



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:18 AM UTC

PDB ID : 2E4Y / pdb_00002e4y
Title : Crystal structure of the extracellular region of the group II metabotropic glutamate receptor complexed with 2R,4R-APDC
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.
Deposited on : 2006-12-17
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

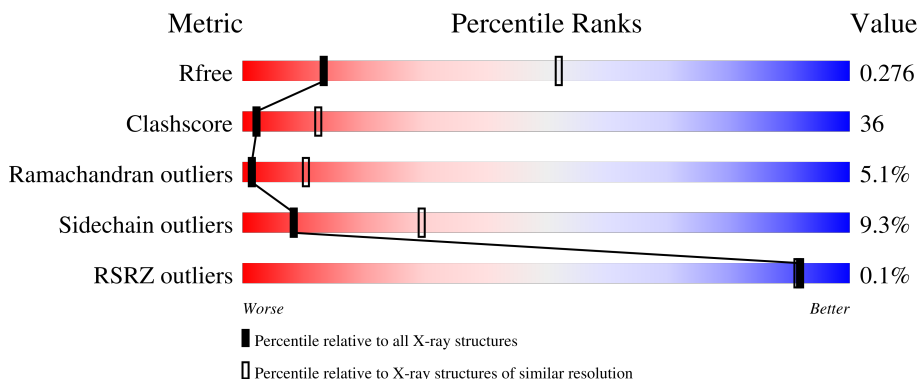
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	
1	B	555	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7823 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.

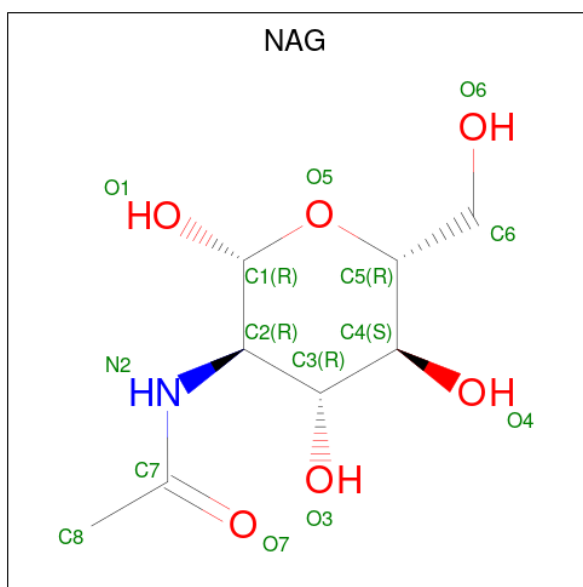
- Molecule 1 is a protein called Metabotropic glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	23	0	0
			4118	2606	709	776	27			
1	B	459	Total	C	N	O	S	23	0	0
			3667	2325	642	685	15			

There are 12 discrepancies between the modelled and reference sequences:

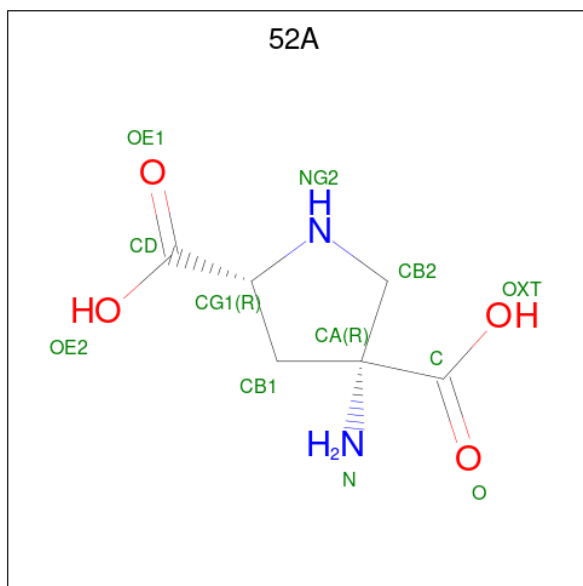
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	engineered mutation	UNP P31422
A	439	GLN	ASN	engineered mutation	UNP P31422
A	576	LEU	-	cloning artifact	UNP P31422
A	577	VAL	-	cloning artifact	UNP P31422
A	578	PRO	-	cloning artifact	UNP P31422
A	579	ARG	-	cloning artifact	UNP P31422
B	414	GLN	ASN	engineered mutation	UNP P31422
B	439	GLN	ASN	engineered mutation	UNP P31422
B	576	LEU	-	cloning artifact	UNP P31422
B	577	VAL	-	cloning artifact	UNP P31422
B	578	PRO	-	cloning artifact	UNP P31422
B	579	ARG	-	cloning artifact	UNP P31422

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is (2R,4R)-4-aminopyrrolidine-2,4-dicarboxylic acid (CCD ID: 52A) (formula: $C_6H_{10}N_2O_4$).

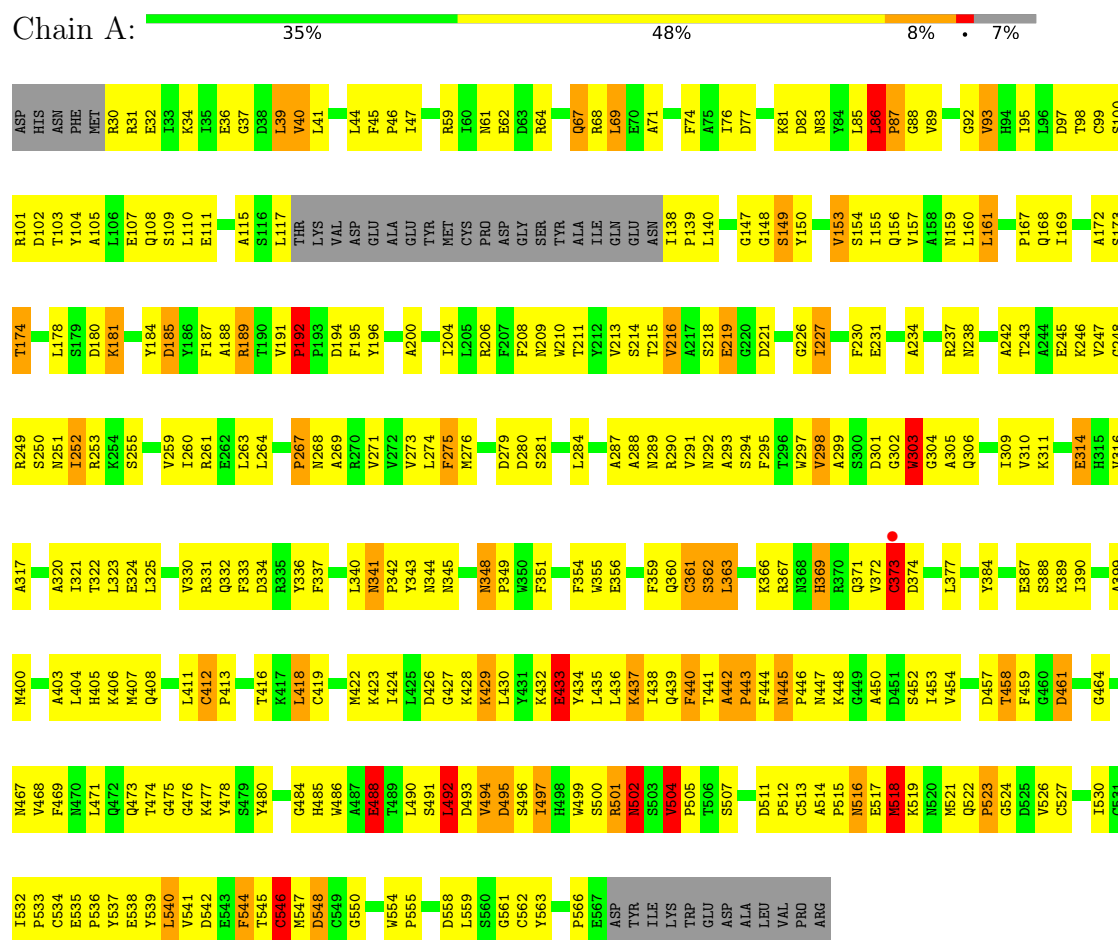


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	2	4		
3	B	1	Total	C	N	O	0	0
			12	6	2	4		

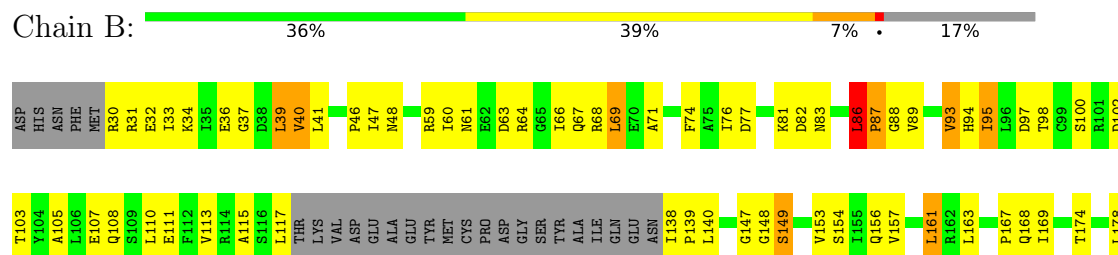
3 Residue-property plots

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: Metabotropic glutamate receptor 3



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PHE	THR	CYS	MET	ASP	CYS	GLY	PRO	GLY	GLN	TRP	PRO	THR	ALA	ASP	LEU	SER	GLY	CYS	TYR	ASN	LEU	PRO	PRO	GLU	ASP	TYR	ILE	LYS	TRP	GLU	ALA	LEU	VAL	PRO	ARG																		
Y480	G484	H485	W486	A487	E488	T489	L490	S491	L492	D493	W494	D495	S496	W499	S500	R501	N502	S503	V504	P505	G508	CYS	SER	ASP	PRO	LYS	TRP	GLU	ASP	ALA	LEU	VAL	PRO	ARG																			
T416	K417	L418	C419	M422	K423	I424	L425	D426	G427	K428	K429	L430	Y431	K432	Y434	L435	L436	K437	I438	Q439	F440	T441	A442	P443	F444	N445	P446	N447	K448	G449	A450	S451	S452	I453	V454	K455	F456	D457	T458	F459	G460	D461	G464	N467	V468	F469	N470	L471	Q472	Q473	G476	K477	S479
T416	K417	L418	C419	M422	K423	I424	L425	D426	G427	K428	K429	L430	Y431	K432	Y434	L435	L436	K437	I438	Q439	F440	T441	A442	P443	F444	N445	P446	N447	K448	G449	A450	S451	S452	I453	V454	K455	F456	D457	T458	F459	G460	D461	G464	N467	V468	F469	N470	L471	Q472	Q473	G476	K477	S479
Q332	F333	D334	R335	Y336	F337	L340	N341	P342	Y343	N344	N345	N348	P349	W350	W355	E356	F359	Q360	C361	S362	L363	K366	R367	N368	H369	R370	Q371	V372	C373	D374	K375	H376	L377	E387	S388	K389	I390	K391	F392	A399	M400	A403	L404	H405	Q408	L411	C412	P413					
Q332	F333	D334	R335	Y336	F337	L340	N341	P342	Y343	N344	N345	N348	P349	W350	W355	E356	F359	Q360	C361	S362	L363	K366	R367	N368	H369	R370	Q371	V372	C373	D374	K375	H376	L377	E387	S388	K389	I390	K391	F392	A399	M400	A403	L404	H405	Q408	L411	C412	P413					
L260	R261	E262	L263	L264	P267	N268	V271	V272	V273	L274	F275	M276	D279	D280	S281	L284	A287	A288	N289	R290	V291	N292	A293	W297	V298	A299	S300	D301	G302	K303	G304	A305	Q306	V310	K311	E314	H315	V316	A317	A320	I321	T322	L323	E324	L325	H328	P329	V330	R331				
L260	R261	E262	L263	L264	P267	N268	V271	V272	V273	L274	F275	M276	D279	D280	S281	L284	A287	A288	N289	R290	V291	N292	A293	W297	V298	A299	S300	D301	G302	K303	G304	A305	Q306	V310	K311	E314	H315	V316	A317	A320	I321	T322	L323	E324	L325	H328	P329	V330	R331				
S179	D180	K181	Y184	D185	Y186	F187	A188	R189	T190	V191	P192	P193	D194	F195	Y196	A200	I204	L205	F208	N209	W210	V213	S214	T215	V216	A217	S218	E219	G220	D221	Y222	I227	F230	E231	A242	T243	A244	E245	K246	V247	G248	N251	I252	R253	K254	S255	Y256	D257	S258	V259			
S179	D180	K181	Y184	D185	Y186	F187	A188	R189	T190	V191	P192	P193	D194	F195	Y196	A200	I204	L205	F208	N209	W210	V213	S214	T215	V216	A217	S218	E219	G220	D221	Y222	I227	F230	E231	A242	T243	A244	E245	K246	V247	G248	N251	I252	R253	K254	S255	Y256	D257	S258	V259			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.39Å 91.80Å 112.97Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	12.00 – 3.40 12.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.40) 97.3 (12.00-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.284 0.220 , 0.276	Depositor DCC
R_{free} test set	1632 reflections (6.85%)	wwPDB-VP
Wilson B-factor (Å ²)	122.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 101.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7823	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: NAG, 52A

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	0.63	0/4212	1.11	41/5704 (0.7%)
1	B	0.45	0/3745	1.02	26/5062 (0.5%)
All	All	0.56	0/7957	1.07	67/10766 (0.6%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	GLU	N-CA-C	-9.62	99.93	114.16
1	A	442	ALA	CA-C-N	8.31	130.22	119.84
1	A	442	ALA	C-N-CA	8.31	130.22	119.84
1	A	373	CYS	N-CA-C	8.25	122.35	108.90
1	B	412	CYS	CA-C-N	8.06	128.51	119.32
1	B	412	CYS	C-N-CA	8.06	128.51	119.32
1	A	147	GLY	N-CA-C	7.82	121.97	110.63
1	A	448	LYS	N-CA-C	-7.76	105.77	114.62
1	B	442	ALA	CA-C-N	7.74	129.52	119.84
1	B	442	ALA	C-N-CA	7.74	129.52	119.84
1	B	373	CYS	N-CA-C	7.40	120.96	108.90
1	A	219	GLU	N-CA-C	-7.24	99.77	110.48
1	A	303	TRP	N-CA-C	-7.22	101.64	112.04
1	B	448	LYS	N-CA-C	-7.13	106.49	114.62
1	A	412	CYS	CA-C-N	6.94	127.24	119.32
1	A	412	CYS	C-N-CA	6.94	127.24	119.32
1	B	61	ASN	N-CA-C	-6.94	97.91	108.67
1	B	147	GLY	N-CA-C	6.72	120.38	110.63
1	A	501	ARG	N-CA-C	-6.55	104.58	112.58
1	B	219	GLU	N-CA-C	-6.54	101.28	110.50
1	B	501	ARG	N-CA-C	-6.47	104.69	112.58
1	B	412	CYS	N-CA-C	6.25	119.38	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	TRP	N-CA-C	-6.21	103.09	112.04
1	B	369	HIS	N-CA-C	6.09	116.33	108.34
1	A	504	VAL	CA-C-N	6.02	127.37	119.84
1	A	504	VAL	C-N-CA	6.02	127.37	119.84
1	A	61	ASN	N-CA-C	-5.97	98.80	108.41
1	A	369	HIS	N-CA-C	5.83	115.98	108.34
1	B	419	CYS	CA-CB-SG	-5.82	101.01	114.40
1	A	419	CYS	CA-CB-SG	-5.72	101.25	114.40
1	A	546	CYS	CA-CB-SG	-5.70	101.30	114.40
1	A	62	GLU	N-CA-C	5.62	117.27	111.03
1	A	192	PRO	CA-C-N	5.62	125.57	119.78
1	A	192	PRO	C-N-CA	5.62	125.57	119.78
1	A	388	SER	N-CA-C	5.52	118.01	111.33
1	A	497	ILE	N-CA-C	5.51	116.18	109.30
1	A	518	MET	N-CA-C	5.47	122.45	110.80
1	B	40	VAL	N-CA-C	5.47	117.27	108.85
1	A	458	THR	N-CA-C	-5.45	106.71	113.19
1	A	348	ASN	CA-C-N	5.44	125.78	119.47
1	A	348	ASN	C-N-CA	5.44	125.78	119.47
1	B	257	ASP	N-CA-C	-5.43	105.36	111.28
1	B	433	GLU	N-CA-C	-5.41	99.28	110.80
1	B	416	THR	N-CA-C	-5.40	106.61	114.12
1	B	388	SER	N-CA-C	5.34	117.10	111.28
1	A	406	LYS	N-CA-C	-5.31	105.41	111.14
1	A	40	VAL	N-CA-C	5.30	117.01	108.85
1	B	185	ASP	N-CA-C	5.27	119.19	112.87
1	A	86	LEU	CA-C-N	5.20	126.34	119.84
1	A	86	LEU	C-N-CA	5.20	126.34	119.84
1	A	550	GLY	CA-C-N	5.17	125.98	120.13
1	A	550	GLY	C-N-CA	5.17	125.98	120.13
1	A	263	LEU	N-CA-C	-5.17	106.48	112.89
1	A	500	SER	N-CA-C	-5.14	102.67	110.28
1	B	63	ASP	N-CA-C	5.13	118.00	111.69
1	B	86	LEU	CA-C-N	5.12	126.24	119.84
1	B	86	LEU	C-N-CA	5.12	126.24	119.84
1	B	66	ILE	N-CA-C	5.11	116.45	110.62
1	A	412	CYS	N-CA-C	5.11	119.03	108.71
1	A	488	GLU	N-CA-C	-5.09	99.96	110.80
1	A	416	THR	N-CA-C	-5.08	107.11	113.72
1	A	384	TYR	N-CA-C	5.08	117.62	108.48
1	B	263	LEU	N-CA-C	-5.08	106.59	112.89
1	A	191	VAL	CA-C-N	5.06	125.59	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	VAL	C-N-CA	5.06	125.59	120.38
1	A	185	ASP	N-CA-C	5.04	118.92	112.87
1	B	496	SER	N-CA-C	-5.04	107.68	113.88

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	4118	0	3994	322	0
1	B	3667	0	3605	235	0
2	A	14	0	13	0	0
3	A	12	0	8	2	0
3	B	12	0	8	1	0
All	All	7823	0	7628	553	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 36.

All (553) 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:437:LYS:HE3	1:B:437:LYS:HA	1.40	1.02
1:B:181:LYS:HE2	1:B:459:PHE:O	1.64	0.98
1:A:437:LYS:HE3	1:A:437:LYS:HA	1.44	0.97
1:A:519:LYS:HD2	1:A:546:CYS:HB2	1.45	0.96
1:A:181:LYS:HE2	1:A:459:PHE:O	1.67	0.95
1:B:274:LEU:HD22	1:B:276:MET:HE2	1.50	0.94
1:A:514:ALA:HB3	1:A:518:MET:HG3	1.47	0.94
1:B:39:LEU:HD23	1:B:404:LEU:HD13	1.49	0.94
1:A:493:ASP:OD2	1:A:496:SER:HB3	1.69	0.93
1:A:39:LEU:HD23	1:A:404:LEU:HD13	1.51	0.93
1:A:538:GLU:HB3	1:A:548:ASP:HA	1.51	0.92
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:HD22	1:A:343:TYR:H	1.16	0.90
1:B:400:MET:HE3	1:B:400:MET:HA	1.53	0.90
1:A:274:LEU:HD22	1:A:276:MET:HE2	1.53	0.89
1:A:442:ALA:O	1:A:444:PHE:N	2.08	0.87
1:A:213:VAL:HG12	1:A:271:VAL:HB	1.57	0.86
1:B:299:ALA:HB3	1:B:322:THR:HG22	1.56	0.86
1:B:341:ASN:HD22	1:B:343:TYR:H	1.17	0.85
1:B:216:VAL:HG13	1:B:274:LEU:HD23	1.59	0.85
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.59	0.84
1:B:252:ILE:HG22	1:B:253:ARG:H	1.42	0.84
1:B:213:VAL:HG12	1:B:271:VAL:HB	1.61	0.82
1:B:493:ASP:OD2	1:B:496:SER:HB3	1.80	0.82
1:A:494:VAL:C	1:A:496:SER:H	1.87	0.81
1:A:252:ILE:HG22	1:A:253:ARG:H	1.43	0.81
1:A:366:LYS:HG2	1:A:367:ARG:H	1.45	0.80
1:A:216:VAL:HG13	1:A:274:LEU:HD23	1.65	0.79
1:B:442:ALA:O	1:B:444:PHE:N	2.16	0.79
1:A:442:ALA:C	1:A:444:PHE:H	1.90	0.78
1:A:148:GLY:HA3	1:A:154:SER:OG	1.85	0.77
1:A:310:VAL:HG13	1:A:317:ALA:HB3	1.66	0.77
1:B:366:LYS:HG2	1:B:367:ARG:H	1.46	0.77
1:B:287:ALA:HA	1:B:290:ARG:NH1	1.99	0.76
1:A:515:PRO:HG2	1:A:516:ASN:H	1.49	0.76
1:B:216:VAL:HA	1:B:245:GLU:O	1.86	0.75
1:B:441:THR:HG23	1:B:452:SER:O	1.86	0.75
1:B:362:SER:O	1:B:363:LEU:HD22	1.87	0.74
1:A:310:VAL:HG12	1:A:314:GLU:HA	1.70	0.74
1:B:310:VAL:HG12	1:B:314:GLU:HA	1.70	0.74
1:A:540:LEU:N	1:A:540:LEU:HD12	2.02	0.73
1:A:287:ALA:HA	1:A:290:ARG:NH1	2.04	0.73
1:A:400:MET:HE3	1:A:400:MET:HA	1.69	0.72
1:B:148:GLY:HA3	1:B:154:SER:OG	1.90	0.72
1:A:216:VAL:HA	1:A:245:GLU:O	1.90	0.72
1:B:311:LYS:HA	1:B:314:GLU:OE2	1.89	0.71
1:A:299:ALA:HB3	1:A:322:THR:HG22	1.72	0.71
1:A:372:VAL:HG22	1:A:373:CYS:H	1.56	0.71
1:A:490:LEU:HG	1:A:492:LEU:HD22	1.72	0.71
1:B:408:GLN:HA	1:B:422:MET:HE2	1.71	0.70
1:A:538:GLU:CB	1:A:548:ASP:HA	2.21	0.70
1:A:74:PHE:HB2	1:A:336:TYR:CE2	2.26	0.70
1:A:362:SER:O	1:A:363:LEU:HD22	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ALA:C	1:B:444:PHE:H	1.96	0.70
1:B:74:PHE:HB2	1:B:336:TYR:CE2	2.27	0.70
1:A:535:GLU:OE2	1:A:535:GLU:HA	1.91	0.69
1:A:187:PHE:HE2	1:A:189:ARG:HD2	1.57	0.69
1:A:438:ILE:HG23	1:A:453:ILE:HD12	1.75	0.68
1:A:521:MET:HB2	1:A:530:ILE:HG13	1.75	0.68
1:A:441:THR:HG23	1:A:452:SER:O	1.92	0.68
1:B:255:SER:O	1:B:259:VAL:HG23	1.93	0.68
1:B:310:VAL:HG13	1:B:317:ALA:HB3	1.74	0.68
1:A:213:VAL:CG1	1:A:271:VAL:HB	2.24	0.67
1:B:494:VAL:C	1:B:496:SER:H	1.98	0.67
1:A:311:LYS:HA	1:A:314:GLU:OE2	1.94	0.67
1:A:342:PRO:HD3	1:A:355:TRP:CD2	2.31	0.66
1:A:518:MET:HA	1:A:532:ILE:O	1.96	0.66
1:A:408:GLN:HA	1:A:422:MET:HE2	1.76	0.66
1:A:342:PRO:HD3	1:A:355:TRP:CE3	2.31	0.66
1:B:115:ALA:HB1	1:B:140:LEU:O	1.96	0.66
1:B:342:PRO:HD3	1:B:355:TRP:CD2	2.31	0.66
1:A:115:ALA:HB1	1:A:140:LEU:O	1.95	0.65
1:A:255:SER:O	1:A:259:VAL:HG23	1.96	0.65
1:B:252:ILE:HD12	1:B:252:ILE:N	2.12	0.65
1:A:216:VAL:HG13	1:A:274:LEU:CD2	2.26	0.65
1:A:87:PRO:HG2	1:A:88:GLY:H	1.61	0.65
1:B:98:THR:HB	1:B:105:ALA:HB2	1.79	0.65
1:A:341:ASN:ND2	1:A:343:TYR:H	1.93	0.65
1:A:298:VAL:HA	1:A:321:ILE:O	1.98	0.64
1:B:372:VAL:HG22	1:B:373:CYS:H	1.63	0.64
1:A:274:LEU:HD11	1:A:297:TRP:CE3	2.32	0.64
1:A:518:MET:HA	1:A:533:PRO:HA	1.80	0.63
1:B:366:LYS:HE2	1:B:369:HIS:HD2	1.64	0.63
1:A:264:LEU:O	1:A:267:PRO:HD3	1.99	0.63
1:B:297:TRP:HB2	1:B:320:ALA:HB1	1.81	0.63
1:A:64:ARG:HD3	3:A:1001:52A:OE1	1.99	0.62
1:B:264:LEU:O	1:B:267:PRO:HD3	1.98	0.62
1:B:260:ILE:CD1	1:B:288:ALA:HB2	2.29	0.62
1:A:490:LEU:HD12	1:A:491:SER:H	1.65	0.62
1:B:41:LEU:HD22	1:B:400:MET:HG2	1.82	0.62
1:A:366:LYS:HE2	1:A:369:HIS:HD2	1.63	0.62
1:B:86:LEU:CD1	1:B:405:HIS:HA	2.30	0.61
1:B:323:LEU:HD23	1:B:468:VAL:HA	1.82	0.61
1:B:169:ILE:HA	1:B:188:ALA:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HD12	1:A:252:ILE:N	2.16	0.61
1:A:64:ARG:O	1:A:68:ARG:HD2	2.00	0.61
1:B:216:VAL:HB	1:B:245:GLU:HB2	1.83	0.61
1:A:539:TYR:C	1:A:540:LEU:HD12	2.25	0.60
1:B:32:GLU:OE2	1:B:34:LYS:HE3	2.01	0.60
1:B:473:GLN:NE2	1:B:476:GLY:H	1.99	0.60
1:B:64:ARG:HD3	3:B:2001:52A:OE1	2.01	0.60
1:A:260:ILE:CD1	1:A:288:ALA:HB2	2.30	0.60
1:A:340:LEU:HD22	1:A:345:ASN:ND2	2.16	0.60
1:A:467:ASN:HB3	1:A:469:PHE:HE1	1.66	0.60
1:A:246:LYS:O	1:A:246:LYS:HG3	2.00	0.60
1:B:340:LEU:HD22	1:B:345:ASN:ND2	2.17	0.60
1:B:490:LEU:HD12	1:B:491:SER:H	1.66	0.60
1:A:227:ILE:HD13	1:A:230:PHE:HB3	1.84	0.60
1:B:87:PRO:HG2	1:B:88:GLY:H	1.65	0.60
1:A:490:LEU:CD1	1:A:491:SER:H	2.15	0.60
1:B:298:VAL:HA	1:B:321:ILE:O	2.01	0.60
1:B:342:PRO:HD3	1:B:355:TRP:CE3	2.37	0.59
1:A:178:LEU:HA	1:A:184:TYR:CD1	2.38	0.59
1:A:40:VAL:HG13	1:A:92:GLY:C	2.28	0.59
1:A:110:LEU:HD21	1:B:113:VAL:HG23	1.83	0.59
1:B:341:ASN:ND2	1:B:343:TYR:H	1.96	0.59
1:A:424:ILE:O	1:A:424:ILE:HG13	2.01	0.59
1:A:169:ILE:HA	1:A:188:ALA:O	2.02	0.58
1:B:82:ASP:OD2	1:B:83:ASN:N	2.36	0.58
1:A:138:ILE:N	1:A:139:PRO:HD2	2.18	0.58
1:B:298:VAL:HG12	1:B:298:VAL:O	2.04	0.58
1:A:535:GLU:O	1:A:537:TYR:N	2.36	0.58
1:A:341:ASN:HA	1:A:355:TRP:CZ3	2.38	0.58
1:B:64:ARG:O	1:B:68:ARG:HD2	2.02	0.58
1:A:323:LEU:HD23	1:A:468:VAL:HA	1.85	0.58
1:A:493:ASP:O	1:A:495:ASP:N	2.36	0.58
1:A:341:ASN:HD22	1:A:343:TYR:N	1.94	0.58
1:A:490:LEU:CG	1:A:491:SER:H	2.17	0.58
1:B:178:LEU:HA	1:B:184:TYR:CD1	2.38	0.58
1:A:39:LEU:HD22	1:A:89:VAL:HG11	1.85	0.58
1:A:41:LEU:HD22	1:A:400:MET:HG2	1.85	0.58
1:A:517:GLU:HG2	1:A:533:PRO:HB2	1.86	0.58
1:B:430:LEU:O	1:B:434:TYR:HB2	2.04	0.58
1:A:491:SER:C	1:A:492:LEU:HD22	2.29	0.57
1:B:216:VAL:HG13	1:B:274:LEU:CD2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ILE:HG23	1:B:453:ILE:HD12	1.85	0.57
1:B:411:LEU:HD12	1:B:422:MET:HG2	1.86	0.57
1:B:362:SER:HA	1:B:366:LYS:HD2	1.87	0.57
1:A:86:LEU:CD1	1:A:405:HIS:HA	2.35	0.57
1:A:108:GLN:O	1:A:111:GLU:HB2	2.05	0.57
1:A:168:GLN:C	1:A:169:ILE:HG13	2.29	0.57
1:B:276:MET:HE3	1:B:281:SER:HA	1.86	0.57
1:B:493:ASP:O	1:B:495:ASP:N	2.37	0.57
1:A:98:THR:HB	1:A:105:ALA:HB2	1.86	0.57
1:A:539:TYR:CD1	1:A:540:LEU:N	2.73	0.57
1:A:555:PRO:HA	1:A:561:GLY:O	2.05	0.57
1:B:227:ILE:HD13	1:B:230:PHE:HB3	1.87	0.57
1:B:138:ILE:N	1:B:139:PRO:HD2	2.20	0.56
1:B:213:VAL:CG1	1:B:271:VAL:HB	2.32	0.56
1:B:252:ILE:HD12	1:B:252:ILE:H	1.70	0.56
1:A:435:LEU:C	1:A:437:LYS:H	2.13	0.56
1:A:519:LYS:HE2	1:A:521:MET:SD	2.45	0.56
1:A:490:LEU:HG	1:A:491:SER:N	2.20	0.56
1:B:314:GLU:H	1:B:314:GLU:CD	2.13	0.56
1:B:341:ASN:HD22	1:B:343:TYR:N	1.96	0.56
1:A:298:VAL:HG12	1:A:298:VAL:O	2.06	0.56
1:A:473:GLN:NE2	1:A:476:GLY:H	2.03	0.56
1:A:453:ILE:O	1:A:453:ILE:HG13	2.05	0.55
1:B:411:LEU:C	1:B:412:CYS:SG	2.89	0.55
1:B:435:LEU:C	1:B:437:LYS:H	2.14	0.55
1:B:279:ASP:OD1	1:B:280:ASP:N	2.39	0.55
1:B:437:LYS:HE2	1:B:438:ILE:H	1.71	0.55
1:B:442:ALA:C	1:B:444:PHE:N	2.64	0.55
1:A:216:VAL:HB	1:A:245:GLU:HB2	1.87	0.55
1:B:424:ILE:O	1:B:424:ILE:HG13	2.06	0.55
1:A:411:LEU:C	1:A:412:CYS:SG	2.90	0.55
1:B:260:ILE:HD12	1:B:288:ALA:HB2	1.89	0.55
1:A:341:ASN:HD22	1:A:341:ASN:C	2.14	0.54
1:B:218:SER:N	1:B:276:MET:HG2	2.22	0.54
1:A:540:LEU:HG	1:A:546:CYS:SG	2.47	0.54
1:A:271:VAL:HG23	1:A:507:SER:HB2	1.89	0.54
1:B:362:SER:C	1:B:363:LEU:HD22	2.32	0.54
1:A:260:ILE:HD12	1:A:288:ALA:HB2	1.88	0.54
1:A:430:LEU:O	1:A:434:TYR:HB2	2.07	0.54
1:B:31:ARG:HD2	1:B:349:PRO:HB2	1.88	0.54
1:B:437:LYS:HA	1:B:437:LYS:CE	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:O	1:A:157:VAL:HG23	2.07	0.54
1:B:437:LYS:HE3	1:B:437:LYS:CA	2.27	0.54
1:A:156:GLN:OE1	1:A:156:GLN:HA	2.06	0.54
1:A:192:PRO:HG3	1:A:464:GLY:HA2	1.90	0.54
1:A:211:THR:HG22	1:A:527:CYS:SG	2.48	0.54
1:B:214:SER:OG	1:B:243:THR:HG22	2.07	0.54
1:B:366:LYS:HE2	1:B:369:HIS:CD2	2.43	0.53
1:A:297:TRP:HB2	1:A:320:ALA:HB1	1.90	0.53
1:A:314:GLU:CD	1:A:314:GLU:H	2.15	0.53
1:A:341:ASN:ND2	1:A:341:ASN:C	2.66	0.53
1:A:200:ALA:O	1:A:204:ILE:HG13	2.09	0.53
1:A:226:GLY:HA3	1:A:275:PHE:CE2	2.44	0.53
1:A:169:ILE:HD11	1:A:400:MET:SD	2.48	0.53
1:B:102:ASP:OD2	1:B:103:THR:N	2.37	0.53
1:B:74:PHE:HB2	1:B:336:TYR:CD2	2.43	0.53
1:B:461:ASP:OD2	1:B:461:ASP:N	2.38	0.53
1:A:426:ASP:O	1:A:427:GLY:C	2.52	0.53
1:A:362:SER:HA	1:A:366:LYS:HD2	1.90	0.53
1:A:519:LYS:HE3	1:A:544:PHE:O	2.08	0.53
1:A:493:ASP:CG	1:A:496:SER:HB3	2.33	0.53
1:A:82:ASP:OD2	1:A:83:ASN:N	2.41	0.53
1:B:284:LEU:C	1:B:284:LEU:HD13	2.34	0.53
1:B:453:ILE:HG13	1:B:453:ILE:O	2.08	0.53
1:A:490:LEU:CG	1:A:491:SER:N	2.73	0.52
1:B:214:SER:OG	1:B:242:ALA:HB3	2.10	0.52
1:A:160:LEU:HB2	1:B:163:LEU:HD23	1.92	0.52
1:A:284:LEU:HD13	1:A:284:LEU:C	2.34	0.52
1:B:76:ILE:HG13	1:B:93:VAL:HG11	1.91	0.52
1:A:515:PRO:CG	1:A:516:ASN:H	2.21	0.52
1:A:535:GLU:C	1:A:537:TYR:H	2.18	0.52
1:B:185:ASP:OD2	1:B:185:ASP:N	2.42	0.52
1:A:366:LYS:HE2	1:A:369:HIS:CD2	2.42	0.52
1:A:86:LEU:HD13	1:A:405:HIS:HA	1.91	0.52
1:A:490:LEU:HG	1:A:491:SER:H	1.73	0.52
1:A:31:ARG:HD2	1:A:349:PRO:HB2	1.92	0.52
1:A:74:PHE:HB2	1:A:336:TYR:CD2	2.45	0.52
1:A:252:ILE:HD12	1:A:252:ILE:H	1.73	0.52
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.91	0.52
1:B:191:VAL:HG12	1:B:392:PHE:CD2	2.45	0.52
1:B:260:ILE:HD11	1:B:288:ALA:HB2	1.92	0.52
1:A:32:GLU:OE2	1:A:34:LYS:HE3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ASP:OD2	1:A:545:THR:N	2.40	0.52
1:B:252:ILE:HG22	1:B:253:ARG:N	2.21	0.52
1:A:303:TRP:CD1	1:A:303:TRP:C	2.87	0.52
1:B:297:TRP:HB2	1:B:320:ALA:CB	2.39	0.51
1:A:46:PRO:HD3	1:A:149:SER:HB2	1.92	0.51
1:B:494:VAL:C	1:B:496:SER:N	2.68	0.51
1:A:554:TRP:CG	1:A:555:PRO:HD2	2.45	0.51
1:B:117:LEU:N	1:B:117:LEU:HD12	2.24	0.51
1:A:76:ILE:HG13	1:A:93:VAL:HG11	1.91	0.51
1:A:441:THR:O	1:A:442:ALA:C	2.54	0.51
1:A:411:LEU:HD12	1:A:422:MET:HG2	1.93	0.51
1:A:428:LYS:O	1:A:432:LYS:HG2	2.10	0.51
1:B:169:ILE:HD11	1:B:400:MET:SD	2.50	0.51
1:A:86:LEU:HG	1:A:89:VAL:HB	1.93	0.51
1:B:69:LEU:C	1:B:69:LEU:HD23	2.35	0.51
1:B:341:ASN:HD22	1:B:341:ASN:C	2.19	0.51
1:B:441:THR:O	1:B:442:ALA:C	2.54	0.51
1:A:521:MET:HB2	1:A:530:ILE:CG1	2.41	0.51
1:B:204:ILE:HG22	1:B:205:LEU:HD23	1.92	0.51
1:B:301:ASP:HA	1:B:323:LEU:O	2.11	0.51
1:B:291:VAL:O	1:B:293:ALA:N	2.44	0.51
1:A:372:VAL:HG22	1:A:373:CYS:N	2.23	0.51
1:B:108:GLN:O	1:B:111:GLU:HB2	2.10	0.51
1:B:205:LEU:HD22	1:B:210:TRP:CE3	2.46	0.51
1:B:490:LEU:HG	1:B:492:LEU:HD22	1.92	0.51
1:A:305:ALA:HA	1:A:480:TYR:CE2	2.47	0.50
1:A:491:SER:C	1:A:492:LEU:CD2	2.84	0.50
1:A:332:GLN:OE1	1:A:332:GLN:N	2.40	0.50
1:B:69:LEU:C	1:B:69:LEU:CD2	2.85	0.50
1:A:494:VAL:O	1:A:496:SER:N	2.44	0.50
1:B:246:LYS:O	1:B:246:LYS:HG3	2.12	0.50
1:A:535:GLU:C	1:A:537:TYR:N	2.69	0.50
1:B:486:TRP:CH2	1:B:488:GLU:HA	2.47	0.50
1:A:558:ASP:O	1:A:559:LEU:HB2	2.11	0.50
1:B:33:ILE:O	1:B:94:HIS:HA	2.12	0.50
1:A:59:ARG:HH11	1:A:59:ARG:HB2	1.76	0.50
1:A:157:VAL:HG12	1:A:161:LEU:HD22	1.93	0.50
1:A:185:ASP:OD2	1:A:185:ASP:N	2.44	0.50
1:A:461:ASP:OD2	1:A:461:ASP:N	2.39	0.50
1:A:359:PHE:O	1:A:360:GLN:HB2	2.12	0.50
1:B:76:ILE:HG13	1:B:93:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:HD2	1:B:196:TYR:CE1	2.30	0.50
1:B:314:GLU:HG3	1:B:478:TYR:CD2	2.47	0.50
1:A:261:ARG:O	1:A:264:LEU:HB2	2.11	0.49
1:A:322:THR:O	1:A:469:PHE:HB2	2.12	0.49
1:B:303:TRP:CD1	1:B:303:TRP:C	2.91	0.49
1:B:341:ASN:HA	1:B:355:TRP:CZ3	2.46	0.49
1:B:156:GLN:OE1	1:B:156:GLN:HA	2.12	0.49
1:A:41:LEU:CD2	1:A:400:MET:HG2	2.42	0.49
1:A:301:ASP:HA	1:A:323:LEU:O	2.12	0.49
1:A:64:ARG:HG2	1:A:68:ARG:CZ	2.42	0.49
1:A:301:ASP:O	1:A:304:GLY:N	2.46	0.49
1:A:457:ASP:HB2	1:A:461:ASP:OD2	2.13	0.49
1:A:515:PRO:O	1:A:517:GLU:N	2.46	0.49
1:A:522:GLN:HE21	1:A:522:GLN:HA	1.77	0.49
1:A:117:LEU:HD12	1:A:117:LEU:N	2.26	0.49
1:A:260:ILE:HD11	1:A:288:ALA:HB2	1.94	0.49
1:A:437:LYS:HE3	1:A:437:LYS:CA	2.30	0.49
1:B:341:ASN:ND2	1:B:341:ASN:C	2.71	0.49
1:B:437:LYS:CE	1:B:438:ILE:H	2.25	0.49
1:A:434:TYR:O	1:A:437:LYS:HB2	2.13	0.49
1:B:205:LEU:HD22	1:B:210:TRP:HE3	1.78	0.49
1:B:387:GLU:HB3	1:B:390:ILE:HG12	1.95	0.49
1:B:422:MET:O	1:B:423:LYS:C	2.55	0.49
1:A:544:PHE:CD1	1:A:544:PHE:N	2.81	0.48
1:B:192:PRO:HG3	1:B:464:GLY:HA2	1.95	0.48
1:A:159:ASN:HB3	1:B:163:LEU:HD11	1.95	0.48
1:A:289:ASN:CB	1:A:316:VAL:HG21	2.44	0.48
1:A:306:GLN:HB2	1:A:309:ILE:HD12	1.94	0.48
1:B:219:GLU:HB2	1:B:248:GLY:HA2	1.94	0.48
1:B:372:VAL:HG22	1:B:373:CYS:N	2.27	0.48
1:A:355:TRP:CE2	1:A:359:PHE:CE1	3.01	0.48
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.78	0.48
1:B:46:PRO:HD3	1:B:149:SER:HB2	1.95	0.48
1:B:187:PHE:HE2	1:B:189:ARG:HD2	1.78	0.48
1:A:40:VAL:HG12	1:A:41:LEU:N	2.29	0.48
1:A:279:ASP:OD1	1:A:280:ASP:N	2.46	0.48
1:A:445:ASN:ND2	1:A:447:ASN:O	2.47	0.48
1:A:563:TYR:O	1:A:563:TYR:CD1	2.66	0.48
1:B:330:VAL:HG13	1:B:444:PHE:HB3	1.94	0.48
1:A:36:GLU:HG2	1:A:37:GLY:N	2.28	0.48
1:A:554:TRP:O	1:A:562:CYS:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:SER:HA	3:A:1001:52A:OXT	2.13	0.48
1:B:36:GLU:HG2	1:B:37:GLY:N	2.28	0.48
1:B:64:ARG:CZ	1:B:306:GLN:NE2	2.77	0.48
1:B:289:ASN:HA	1:B:316:VAL:HG21	1.96	0.48
1:B:440:PHE:CD2	1:B:453:ILE:HG22	2.49	0.48
1:A:69:LEU:C	1:A:69:LEU:CD2	2.87	0.48
1:A:486:TRP:CH2	1:A:488:GLU:HA	2.49	0.48
1:B:47:ILE:HB	1:B:97:ASP:CG	2.39	0.48
1:A:301:ASP:O	1:A:302:GLY:C	2.57	0.48
1:B:200:ALA:HA	1:B:486:TRP:CD1	2.49	0.48
1:B:322:THR:O	1:B:469:PHE:HB2	2.14	0.48
1:B:331:ARG:O	1:B:334:ASP:HB2	2.13	0.48
1:A:362:SER:C	1:A:363:LEU:HD22	2.39	0.47
1:B:418:LEU:HD22	1:B:422:MET:HE3	1.96	0.47
1:A:59:ARG:NH1	1:A:59:ARG:CB	2.76	0.47
1:A:306:GLN:HB2	1:A:309:ILE:CD1	2.45	0.47
1:A:276:MET:HB2	1:A:281:SER:OG	2.14	0.47
1:A:99:CYS:HB2	1:A:104:TYR:CD2	2.50	0.47
1:A:99:CYS:SG	1:A:104:TYR:CE2	3.07	0.47
1:A:101:ARG:HD3	1:A:103:THR:OG1	2.14	0.47
1:A:138:ILE:N	1:A:139:PRO:CD	2.78	0.47
1:A:324:GLU:HG3	1:A:325:LEU:N	2.29	0.47
1:A:492:LEU:HD23	1:A:492:LEU:N	2.30	0.47
1:B:324:GLU:HG3	1:B:325:LEU:N	2.29	0.47
1:A:71:ALA:HA	1:A:333:PHE:CE1	2.49	0.47
1:A:187:PHE:CE2	1:A:189:ARG:HB3	2.49	0.47
1:A:276:MET:HE3	1:A:281:SER:HA	1.96	0.47
1:A:403:ALA:HB2	1:A:434:TYR:CD1	2.50	0.47
1:A:443:PRO:C	1:A:445:ASN:H	2.21	0.47
1:A:484:GLY:HA3	1:A:492:LEU:HA	1.97	0.47
1:A:514:ALA:CB	1:A:518:MET:HG3	2.32	0.47
1:B:59:ARG:HH11	1:B:59:ARG:HB2	1.79	0.47
1:B:227:ILE:O	1:B:231:GLU:HG3	2.15	0.47
1:B:337:PHE:CD1	1:B:340:LEU:HD12	2.48	0.47
1:B:445:ASN:ND2	1:B:447:ASN:O	2.47	0.47
1:A:219:GLU:HB2	1:A:248:GLY:HA2	1.97	0.47
1:A:433:GLU:O	1:A:433:GLU:HG3	2.14	0.47
1:A:539:TYR:HE1	1:A:541:VAL:HA	1.80	0.47
1:B:359:PHE:HB3	1:B:377:LEU:HD21	1.97	0.47
1:A:68:ARG:NH1	1:A:149:SER:OG	2.48	0.47
1:A:330:VAL:HG13	1:A:444:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:PHE:HB3	1:B:460:GLY:HA2	1.97	0.47
1:A:76:ILE:HG13	1:A:93:VAL:CG1	2.44	0.47
1:A:499:TRP:CD2	1:A:505:PRO:HD3	2.50	0.47
1:A:40:VAL:HG13	1:A:92:GLY:O	2.15	0.47
1:A:102:ASP:OD2	1:A:103:THR:N	2.41	0.47
1:B:490:LEU:CD1	1:B:491:SER:H	2.27	0.47
1:A:227:ILE:O	1:A:231:GLU:HG3	2.16	0.46
1:A:540:LEU:HB3	1:A:542:ASP:O	2.15	0.46
1:A:497:ILE:HG21	1:A:499:TRP:CZ2	2.50	0.46
1:B:399:ALA:O	1:B:400:MET:C	2.58	0.46
1:B:440:PHE:O	1:B:441:THR:C	2.56	0.46
1:B:467:ASN:HB3	1:B:469:PHE:HE1	1.79	0.46
1:A:519:LYS:HG2	1:A:532:ILE:O	2.16	0.46
1:B:443:PRO:C	1:B:445:ASN:H	2.22	0.46
1:A:540:LEU:N	1:A:540:LEU:CD1	2.76	0.46
1:B:157:VAL:HG12	1:B:161:LEU:HD22	1.96	0.46
1:A:310:VAL:HG21	1:A:471:LEU:HD22	1.97	0.46
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.98	0.46
1:A:86:LEU:HD13	1:A:405:HIS:CA	2.46	0.46
1:A:211:THR:HG23	1:A:238:ASN:O	2.16	0.46
1:B:107:GLU:O	1:B:110:LEU:HB2	2.16	0.46
1:B:195:PHE:HD2	1:B:196:TYR:HE1	1.64	0.46
1:A:174:THR:HB	1:A:194:ASP:OD1	2.15	0.46
1:A:206:ARG:HD2	1:A:237:ARG:HB3	1.97	0.46
1:A:492:LEU:CD2	1:A:492:LEU:N	2.79	0.46
1:B:426:ASP:O	1:B:427:GLY:C	2.57	0.46
1:A:422:MET:O	1:A:423:LYS:C	2.57	0.46
1:B:196:TYR:CD1	1:B:196:TYR:N	2.84	0.46
1:B:287:ALA:HA	1:B:290:ARG:CZ	2.44	0.46
1:A:230:PHE:CZ	1:A:273:VAL:HG21	2.52	0.45
1:B:433:GLU:HG3	1:B:433:GLU:O	2.15	0.45
1:B:491:SER:O	1:B:492:LEU:HB3	2.16	0.45
1:A:231:GLU:O	1:A:234:ALA:HB3	2.15	0.45
1:A:412:CYS:HA	1:A:413:PRO:HD2	1.73	0.45
1:A:539:TYR:HD1	1:A:540:LEU:N	2.15	0.45
1:B:196:TYR:N	1:B:196:TYR:HD1	2.14	0.45
1:A:85:LEU:O	1:A:86:LEU:C	2.59	0.45
1:B:403:ALA:HB2	1:B:434:TYR:CD1	2.51	0.45
1:B:86:LEU:HD13	1:B:405:HIS:CA	2.46	0.45
1:B:167:PRO:HG3	1:B:430:LEU:HD23	1.98	0.45
1:B:374:ASP:O	1:B:377:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:CYS:HB3	1:A:362:SER:H	1.39	0.45
1:A:435:LEU:O	1:A:437:LYS:N	2.49	0.45
1:B:86:LEU:HD13	1:B:405:HIS:HA	1.99	0.45
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.77	0.45
1:B:426:ASP:CG	1:B:429:LYS:HB2	2.42	0.45
1:A:437:LYS:CE	1:A:438:ILE:H	2.30	0.45
1:A:437:LYS:HE2	1:A:438:ILE:H	1.80	0.45
1:B:86:LEU:HG	1:B:89:VAL:HB	1.98	0.45
1:A:64:ARG:CZ	1:A:306:GLN:NE2	2.80	0.45
1:A:535:GLU:O	1:A:538:GLU:HG2	2.17	0.45
1:A:69:LEU:C	1:A:69:LEU:HD23	2.42	0.45
1:A:44:LEU:C	1:A:45:PHE:CD1	2.95	0.44
1:A:155:ILE:O	1:A:156:GLN:C	2.59	0.44
1:A:314:GLU:HG3	1:A:478:TYR:CD2	2.53	0.44
1:B:426:ASP:HB3	1:B:429:LYS:HB2	1.99	0.44
1:A:418:LEU:HD22	1:A:422:MET:HE3	1.98	0.44
1:B:389:LYS:O	1:B:390:ILE:C	2.61	0.44
1:A:387:GLU:HB3	1:A:390:ILE:HG12	1.99	0.44
1:B:138:ILE:N	1:B:139:PRO:CD	2.79	0.44
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.81	0.44
1:A:87:PRO:HG2	1:A:88:GLY:N	2.30	0.44
1:A:517:GLU:HB3	1:A:518:MET:H	1.61	0.44
1:A:59:ARG:HH11	1:A:59:ARG:CB	2.30	0.44
1:A:442:ALA:HA	1:A:443:PRO:HD2	1.63	0.44
1:A:323:LEU:HD21	1:A:468:VAL:HG22	1.99	0.44
1:A:355:TRP:CE2	1:A:359:PHE:HE1	2.36	0.44
1:B:97:ASP:OD1	1:B:98:THR:N	2.50	0.44
1:B:178:LEU:O	1:B:181:LYS:NZ	2.48	0.44
1:A:359:PHE:HB3	1:A:377:LEU:HD21	1.99	0.44
1:B:48:ASN:OD1	1:B:60:ILE:HD13	2.17	0.44
1:B:218:SER:OG	1:B:280:ASP:HB2	2.18	0.44
1:A:490:LEU:HG	1:A:492:LEU:CD2	2.45	0.44
1:B:86:LEU:HD13	1:B:405:HIS:HB2	2.00	0.44
1:B:442:ALA:HA	1:B:443:PRO:HD2	1.71	0.44
1:A:287:ALA:HA	1:A:290:ARG:CZ	2.47	0.44
1:A:374:ASP:O	1:A:377:LEU:HB2	2.18	0.44
1:A:473:GLN:NE2	1:A:476:GLY:N	2.66	0.44
1:B:332:GLN:OE1	1:B:332:GLN:N	2.40	0.44
1:B:457:ASP:HB2	1:B:461:ASP:OD2	2.17	0.44
1:A:291:VAL:O	1:A:293:ALA:N	2.51	0.43
1:B:446:PRO:HG2	1:B:447:ASN:H	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:O	1:A:390:ILE:C	2.59	0.43
1:A:440:PHE:CD2	1:A:453:ILE:HG22	2.53	0.43
1:A:499:TRP:CG	1:A:505:PRO:HD3	2.53	0.43
1:A:515:PRO:HG2	1:A:516:ASN:N	2.24	0.43
1:B:220:GLY:O	1:B:222:TYR:N	2.50	0.43
1:B:289:ASN:CB	1:B:316:VAL:HG21	2.48	0.43
1:B:366:LYS:HG2	1:B:367:ARG:N	2.24	0.43
1:A:150:TYR:HB2	1:A:153:VAL:HG12	2.00	0.43
1:A:310:VAL:HG21	1:A:471:LEU:CD2	2.48	0.43
1:A:310:VAL:HG11	1:A:471:LEU:HD21	2.01	0.43
1:A:310:VAL:CG1	1:A:317:ALA:HB3	2.44	0.43
1:A:459:PHE:HB2	1:A:461:ASP:OD2	2.18	0.43
1:B:187:PHE:CE2	1:B:189:ARG:HB3	2.54	0.43
1:A:208:PHE:O	1:A:210:TRP:N	2.51	0.43
1:A:269:ALA:HA	1:A:507:SER:OG	2.18	0.43
1:B:168:GLN:C	1:B:169:ILE:HG13	2.43	0.43
1:B:301:ASP:O	1:B:302:GLY:C	2.60	0.43
1:B:499:TRP:CG	1:B:505:PRO:HD3	2.53	0.43
1:A:348:ASN:OD1	1:A:348:ASN:C	2.62	0.43
1:A:443:PRO:C	1:A:445:ASN:N	2.77	0.43
1:A:501:ARG:O	1:A:502:ASN:C	2.61	0.43
1:A:473:GLN:NE2	1:A:474:THR:C	2.77	0.43
1:B:174:THR:O	1:B:193:PRO:HA	2.19	0.43
1:B:434:TYR:O	1:B:437:LYS:HB2	2.19	0.43
1:B:473:GLN:HE21	1:B:476:GLY:N	2.17	0.43
1:A:511:ASP:HB3	1:A:512:PRO:HD2	2.00	0.43
1:A:540:LEU:CD1	1:A:559:LEU:HB3	2.49	0.43
1:A:554:TRP:CD2	1:A:555:PRO:HD2	2.54	0.43
1:B:47:ILE:HD13	1:B:350:TRP:CE3	2.54	0.43
1:A:435:LEU:C	1:A:437:LYS:N	2.77	0.43
1:B:208:PHE:O	1:B:210:TRP:N	2.52	0.43
1:B:261:ARG:O	1:B:264:LEU:HB2	2.19	0.43
1:A:196:TYR:CD1	1:A:196:TYR:N	2.86	0.43
1:A:260:ILE:O	1:A:261:ARG:C	2.62	0.43
1:B:41:LEU:CD2	1:B:400:MET:HG2	2.47	0.43
1:B:469:PHE:HD2	1:B:480:TYR:HB3	1.84	0.43
1:A:337:PHE:CD1	1:A:340:LEU:HD12	2.54	0.42
1:B:359:PHE:O	1:B:360:GLN:HB2	2.19	0.42
1:A:93:VAL:HG23	1:A:95:ILE:HG13	2.00	0.42
1:A:157:VAL:HG12	1:A:161:LEU:CD2	2.49	0.42
1:A:441:THR:HG23	1:A:452:SER:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:NH1	1:B:59:ARG:CB	2.82	0.42
1:B:389:LYS:O	1:B:392:PHE:N	2.52	0.42
1:B:400:MET:O	1:B:403:ALA:HB3	2.19	0.42
1:A:97:ASP:OD1	1:A:98:THR:N	2.52	0.42
1:A:195:PHE:HD2	1:A:196:TYR:CE1	2.36	0.42
1:A:515:PRO:O	1:A:516:ASN:C	2.62	0.42
1:A:517:GLU:HG3	1:A:534:CYS:H	1.84	0.42
1:B:484:GLY:HA3	1:B:492:LEU:HA	2.00	0.42
1:A:303:TRP:C	1:A:303:TRP:HD1	2.26	0.42
1:B:71:ALA:HA	1:B:333:PHE:CE1	2.55	0.42
1:B:93:VAL:HG23	1:B:95:ILE:HG13	2.00	0.42
1:B:317:ALA:O	1:B:471:LEU:HD23	2.20	0.42
1:A:196:TYR:N	1:A:196:TYR:HD1	2.18	0.42
1:B:473:GLN:NE2	1:B:476:GLY:N	2.64	0.42
1:A:167:PRO:HG3	1:A:430:LEU:HD23	2.01	0.42
1:A:252:ILE:HG22	1:A:253:ARG:N	2.22	0.42
1:A:467:ASN:CB	1:A:469:PHE:HE1	2.33	0.42
1:A:513:CYS:HB3	1:A:518:MET:HB2	2.00	0.42
1:B:187:PHE:CD2	1:B:188:ALA:N	2.88	0.42
1:B:219:GLU:HB2	1:B:247:VAL:O	2.19	0.42
1:B:441:THR:HG23	1:B:452:SER:C	2.43	0.42
1:A:107:GLU:O	1:A:110:LEU:HB2	2.19	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.82	0.42
1:A:475:GLY:C	1:A:477:LYS:H	2.28	0.42
1:A:540:LEU:C	1:A:542:ASP:N	2.76	0.42
1:B:303:TRP:CD1	1:B:322:THR:HG21	2.54	0.42
1:A:294:SER:C	1:A:295:PHE:CD1	2.97	0.42
1:A:215:THR:HG22	1:A:273:VAL:HB	2.02	0.42
1:A:426:ASP:HB3	1:A:429:LYS:HB2	2.02	0.42
1:B:412:CYS:HA	1:B:413:PRO:HD2	1.66	0.42
1:B:341:ASN:OD1	1:B:344:ASN:ND2	2.53	0.42
1:A:76:ILE:O	1:A:77:ASP:C	2.63	0.41
1:A:218:SER:N	1:A:276:MET:HG2	2.35	0.41
1:A:407:MET:HG2	1:A:422:MET:SD	2.60	0.41
1:A:523:PRO:HG2	1:A:524:GLY:H	1.84	0.41
1:A:541:VAL:HG23	1:A:547:MET:CB	2.50	0.41
1:A:41:LEU:HD12	1:A:76:ILE:HD11	2.02	0.41
1:A:468:VAL:HG23	1:A:485:HIS:HA	2.02	0.41
1:B:40:VAL:HG12	1:B:41:LEU:N	2.35	0.41
1:B:215:THR:O	1:B:245:GLU:N	2.41	0.41
1:B:305:ALA:HA	1:B:480:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:HB2	1:A:247:VAL:O	2.20	0.41
1:B:205:LEU:HA	1:B:210:TRP:HE3	1.86	0.41
1:B:356:GLU:OE1	1:B:363:LEU:HB2	2.21	0.41
1:A:67:GLN:HB3	1:A:390:ILE:HD11	2.02	0.41
1:A:486:TRP:HE3	1:A:486:TRP:O	2.03	0.41
1:B:76:ILE:O	1:B:77:ASP:C	2.63	0.41
1:B:251:ASN:HD22	1:B:255:SER:HB3	1.85	0.41
1:B:355:TRP:CE2	1:B:359:PHE:CE1	3.08	0.41
1:A:305:ALA:HA	1:A:480:TYR:CD2	2.56	0.41
1:A:331:ARG:O	1:A:334:ASP:HB2	2.21	0.41
1:B:40:VAL:HG21	1:B:140:LEU:HD22	2.02	0.41
1:B:328:HIS:HA	1:B:329:PRO:HD2	1.87	0.41
1:B:443:PRO:C	1:B:445:ASN:N	2.78	0.41
1:B:459:PHE:HB2	1:B:461:ASP:OD2	2.21	0.41
1:A:213:VAL:HB	1:A:271:VAL:O	2.20	0.41
1:A:289:ASN:OD1	1:A:316:VAL:HG21	2.21	0.41
1:A:440:PHE:O	1:A:441:THR:C	2.64	0.41
1:A:514:ALA:O	1:A:515:PRO:C	2.63	0.41
1:A:274:LEU:HD22	1:A:276:MET:CE	2.38	0.41
1:A:399:ALA:O	1:A:400:MET:C	2.62	0.41
1:B:348:ASN:C	1:B:348:ASN:OD1	2.63	0.41
1:B:375:LYS:C	1:B:377:LEU:H	2.29	0.41
1:A:208:PHE:HB2	1:A:210:TRP:CE3	2.56	0.41
1:A:310:VAL:HG13	1:A:317:ALA:CB	2.45	0.41
1:B:68:ARG:NH1	1:B:149:SER:OG	2.54	0.41
1:B:435:LEU:O	1:B:437:LYS:N	2.51	0.41
1:A:289:ASN:HA	1:A:316:VAL:HG21	2.03	0.41
1:A:515:PRO:CG	1:A:516:ASN:N	2.84	0.41
1:A:40:VAL:HA	1:A:92:GLY:O	2.21	0.40
1:A:47:ILE:HB	1:A:97:ASP:CG	2.46	0.40
1:A:214:SER:OG	1:A:243:THR:HG22	2.21	0.40
1:A:215:THR:O	1:A:245:GLU:N	2.46	0.40
1:A:356:GLU:OE1	1:A:363:LEU:HB2	2.20	0.40
1:A:109:SER:C	1:A:111:GLU:N	2.79	0.40
1:A:249:ARG:C	1:A:251:ASN:N	2.78	0.40
1:A:351:PHE:O	1:A:354:PHE:HB3	2.21	0.40
1:A:504:VAL:HA	1:A:505:PRO:HD3	1.76	0.40
1:A:519:LYS:N	1:A:532:ILE:O	2.53	0.40
1:A:541:VAL:HG23	1:A:547:MET:HB2	2.02	0.40
1:B:301:ASP:O	1:B:304:GLY:N	2.54	0.40
1:A:341:ASN:ND2	1:A:341:ASN:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HG12	1:B:434:TYR:OH	2.22	0.40
1:B:291:VAL:O	1:B:292:ASN:C	2.64	0.40
1:A:341:ASN:OD1	1:A:344:ASN:ND2	2.54	0.40
1:B:215:THR:HG22	1:B:273:VAL:HB	2.03	0.40
1:B:399:ALA:HB1	1:B:434:TYR:HE1	1.85	0.40
1:A:159:ASN:C	1:B:163:LEU:HD21	2.46	0.40
1:B:181:LYS:CE	1:B:459:PHE:O	2.53	0.40
1:B:428:LYS:O	1:B:432:LYS:HG2	2.21	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	514/555 (93%)	415 (81%)	71 (14%)	28 (5%)	1	10
1	B	455/555 (82%)	368 (81%)	66 (14%)	21 (5%)	2	12
All	All	969/1110 (87%)	783 (81%)	137 (14%)	49 (5%)	1	10

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	ALA
1	A	292	ASN
1	A	361	CYS
1	A	443	PRO
1	A	494	VAL
1	A	518	MET
1	B	242	ALA
1	B	292	ASN
1	B	361	CYS
1	B	443	PRO

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Mol	Chain	Res	Type
1	B	494	VAL
1	A	87	PRO
1	A	209	ASN
1	A	221	ASP
1	A	371	GLN
1	A	436	LEU
1	A	488	GLU
1	A	495	ASP
1	A	516	ASN
1	A	523	PRO
1	A	566	PRO
1	B	87	PRO
1	B	100	SER
1	B	209	ASN
1	B	221	ASP
1	B	314	GLU
1	B	371	GLN
1	B	436	LEU
1	B	488	GLU
1	B	495	ASP
1	B	502	ASN
1	A	100	SER
1	A	314	GLU
1	A	450	ALA
1	A	502	ASN
1	B	441	THR
1	A	172	ALA
1	A	180	ASP
1	A	362	SER
1	A	492	LEU
1	A	536	PRO
1	B	180	ASP
1	B	362	SER
1	B	450	ALA
1	B	492	LEU
1	A	250	SER
1	A	446	PRO
1	B	446	PRO
1	A	267	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/481 (93%)	405 (91%)	42 (9%)	8	29
1	B	394/481 (82%)	358 (91%)	36 (9%)	9	30
All	All	841/962 (87%)	763 (91%)	78 (9%)	8	29

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	67	GLN
1	A	69	LEU
1	A	81	LYS
1	A	86	LEU
1	A	93	VAL
1	A	149	SER
1	A	153	VAL
1	A	161	LEU
1	A	174	THR
1	A	181	LYS
1	A	189	ARG
1	A	192	PRO
1	A	216	VAL
1	A	227	ILE
1	A	252	ILE
1	A	268	ASN
1	A	275	PHE
1	A	298	VAL
1	A	303	TRP
1	A	341	ASN
1	A	363	LEU
1	A	373	CYS
1	A	418	LEU
1	A	429	LYS
1	A	433	GLU
1	A	437	LYS

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Mol	Chain	Res	Type
1	A	439	GLN
1	A	440	PHE
1	A	445	ASN
1	A	454	VAL
1	A	458	THR
1	A	461	ASP
1	A	492	LEU
1	A	502	ASN
1	A	504	VAL
1	A	518	MET
1	A	526	VAL
1	A	540	LEU
1	A	544	PHE
1	A	546	CYS
1	A	548	ASP
1	B	39	LEU
1	B	67	GLN
1	B	69	LEU
1	B	81	LYS
1	B	86	LEU
1	B	93	VAL
1	B	95	ILE
1	B	149	SER
1	B	153	VAL
1	B	161	LEU
1	B	181	LYS
1	B	189	ARG
1	B	204	ILE
1	B	216	VAL
1	B	227	ILE
1	B	252	ILE
1	B	268	ASN
1	B	275	PHE
1	B	298	VAL
1	B	303	TRP
1	B	341	ASN
1	B	363	LEU
1	B	373	CYS
1	B	418	LEU
1	B	429	LYS
1	B	433	GLU
1	B	437	LYS

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Mol	Chain	Res	Type
1	B	439	GLN
1	B	440	PHE
1	B	445	ASN
1	B	454	VAL
1	B	458	THR
1	B	461	ASP
1	B	492	LEU
1	B	502	ASN
1	B	504	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	292	ASN
1	A	306	GLN
1	A	328	HIS
1	A	341	ASN
1	A	365	ASN
1	A	369	HIS
1	A	467	ASN
1	A	473	GLN
1	A	520	ASN
1	A	522	GLN
1	B	61	ASN
1	B	251	ASN
1	B	265	GLN
1	B	292	ASN
1	B	306	GLN
1	B	328	HIS
1	B	341	ASN
1	B	344	ASN
1	B	365	ASN
1	B	369	HIS
1	B	408	GLN
1	B	467	ASN
1	B	473	GLN

5.3.3 RNA ⓘ

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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	52A	B	2001	-	9,12,12	1.00	0	13,18,18	1.10	1 (7%)
2	NAG	A	801	1	14,14,15	0.81	1 (7%)	17,19,21	0.55	0
3	52A	A	1001	-	9,12,12	1.05	0	13,18,18	1.13	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	52A	B	2001	-	-	5/10/21/21	0/1/1/1
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
3	52A	A	1001	-	-	5/10/21/21	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAG	C1-C2	2.31	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	52A	OXT-C-CA	2.29	119.79	113.69
3	B	2001	52A	OXT-C-CA	2.16	119.45	113.69

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
3	A	1001	52A	O-C-CA-N
3	A	1001	52A	OE1-CD-CG1-CB1
3	A	1001	52A	OE2-CD-CG1-CB1
3	A	1001	52A	OE1-CD-CG1-NG2
3	A	1001	52A	OE2-CD-CG1-NG2
3	B	2001	52A	O-C-CA-N
3	B	2001	52A	OE1-CD-CG1-CB1
3	B	2001	52A	OE2-CD-CG1-CB1
3	B	2001	52A	OE1-CD-CG1-NG2
3	B	2001	52A	OE2-CD-CG1-NG2
2	A	801	NAG	O5-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	52A	1	0
3	A	1001	52A	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/555 (93%)	-0.62	1 (0%) 91 87	38, 97, 201, 302	5 (0%)
1	B	459/555 (82%)	-0.43	0 100 100	41, 150, 267, 371	5 (1%)
All	All	977/1110 (88%)	-0.53	1 (0%) 92 91	38, 116, 246, 371	10 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	CYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	801	14/15	0.44	0.10	210,210,210,210	0
3	52A	B	2001	12/12	0.93	0.06	94,94,94,94	0
3	52A	A	1001	12/12	0.96	0.06	64,64,64,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.