2.05	0.55
1:B:75:ASN:OD1	1:B:92:ASN:CB	2.54	0.55
1:B:143:ILE:HD12	1:B:145:GLU:O	2.04	0.55
1:B:596:ARG:C	1:B:597:ARG:HG3	2.31	0.55
1:A:109:PRO:HD2	1:A:161:GLY:O	2.07	0.55
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.41	0.55
1:A:735:TYR:OH	1:A:750:HIS:CD2	2.46	0.55
1:B:46:THR:CG2	1:B:50:LYS:HD2	2.36	0.55
1:A:519:LEU:C	1:A:520:ASN:O	2.48	0.55
1:A:543:LEU:HD22	1:A:543:LEU:C	2.32	0.55
1:A:612:GLN:O	1:A:613:PHE:C	2.49	0.55
1:A:629:TRP:O	1:A:632:GLY:N	2.41	0.54
1:A:43:TYR:CD2	1:A:565:THR:CG2	2.90	0.54
1:A:123:GLN:CG	1:A:124:TRP:N	2.69	0.54
1:B:63:ILE:HD13	1:B:69:LEU:CG	2.35	0.54
1:A:158:SER:OG	1:A:163:LYS:HB2	2.07	0.54
1:A:163:LYS:NZ	1:A:273:THR:HG22	2.19	0.54
1:B:155:VAL:CG1	1:B:156:THR:N	2.71	0.54
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.38	0.54
1:A:327:ILE:HB	1:A:343:ARG:HG3	1.89	0.54
1:A:751:ILE:O	1:A:755:MET:HG3	2.07	0.54
1:B:600:THR:HG22	1:B:601:PHE:N	2.05	0.54
1:A:422:TYR:C	1:A:424:GLY:H	2.16	0.53
1:A:479:LEU:HD13	1:A:481:THR:HG23	1.89	0.53
1:A:680:LEU:CD1	1:A:684:ARG:CD	2.86	0.53
1:A:680:LEU:CD1	1:A:684:ARG:HD3	2.36	0.53
1:A:414:TYR:CE2	1:A:435:GLN:HG3	2.44	0.53
1:B:63:ILE:CD1	1:B:69:LEU:CD1	2.86	0.53
1:A:208:PHE:HZ	1:A:300:LEU:HD13	1.73	0.53
1:A:381:TYR:CZ	1:A:401:THR:HG23	2.43	0.53
1:A:431:LEU:HD13	1:A:445:LEU:HB2	1.91	0.53
1:B:482:LEU:HB2	1:B:494:LEU:HD11	1.90	0.53
1:A:272:ASN:OD1	1:A:274:ASP:N	2.35	0.53
1:A:420:ASN:C	1:A:420:ASN:HD22	2.15	0.53
1:A:739:ASP:C	1:A:739:ASP:OD1	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASN:OD1	1:B:92:ASN:CG	2.52	0.53
1:A:626:ILE:O	1:A:650:GLY:HA2	2.09	0.53
1:A:357:PHE:HD1	1:A:669:ARG:HH21	1.56	0.52
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.91	0.52
1:B:680:LEU:CD2	1:B:684:ARG:NE	2.72	0.52
1:B:46:THR:HG22	1:B:50:LYS:HD3	1.91	0.52
1:B:693:GLU:O	1:B:696:LYS:HG2	2.09	0.52
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.75	0.52
1:B:92:ASN:HD21	2:B:797:NAG:C1	2.18	0.52
1:B:107:ILE:CG1	1:B:114:ILE:CD1	2.87	0.52
1:A:540:TYR:CD1	1:A:540:TYR:N	2.75	0.52
1:A:540:TYR:HB3	1:A:541:PRO:HD2	1.92	0.52
1:A:487:ASN:O	1:A:488:ASP:C	2.53	0.52
1:A:654:ALA:N	1:A:655:PRO:HD3	2.25	0.52
1:A:666:TYR:CZ	3:A:900:5AP:H13	2.44	0.52
1:A:357:PHE:HB2	1:A:358:ARG:NH1	2.25	0.51
1:A:621:ASN:C	1:A:621:ASN:ND2	2.54	0.51
1:A:571:GLU:HB2	1:A:573:ILE:HD12	1.92	0.51
1:A:431:LEU:HD13	1:A:445:LEU:HD12	1.91	0.51
1:A:331:ASP:OD1	1:A:331:ASP:C	2.53	0.51
1:A:356:ARG:NH2	1:A:403:GLU:OE1	2.43	0.51
1:B:377:ASN:ND2	1:B:378:GLU:N	2.59	0.51
1:A:48:TYR:CD2	1:A:49:LEU:HD13	2.45	0.51
1:B:236:ILE:HG12	1:B:237:GLU:N	2.26	0.51
1:B:293:MET:O	1:B:298:HIS:CD2	2.64	0.51
1:B:46:THR:CG2	1:B:50:LYS:HD3	2.41	0.51
1:B:215:TRP:CH2	1:B:303:VAL:HG21	2.46	0.51
1:B:463:LYS:O	1:B:464:GLU:HB2	2.11	0.51
1:B:614:SER:OG	1:B:624:ILE:HD11	2.11	0.51
1:B:651:ILE:CD1	1:B:759:ILE:HD11	2.41	0.51
1:B:651:ILE:CD1	1:B:759:ILE:CD1	2.89	0.51
1:A:105:TYR:HA	1:A:115:LEU:O	2.12	0.50
1:A:422:TYR:C	1:A:424:GLY:N	2.64	0.50
1:B:125:ARG:HD2	1:B:126:HIS:CE1	2.47	0.50
1:B:387:PHE:CD2	1:B:394:CYS:HB3	2.46	0.50
1:B:651:ILE:HD12	1:B:759:ILE:HD11	1.93	0.50
1:B:680:LEU:HD21	1:B:684:ARG:NE	2.26	0.50
1:B:429:ARG:HG3	1:B:456:TYR:CE2	2.47	0.50
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.47	0.50
1:B:267:LYS:CD	1:B:286:GLN:HE22	1.99	0.50
1:A:500:LEU:HA	1:A:503:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LEU:C	1:A:543:LEU:CD2	2.85	0.50
1:A:300:LEU:C	1:A:300:LEU:HD22	2.36	0.50
1:A:377:ASN:ND2	1:A:379:GLU:H	2.10	0.50
1:B:377:ASN:ND2	1:B:379:GLU:N	2.57	0.50
1:B:758:PHE:CD2	1:B:758:PHE:O	2.65	0.50
1:B:107:ILE:O	1:B:108:SER:C	2.53	0.50
1:B:223:LEU:C	1:B:223:LEU:CD2	2.83	0.50
1:B:227:GLN:O	1:B:266:VAL:HA	2.11	0.50
1:B:236:ILE:HD12	1:B:712:HIS:NE2	2.25	0.50
1:A:221:THR:O	1:A:273:THR:CB	2.54	0.50
1:B:108:SER:OG	1:B:113:PHE:HB2	2.12	0.50
1:A:329:ASP:O	1:A:337:TRP:HA	2.12	0.49
1:A:431:LEU:HD22	1:A:431:LEU:C	2.36	0.49
1:B:63:ILE:HD13	1:B:69:LEU:CD1	2.42	0.49
1:B:383:HIS:HD2	1:B:398:THR:CB	2.23	0.49
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.47	0.49
1:A:198:ILE:HA	1:A:211:TYR:O	2.13	0.49
1:A:42:THR:HG23	1:A:570:THR:OG1	2.13	0.49
1:A:146:GLU:HG3	1:A:180:LEU:C	2.38	0.49
1:A:458:SER:OG	1:A:471:ARG:CG	2.61	0.49
1:B:377:ASN:HD22	1:B:378:GLU:N	2.09	0.49
1:B:736:THR:O	1:B:737:ASP:HB2	2.12	0.49
1:A:431:LEU:C	1:A:431:LEU:CD2	2.85	0.49
1:B:428:GLY:O	1:B:429:ARG:HG2	2.12	0.49
1:B:236:ILE:HD12	1:B:712:HIS:CE1	2.48	0.49
1:B:379:GLU:N	1:B:379:GLU:CD	2.71	0.49
1:B:422:TYR:CE2	1:B:423:LYS:HE3	2.48	0.48
1:B:580:GLY:C	1:B:581:ARG:O	2.52	0.48
1:A:334:SER:OG	1:A:336:ARG:HG3	2.13	0.48
1:A:614:SER:O	1:A:616:MET:N	2.45	0.48
1:B:462:SER:O	1:B:463:LYS:C	2.55	0.48
1:A:446:SER:O	1:A:447:CYS:C	2.55	0.48
1:B:459:VAL:HG22	1:B:460:SER:N	2.28	0.48
1:A:331:ASP:CG	1:A:334:SER:HB3	2.39	0.48
1:A:320:GLN:CD	1:A:669:ARG:HG2	2.34	0.48
1:A:730:PHE:CE2	1:B:733:MET:HE1	2.48	0.48
1:B:386:TYR:HB2	1:B:397:ILE:CD1	2.43	0.48
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.48	0.48
1:B:420:ASN:HD22	1:B:420:ASN:C	2.20	0.48
1:A:167:VAL:HG11	1:A:198:ILE:HG12	1.96	0.48
1:A:173:TYR:OH	1:A:184:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:O	1:A:298:HIS:HD2	1.97	0.48
1:A:621:ASN:HD22	1:A:622:LYS:N	2.09	0.48
1:B:122:LYS:HG2	1:B:123:GLN:N	2.29	0.48
1:B:162:HIS:CD2	1:B:162:HIS:O	2.67	0.48
1:A:594:ILE:HD13	1:A:601:PHE:HB2	1.93	0.47
1:B:522:THR:HG22	1:B:523:LYS:N	2.28	0.47
1:A:554:LYS:NZ	4:A:903:HOH:O	2.47	0.47
1:B:594:ILE:O	1:B:595:ASN:C	2.54	0.47
1:A:327:ILE:HD13	1:A:389:ILE:HD13	1.97	0.47
1:A:653:VAL:C	1:A:655:PRO:HD3	2.39	0.47
1:A:57:LEU:HD22	1:A:480:TYR:OH	2.14	0.47
1:A:622:LYS:O	1:A:648:LYS:HD2	2.15	0.47
1:B:429:ARG:HG3	1:B:456:TYR:CZ	2.50	0.47
1:B:636:THR:O	1:B:640:LEU:HG	2.14	0.47
1:B:415:LEU:HD23	1:B:416:TYR:N	2.29	0.47
1:B:507:VAL:HG23	1:B:508:GLN:N	2.29	0.47
1:A:169:ASN:O	1:A:170:ASN:HB2	2.14	0.47
1:A:431:LEU:CD2	1:A:432:TYR:N	2.78	0.47
1:A:456:TYR:HB2	1:A:557:THR:OG1	2.15	0.47
1:A:314:GLN:HG3	1:A:325:MET:HG3	1.96	0.47
1:A:540:TYR:O	1:A:619:VAL:HA	2.14	0.47
1:B:91:GLU:OE1	1:B:94:THR:OG1	2.31	0.47
1:B:340:LEU:O	1:B:341:VAL:C	2.58	0.47
1:B:110:ASP:HB2	1:B:161:GLY:HA2	1.97	0.47
1:A:500:LEU:HA	1:A:503:MET:CE	2.45	0.47
1:B:117:GLU:HG3	1:B:132:TYR:CE1	2.50	0.47
1:A:680:LEU:HD11	1:A:684:ARG:NE	2.30	0.46
1:A:708:ASP:HA	1:A:739:ASP:HA	1.97	0.46
1:A:741:GLY:O	1:A:742:ILE:C	2.58	0.46
1:B:71:LYS:HB3	1:B:71:LYS:HZ2	1.79	0.46
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.15	0.46
1:B:429:ARG:CZ	1:B:456:TYR:OH	2.63	0.46
1:B:734:TRP:CD1	1:B:734:TRP:C	2.93	0.46
1:A:71:LYS:HA	1:A:75:ASN:O	2.16	0.46
1:A:703:ILE:HA	1:A:733:MET:O	2.15	0.46
1:A:417:TYR:O	1:A:431:LEU:HD23	2.16	0.46
1:B:115:LEU:HD11	1:B:155:VAL:HG11	1.97	0.46
1:B:327:ILE:HG21	1:B:343:ARG:HD3	1.97	0.46
1:B:563:TRP:HH2	1:B:759:ILE:HD13	1.80	0.46
1:B:658:ARG:NH2	1:B:660:GLU:OE1	2.49	0.46
1:A:630:SER:O	1:A:631:TYR:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:ILE:O	1:B:626:ILE:HG23	2.15	0.46
1:B:72:GLN:O	1:B:73:GLU:C	2.58	0.46
2:B:793:NAG:C1	2:B:793:NAG:H82	2.46	0.46
1:A:304:THR:O	1:A:305:TRP:C	2.59	0.46
1:A:763:PHE:O	1:A:765:LEU:HG	2.16	0.46
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.15	0.46
1:A:271:VAL:CG1	1:A:272:ASN:N	2.77	0.46
1:A:658:ARG:HB2	1:A:689:MET:HE1	1.96	0.46
1:A:57:LEU:CD2	1:A:480:TYR:OH	2.64	0.46
1:A:558:VAL:HG12	1:A:559:PHE:N	2.30	0.46
1:B:715:GLN:HE21	1:B:715:GLN:HB3	1.55	0.46
1:B:43:TYR:HB3	1:B:569:SER:HB3	1.99	0.46
1:B:624:ILE:HG22	1:B:647:PHE:CD2	2.50	0.46
1:A:205:GLU:OE2	3:A:900:5AP:N21	2.49	0.45
1:B:163:LYS:NZ	1:B:273:THR:HG22	2.20	0.45
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.69	0.45
1:A:235:LEU:HD23	1:A:255:PRO:HA	1.98	0.45
1:A:615:LYS:O	1:A:616:MET:C	2.59	0.45
1:B:680:LEU:CD2	1:B:684:ARG:CD	2.90	0.45
1:A:327:ILE:HD13	1:A:389:ILE:CD1	2.47	0.45
1:A:567:LEU:HD22	1:A:573:ILE:HD13	1.97	0.45
1:A:558:VAL:CG1	1:A:559:PHE:N	2.79	0.45
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.72	0.45
1:B:51:ASN:OD1	1:B:54:ARG:HG2	2.17	0.45
1:B:272:ASN:OD1	1:B:272:ASN:C	2.60	0.45
1:B:604:GLU:O	1:B:607:ILE:HB	2.16	0.45
3:A:900:5AP:H283	4:A:940:HOH:O	2.17	0.45
1:B:207:VAL:HG12	1:B:208:PHE:CD1	2.51	0.45
1:B:535:ASP:OD1	1:B:535:ASP:C	2.60	0.45
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.82	0.45
1:B:146:GLU:OE1	1:B:181:PRO:HA	2.17	0.45
1:A:44:THR:HG22	1:A:45:LEU:N	2.32	0.45
1:B:107:ILE:HG13	1:B:114:ILE:CD1	2.47	0.45
1:A:406:GLY:O	1:A:417:TYR:HB2	2.17	0.45
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.17	0.45
1:B:107:ILE:O	1:B:108:SER:O	2.34	0.45
1:B:532:PRO:O	1:B:533:HIS:C	2.59	0.45
1:A:554:LYS:H	1:A:579:ASP:CG	2.26	0.44
1:B:403:GLU:H	1:B:420:ASN:ND2	2.08	0.44
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.17	0.44
1:B:599:GLY:N	1:B:602:GLU:OE2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LYS:CE	1:B:527:GLN:CD	2.90	0.44
1:B:594:ILE:HD11	1:B:602:GLU:N	2.30	0.44
1:A:562:ASN:O	1:A:565:THR:N	2.50	0.44
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.17	0.44
1:A:666:TYR:OH	3:A:900:5AP:H13	2.18	0.44
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.53	0.44
1:A:377:ASN:C	1:A:377:ASN:ND2	2.75	0.44
1:A:371:PHE:CE1	1:A:387:PHE:HB2	2.53	0.44
1:A:581:ARG:HB2	1:A:605:ASP:OD2	2.18	0.44
1:A:195:TYR:O	1:A:227:GLN:HA	2.18	0.44
1:B:107:ILE:HG13	1:B:114:ILE:CG1	2.45	0.44
1:A:116:LEU:O	1:A:132:TYR:HA	2.17	0.43
1:A:326:ASP:OD1	1:A:344:GLN:HG2	2.18	0.43
1:A:403:GLU:H	1:A:420:ASN:ND2	2.08	0.43
1:B:82:GLU:OE1	1:B:467:TYR:OH	2.23	0.43
1:B:156:THR:HG22	1:B:157:TRP:O	2.18	0.43
1:A:219:ASN:HB3	1:A:221:THR:OG1	2.18	0.43
1:B:190:LYS:O	1:B:191:GLU:C	2.60	0.43
1:A:414:TYR:HE2	1:A:435:GLN:HG3	1.84	0.43
1:B:405:ILE:HD13	1:B:429:ARG:HD3	2.00	0.43
1:B:510:PRO:HD3	1:B:569:SER:HB2	2.00	0.43
1:B:619:VAL:O	1:B:619:VAL:HG22	2.17	0.43
1:A:224:ALA:HA	1:A:270:VAL:HA	2.00	0.43
1:B:299:TYR:CZ	1:B:665:VAL:HG22	2.54	0.43
1:B:436:LEU:N	1:B:436:LEU:HD23	2.31	0.43
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.84	0.43
1:B:613:PHE:O	1:B:616:MET:HB2	2.18	0.43
1:B:90:LEU:HD11	1:B:95:PHE:HE2	1.83	0.43
1:B:107:ILE:CG1	1:B:114:ILE:HG13	2.47	0.43
1:A:734:TRP:CD1	1:A:734:TRP:C	2.97	0.43
1:B:532:PRO:C	1:B:534:PHE:N	2.75	0.43
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.69	0.43
1:A:562:ASN:OD1	1:A:562:ASN:C	2.61	0.43
1:B:580:GLY:O	1:B:581:ARG:C	2.61	0.43
1:A:44:THR:CG2	1:A:45:LEU:N	2.82	0.43
1:A:327:ILE:CD1	1:A:389:ILE:HD13	2.48	0.43
1:A:349:SER:HB3	1:A:352:GLY:O	2.18	0.43
1:B:107:ILE:C	1:B:108:SER:O	2.62	0.43
1:B:136:ASP:OD1	1:B:136:ASP:C	2.61	0.43
1:B:415:LEU:C	1:B:415:LEU:CD2	2.90	0.43
1:B:94:THR:O	1:B:95:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:CD1	1:B:712:HIS:CG	3.00	0.42
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.84	0.42
1:B:563:TRP:CH2	1:B:759:ILE:HD13	2.54	0.42
1:A:408:GLU:O	1:A:409:ALA:HB2	2.19	0.42
1:A:438:ASP:OD1	1:A:440:THR:OG1	2.36	0.42
1:B:158:SER:OG	1:B:163:LYS:HB2	2.19	0.42
1:B:309:GLU:HB3	1:B:330:TYR:HB3	2.01	0.42
1:A:269:PHE:N	1:A:269:PHE:CD1	2.86	0.42
1:A:281:ASN:ND2	2:A:795:NAG:C7	2.82	0.42
1:A:333:SER:OG	1:A:334:SER:N	2.53	0.42
1:A:357:PHE:HD1	1:A:669:ARG:NH2	2.16	0.42
1:A:702:LEU:O	1:A:732:ALA:HA	2.19	0.42
1:B:150:ASN:ND2	2:B:793:NAG:N2	2.67	0.42
1:A:146:GLU:O	1:A:175:LYS:NZ	2.50	0.42
1:A:420:ASN:C	1:A:420:ASN:ND2	2.78	0.42
1:A:662:TYR:OH	3:A:900:5AP:N21	2.53	0.42
1:A:756:SER:O	1:A:760:LYS:HG3	2.20	0.42
1:B:64:SER:OG	1:B:66:HIS:CD2	2.73	0.42
1:A:141:GLN:HG2	1:A:142:LEU:O	2.19	0.42
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.75	0.42
1:B:362:PRO:O	1:B:362:PRO:HG2	2.19	0.42
1:B:544:LEU:HD12	1:B:576:ALA:O	2.19	0.42
1:A:340:LEU:HD12	1:A:340:LEU:HA	1.87	0.42
1:A:695:PHE:C	1:A:697:GLN:N	2.76	0.42
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.51	0.42
1:B:383:HIS:HD2	1:B:398:THR:HB	1.84	0.42
1:A:40:ARG:HD3	1:A:40:ARG:HA	1.38	0.42
1:A:763:PHE:O	1:A:764:SER:C	2.62	0.42
1:A:387:PHE:CE2	1:A:394:CYS:HB3	2.55	0.42
1:A:594:ILE:HD12	1:A:594:ILE:HA	1.62	0.42
1:B:299:TYR:CE1	1:B:665:VAL:HG22	2.55	0.42
1:A:417:TYR:HE1	1:A:434:ILE:HD11	1.83	0.42
1:A:522:THR:HG22	1:A:523:LYS:N	2.34	0.42
1:A:596:ARG:HA	1:A:670:TYR:O	2.20	0.42
1:A:664:SER:O	1:A:668:GLU:HB2	2.19	0.42
1:B:105:TYR:CE1	1:B:107:ILE:HD12	2.55	0.42
1:B:195:TYR:CD1	1:B:195:TYR:N	2.88	0.42
1:B:206:GLU:OE2	1:B:663:ASP:OD2	2.38	0.42
1:B:596:ARG:HA	1:B:670:TYR:O	2.19	0.42
1:B:191:GLU:O	1:B:193:ILE:HG13	2.19	0.42
1:B:758:PHE:CD2	1:B:758:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:SER:OG	1:A:471:ARG:HG2	2.19	0.41
1:B:327:ILE:CG2	1:B:343:ARG:HD3	2.50	0.41
1:B:421:GLU:O	1:B:422:TYR:C	2.60	0.41
1:B:566:TYR:O	1:B:567:LEU:C	2.61	0.41
1:A:509:MET:HA	1:A:510:PRO:HD3	1.97	0.41
1:A:135:TYR:HD1	1:A:142:LEU:HD23	1.85	0.41
1:A:331:ASP:O	1:A:332:GLU:C	2.62	0.41
1:B:596:ARG:O	1:B:597:ARG:HG3	2.20	0.41
1:A:42:THR:CG2	1:A:570:THR:OG1	2.68	0.41
1:A:49:LEU:HG	1:A:749:GLN:HA	2.01	0.41
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.55	0.41
1:A:433:LYS:HB3	1:A:443:THR:HB	2.02	0.41
1:B:526:TYR:CD2	1:B:526:TYR:C	2.98	0.41
1:B:219:ASN:N	1:B:308:GLN:OE1	2.54	0.41
1:B:666:TYR:CD1	1:B:666:TYR:C	2.99	0.41
1:A:153:GLN:OE1	1:A:169:ASN:N	2.53	0.41
1:B:78:VAL:O	2:B:794:NAG:H81	2.19	0.41
1:B:375:ILE:HD13	1:B:387:PHE:HZ	1.86	0.41
1:A:50:LYS:O	1:A:51:ASN:HB2	2.20	0.41
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.55	0.41
1:A:580:GLY:O	1:A:583:SER:OG	2.30	0.41
1:A:761:GLN:CD	1:A:761:GLN:C	2.89	0.41
1:B:430:ASN:OD1	1:B:446:SER:OG	2.38	0.41
1:A:164:LEU:HB2	1:A:175:LYS:HB2	2.03	0.41
1:A:431:LEU:HD23	1:A:431:LEU:HA	1.89	0.41
1:B:614:SER:C	1:B:616:MET:H	2.27	0.41
1:B:675:THR:C	1:B:680:LEU:HB2	2.45	0.41
1:A:134:ILE:HD11	1:A:164:LEU:CD1	2.50	0.41
1:A:199:THR:OG1	1:A:204:GLU:HB2	2.21	0.41
1:A:384:ILE:HG23	1:A:407:ILE:HD11	2.03	0.41
1:A:562:ASN:O	1:A:565:THR:CB	2.67	0.41
1:A:712:HIS:O	1:A:713:PHE:C	2.62	0.41
1:A:728:VAL:O	1:B:750:HIS:HE1	2.04	0.41
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.51	0.41
1:B:621:ASN:N	1:B:621:ASN:ND2	2.69	0.41
1:B:643:GLY:O	1:B:644:SER:C	2.63	0.41
1:A:62:TRP:CG	1:A:462:SER:HA	2.56	0.41
1:A:305:TRP:CE3	1:A:311:ILE:HG12	2.55	0.41
1:B:742:ILE:O	1:B:742:ILE:CG2	2.67	0.41
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.89	0.40
1:B:103:ASN:O	1:B:104:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:LEU:HA	1:A:640:LEU:HD23	1.82	0.40
1:B:621:ASN:N	1:B:621:ASN:HD22	2.19	0.40
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.56	0.40
1:A:420:ASN:ND2	1:A:420:ASN:H	2.20	0.40
1:A:554:LYS:HB3	1:A:577:SER:HB3	2.02	0.40
1:B:64:SER:OG	1:B:65:ASP:N	2.54	0.40
1:A:50:LYS:HA	1:A:50:LYS:HD3	1.94	0.40
1:A:61:ARG:HB3	4:A:934:HOH:O	2.21	0.40
1:A:90:LEU:HD23	1:A:91:GLU:N	2.35	0.40
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.80	0.40
1:B:341:VAL:C	1:B:343:ARG:N	2.78	0.40
1:B:465:ALA:O	1:B:485:SER:OG	2.25	0.40
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/728 (100%)	665 (92%)	54 (7%)	7 (1%)	12	11
1	B	726/728 (100%)	665 (92%)	58 (8%)	3 (0%)	30	34
All	All	1452/1456 (100%)	1330 (92%)	112 (8%)	10 (1%)	18	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	488	ASP
1	B	111	GLY
1	B	242	SER
1	A	615	LYS

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Mol	Chain	Res	Type
1	A	423	LYS
1	A	614	SER
1	B	108	SER
1	A	714	GLN
1	A	742	ILE

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	653/653 (100%)	585 (90%)	68 (10%)	7	7
1	B	653/653 (100%)	582 (89%)	71 (11%)	6	6
All	All	1306/1306 (100%)	1167 (89%)	139 (11%)	6	6

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	42	THR
1	A	49	LEU
1	A	56	LYS
1	A	60	LEU
1	A	87	SER
1	A	88	VAL
1	A	91	GLU
1	A	107	ILE
1	A	144	THR
1	A	156	THR
1	A	158	SER
1	A	169	ASN
1	A	180	LEU
1	A	195	TYR
1	A	198	ILE
1	A	202	VAL
1	A	223	LEU

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Mol	Chain	Res	Type
1	A	246	LEU
1	A	273	THR
1	A	278	SER
1	A	279	VAL
1	A	294	LEU
1	A	300	LEU
1	A	301	CYS
1	A	312	SER
1	A	316	LEU
1	A	326	ASP
1	A	334	SER
1	A	341	VAL
1	A	343	ARG
1	A	350	THR
1	A	377	ASN
1	A	378	GLU
1	A	379	GLU
1	A	385	CYS
1	A	389	ILE
1	A	410	LEU
1	A	411	THR
1	A	418	ILE
1	A	420	ASN
1	A	431	LEU
1	A	435	GLN
1	A	448	GLU
1	A	452	GLU
1	A	471	ARG
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	502	LYS
1	A	513	LYS
1	A	514	LEU
1	A	517	ILE
1	A	529	ILE
1	A	540	TYR
1	A	543	LEU
1	A	544	LEU
1	A	566	TYR
1	A	594	ILE
1	A	621	ASN

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Mol	Chain	Res	Type
1	A	656	VAL
1	A	669	ARG
1	A	677	GLU
1	A	704	HIS
1	A	715	GLN
1	A	721	LYS
1	A	726	VAL
1	A	736	THR
1	B	40	ARG
1	B	41	LYS
1	B	42	THR
1	B	49	LEU
1	B	51	ASN
1	B	60	LEU
1	B	63	ILE
1	B	71	LYS
1	B	86	SER
1	B	87	SER
1	B	90	LEU
1	B	91	GLU
1	B	93	SER
1	B	94	THR
1	B	143	ILE
1	B	144	THR
1	B	180	LEU
1	B	202	VAL
1	B	214	LEU
1	B	223	LEU
1	B	236	ILE
1	B	242	SER
1	B	246	LEU
1	B	273	THR
1	B	279	VAL
1	B	285	ILE
1	B	295	ILE
1	B	300	LEU
1	B	311	ILE
1	B	314	GLN
1	B	319	ILE
1	B	332	GLU
1	B	365	THR
1	B	375	ILE

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Mol	Chain	Res	Type
1	B	377	ASN
1	B	389	ILE
1	B	392	LYS
1	B	397	ILE
1	B	405	ILE
1	B	420	ASN
1	B	435	GLN
1	B	452	GLU
1	B	471	ARG
1	B	472	CYS
1	B	479	LEU
1	B	480	TYR
1	B	486	VAL
1	B	500	LEU
1	B	507	VAL
1	B	514	LEU
1	B	517	ILE
1	B	521	GLU
1	B	543	LEU
1	B	546	VAL
1	B	552	SER
1	B	558	VAL
1	B	562	ASN
1	B	594	ILE
1	B	600	THR
1	B	619	VAL
1	B	620	ASP
1	B	621	ASN
1	B	626	ILE
1	B	677	GLU
1	B	680	LEU
1	B	684	ARG
1	B	714	GLN
1	B	715	GLN
1	B	726	VAL
1	B	731	GLN
1	B	759	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS

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Mol	Chain	Res	Type
1	A	123	GLN
1	A	247	GLN
1	A	263	ASN
1	A	298	HIS
1	A	363	HIS
1	A	377	ASN
1	A	388	GLN
1	A	420	ASN
1	A	455	GLN
1	A	483	HIS
1	A	508	GLN
1	A	533	HIS
1	A	586	GLN
1	A	592	HIS
1	A	612	GLN
1	A	621	ASN
1	A	679	ASN
1	A	715	GLN
1	A	748	HIS
1	A	750	HIS
1	B	66	HIS
1	B	100	HIS
1	B	126	HIS
1	B	150	ASN
1	B	286	GLN
1	B	298	HIS
1	B	344	GLN
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	430	ASN
1	B	435	GLN
1	B	483	HIS
1	B	487	ASN
1	B	562	ASN
1	B	586	GLN
1	B	621	ASN
1	B	679	ASN
1	B	715	GLN
1	B	750	HIS

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](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	794	1	14,14,15	1.00	1 (7%)	17,19,21	2.15	6 (35%)
2	NAG	B	796	1	14,14,15	0.90	1 (7%)	17,19,21	1.40	3 (17%)
2	NAG	B	793	1	14,14,15	0.67	0	17,19,21	1.27	2 (11%)
2	NAG	A	793	1	14,14,15	0.70	1 (7%)	17,19,21	2.29	6 (35%)
3	5AP	A	900	-	29,29,29	2.05	6 (20%)	37,41,41	2.29	13 (35%)
2	NAG	A	795	1	14,14,15	0.72	0	17,19,21	2.29	4 (23%)
3	5AP	B	1900	-	29,29,29	1.64	6 (20%)	37,41,41	1.89	11 (29%)
2	NAG	B	794	1	14,14,15	0.71	0	17,19,21	1.39	2 (11%)
2	NAG	A	796	1	14,14,15	0.74	0	17,19,21	1.97	5 (29%)
2	NAG	B	797	1	14,14,15	0.62	0	17,19,21	1.83	4 (23%)

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
2	NAG	A	794	1	-	0/6/23/26	0/1/1/1
2	NAG	B	796	1	-	1/6/23/26	0/1/1/1
2	NAG	B	793	1	-	5/6/23/26	0/1/1/1
2	NAG	A	793	1	-	5/6/23/26	0/1/1/1
3	5AP	A	900	-	-	2/12/14/14	0/3/3/3
2	NAG	A	795	1	-	5/6/23/26	0/1/1/1
3	5AP	B	1900	-	-	4/12/14/14	0/3/3/3
2	NAG	B	794	1	-	4/6/23/26	0/1/1/1
2	NAG	A	796	1	-	0/6/23/26	0/1/1/1
2	NAG	B	797	1	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	5AP	C11-C10	-7.98	1.41	1.49
3	B	1900	5AP	C10-N9	-3.88	1.28	1.34
3	B	1900	5AP	C19-C22	3.70	1.47	1.41
3	A	900	5AP	C10-C19	3.38	1.47	1.41
3	B	1900	5AP	C12-C11	-3.13	1.35	1.40
3	A	900	5AP	C19-C22	3.06	1.46	1.41
3	B	1900	5AP	C10-C19	2.83	1.46	1.41
3	B	1900	5AP	C8-C3	-2.59	1.35	1.39
3	B	1900	5AP	C22-N1	-2.52	1.31	1.35
3	A	900	5AP	C11-C17	-2.49	1.35	1.39
3	A	900	5AP	C16-C17	-2.43	1.34	1.38
2	B	796	NAG	C1-C2	2.39	1.55	1.52
3	A	900	5AP	C12-C11	-2.27	1.36	1.40
2	A	794	NAG	O5-C1	-2.03	1.40	1.43
2	A	793	NAG	O5-C1	-2.01	1.40	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	793	NAG	C4-C3-C2	-5.88	102.40	111.02
3	A	900	5AP	C22-N1-C2	5.68	124.22	117.36
3	A	900	5AP	C16-C17-C11	5.11	125.94	121.97
2	A	795	NAG	C4-C3-C2	-5.01	103.67	111.02
2	A	796	NAG	C2-N2-C7	-4.97	116.23	122.90
3	A	900	5AP	C17-C16-C14	-4.75	113.36	118.72
2	A	795	NAG	C2-N2-C7	-4.67	116.64	122.90
2	A	795	NAG	C1-O5-C5	4.60	118.35	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	5AP	N23-C22-N1	4.59	123.22	117.03
2	A	794	NAG	O5-C1-C2	-4.56	104.23	111.29
3	A	900	5AP	C11-C17-CL2	-4.45	114.57	120.67
2	A	794	NAG	C2-N2-C7	4.35	128.73	122.90
3	B	1900	5AP	C12-C13-C14	4.26	123.53	119.24
2	B	797	NAG	C2-N2-C7	-4.11	117.40	122.90
2	A	793	NAG	C2-N2-C7	4.05	128.33	122.90
3	B	1900	5AP	C16-C17-C11	3.80	124.92	121.97
2	A	793	NAG	O3-C3-C2	3.71	117.10	109.40
3	B	1900	5AP	C17-C16-C14	-3.62	114.63	118.72
2	B	794	NAG	C4-C3-C2	-3.56	105.81	111.02
2	A	795	NAG	C1-C2-N2	3.34	115.69	110.43
3	A	900	5AP	C11-C10-N9	3.27	119.57	114.90
2	B	797	NAG	C3-C4-C5	-3.20	104.44	110.23
2	A	796	NAG	C3-C4-C5	-3.18	104.46	110.23
2	A	796	NAG	O4-C4-C5	3.01	116.74	109.32
2	A	796	NAG	O5-C1-C2	-2.95	106.72	111.29
3	B	1900	5AP	C10-N9-C2	2.93	121.64	117.36
3	A	900	5AP	C19-C22-N1	-2.91	116.04	121.33
3	B	1900	5AP	C8-C3-C4	2.88	122.57	118.35
3	B	1900	5AP	C11-C10-N9	2.85	118.98	114.90
3	B	1900	5AP	C19-C10-N9	-2.79	118.38	122.75
2	B	796	NAG	C8-C7-N2	2.76	120.70	116.12
3	B	1900	5AP	N23-C22-N1	2.74	120.73	117.03
2	A	793	NAG	O4-C4-C5	2.74	116.07	109.32
2	B	794	NAG	O5-C5-C6	2.70	112.91	107.66
2	B	793	NAG	C4-C3-C2	-2.66	107.12	111.02
2	B	796	NAG	O7-C7-C8	-2.64	117.36	122.05
3	A	900	5AP	C13-C12-C11	-2.63	115.80	120.33
2	B	797	NAG	O5-C5-C6	2.62	112.77	107.66
2	A	794	NAG	C4-C3-C2	-2.58	107.24	111.02
2	B	797	NAG	O5-C5-C4	-2.54	104.65	110.83
2	A	794	NAG	O7-C7-N2	2.53	126.46	121.98
2	A	794	NAG	C6-C5-C4	-2.45	106.99	113.02
3	B	1900	5AP	C13-C12-C11	-2.44	116.12	120.33
2	A	796	NAG	C4-C3-C2	-2.36	107.56	111.02
2	B	793	NAG	O5-C1-C2	-2.34	107.67	111.29
3	A	900	5AP	C29-O26-C7	-2.32	112.52	117.50
2	A	794	NAG	C8-C7-N2	-2.30	112.31	116.12
2	A	793	NAG	C3-C4-C5	-2.26	106.13	110.23
3	B	1900	5AP	C16-C17-CL2	-2.23	114.80	118.45
3	A	900	5AP	C12-C11-C17	2.19	120.07	117.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1900	5AP	C22-N1-C2	2.14	119.94	117.36
2	B	796	NAG	C6-C5-C4	-2.11	107.83	113.02
3	A	900	5AP	C10-N9-C2	2.08	120.40	117.36
2	A	793	NAG	C8-C7-N2	2.06	119.54	116.12
3	A	900	5AP	C4-C3-C2	2.04	123.11	120.03
3	A	900	5AP	C3-C2-N1	2.01	120.72	117.40

There are no chirality outliers.

All (28) torsion outliers are listed below:

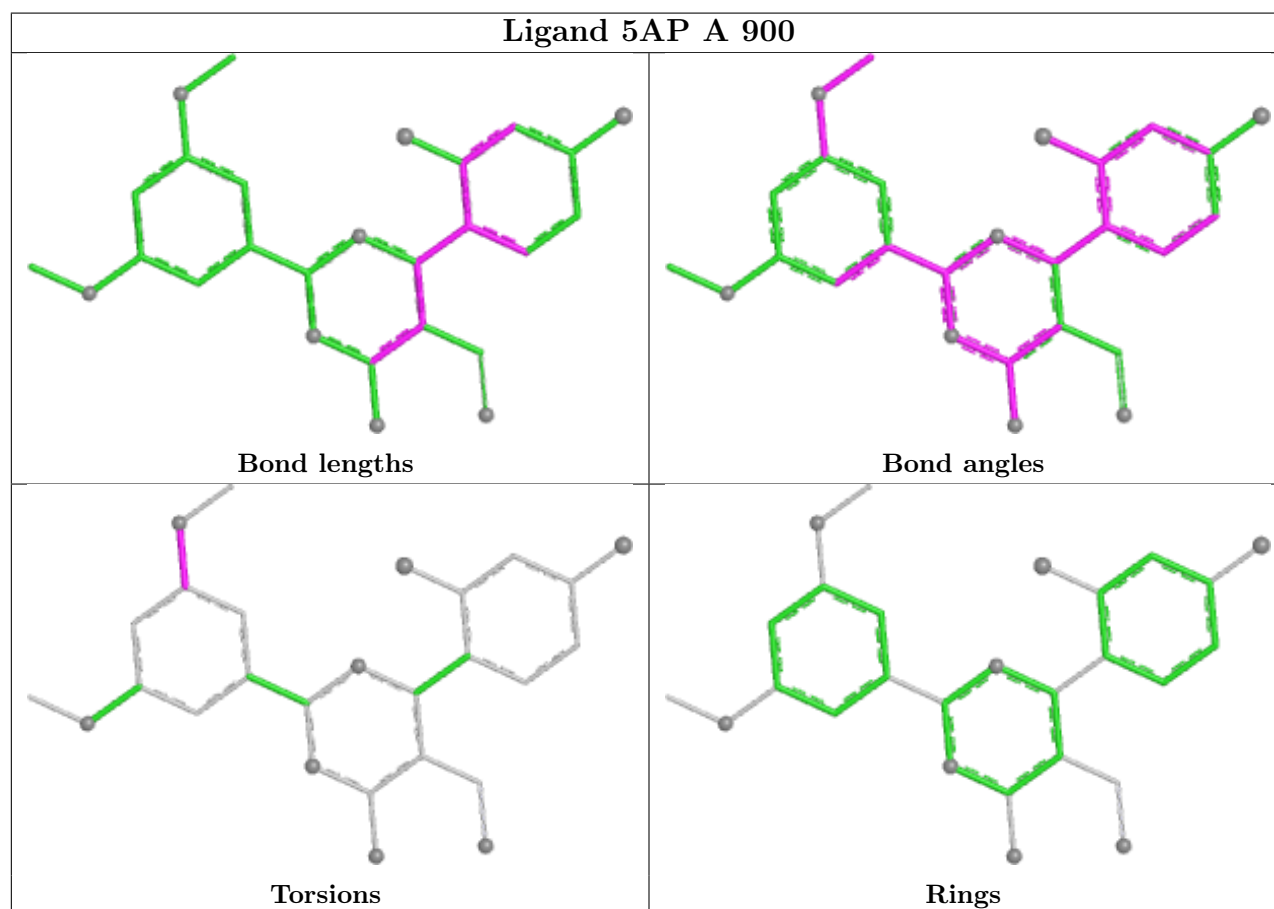
Mol	Chain	Res	Type	Atoms
2	A	793	NAG	C3-C2-N2-C7
2	A	793	NAG	C8-C7-N2-C2
2	A	793	NAG	O7-C7-N2-C2
2	B	793	NAG	C1-C2-N2-C7
2	B	793	NAG	C8-C7-N2-C2
2	B	793	NAG	O7-C7-N2-C2
3	A	900	5AP	C6-C7-O26-C29
3	A	900	5AP	C8-C7-O26-C29
3	B	1900	5AP	C4-C5-O25-C28
3	B	1900	5AP	C6-C5-O25-C28
3	B	1900	5AP	C6-C7-O26-C29
3	B	1900	5AP	C8-C7-O26-C29
2	A	795	NAG	C8-C7-N2-C2
2	A	793	NAG	O5-C5-C6-O6
2	A	795	NAG	O5-C5-C6-O6
2	B	797	NAG	C4-C5-C6-O6
2	A	795	NAG	O7-C7-N2-C2
2	A	793	NAG	C4-C5-C6-O6
2	B	793	NAG	O5-C5-C6-O6
2	A	795	NAG	C4-C5-C6-O6
2	B	794	NAG	C4-C5-C6-O6
2	B	797	NAG	O5-C5-C6-O6
2	B	793	NAG	C4-C5-C6-O6
2	B	794	NAG	O5-C5-C6-O6
2	B	796	NAG	O5-C5-C6-O6
2	A	795	NAG	C1-C2-N2-C7
2	B	794	NAG	C8-C7-N2-C2
2	B	794	NAG	O7-C7-N2-C2

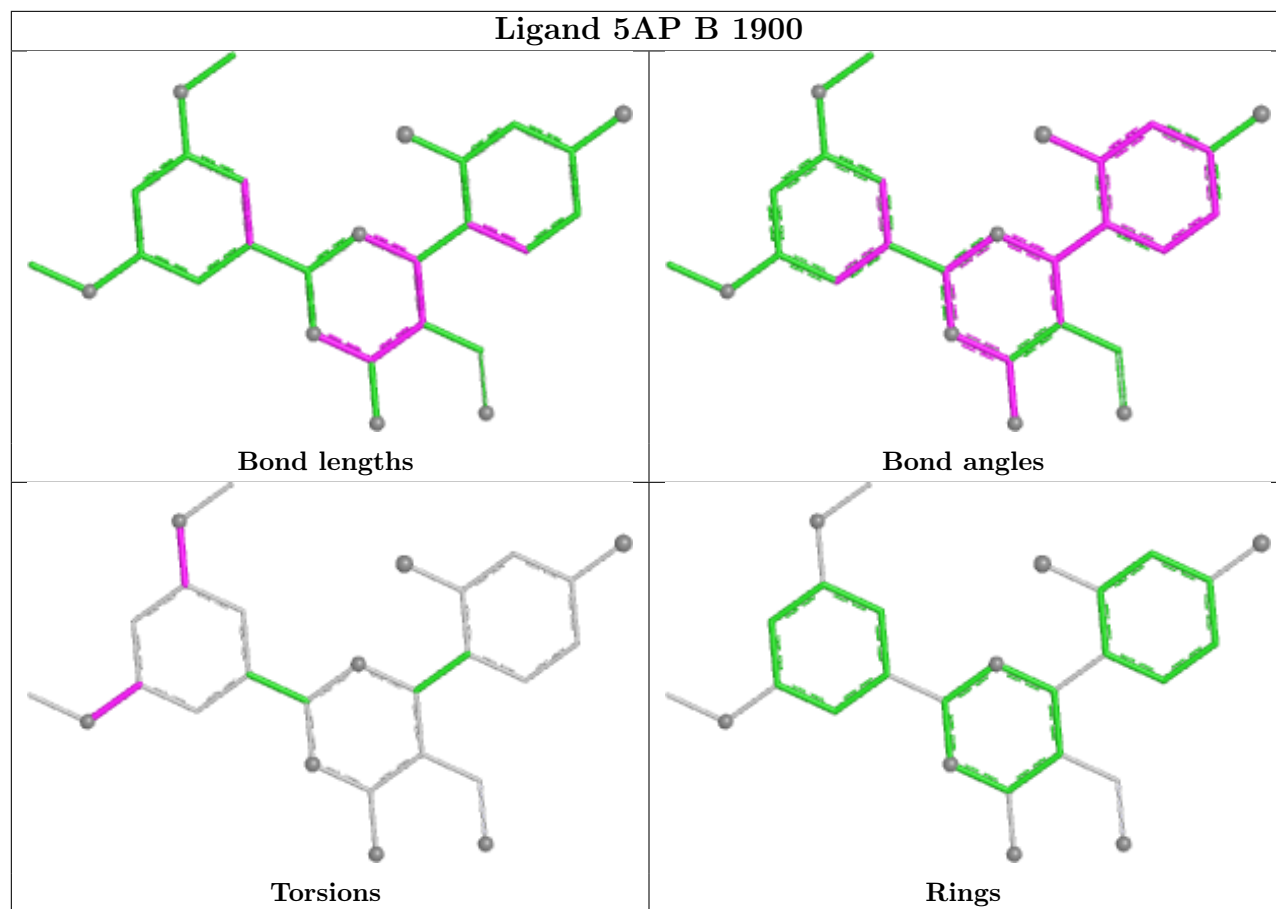
There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	793	NAG	5	0
2	A	793	NAG	1	0
3	A	900	5AP	5	0
2	A	795	NAG	1	0
2	B	794	NAG	2	0
2	B	797	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.