



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:05 PM UTC

PDB ID : 2XQ2 / pdb_00002xq2
Title : Structure of the K294A mutant of vSGLT
Authors : Watanabe, A.; Choe, S.; Chaptal, V.; Rosenberg, J.M.; Wright, E.M.; Grabe, M.; Abramson, J.
Deposited on : 2010-09-01
Resolution : 2.73 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

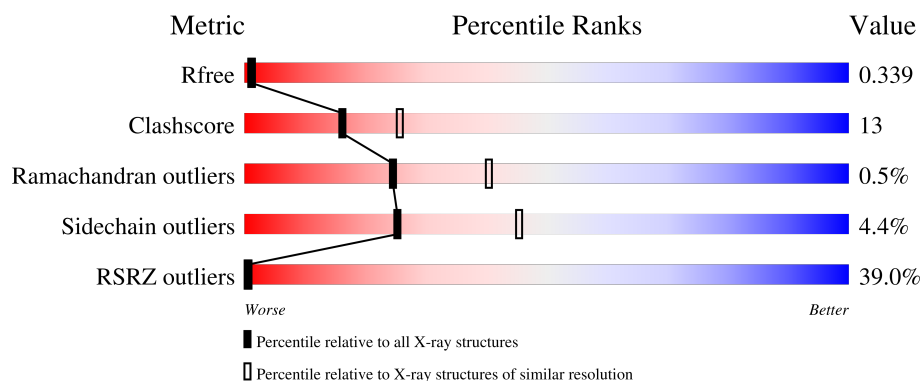
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	593	33% 66% 21% 9%
2	B	593	35% 68% 17% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8090 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 SODIUM/GLUCOSE COTRANSPORTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4107	2762	612	711	22			

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	ALA	LYS	engineered mutation	UNP P96169
A	411	ALA	CYS	engineered mutation	UNP P96169
A	423	CYS	ALA	engineered mutation	UNP P96169
A	544	VAL	-	expression tag	UNP P96169
A	545	ASN	-	expression tag	UNP P96169
A	546	ALA	-	expression tag	UNP P96169
A	547	ASP	-	expression tag	UNP P96169
A	548	ALA	-	expression tag	UNP P96169
A	549	GLU	-	expression tag	UNP P96169
A	550	ILE	-	expression tag	UNP P96169
A	551	THR	-	expression tag	UNP P96169
A	552	LEU	-	expression tag	UNP P96169
A	553	ILE	-	expression tag	UNP P96169
A	554	ILE	-	expression tag	UNP P96169
A	555	PHE	-	expression tag	UNP P96169
A	556	GLY	-	expression tag	UNP P96169
A	557	VAL	-	expression tag	UNP P96169
A	558	MET	-	expression tag	UNP P96169
A	559	ALA	-	expression tag	UNP P96169
A	560	GLY	-	expression tag	UNP P96169
A	561	VAL	-	expression tag	UNP P96169
A	562	ILE	-	expression tag	UNP P96169
A	563	GLY	-	expression tag	UNP P96169
A	564	THR	-	expression tag	UNP P96169
A	565	ILE	-	expression tag	UNP P96169
A	566	LEU	-	expression tag	UNP P96169
A	567	LEU	-	expression tag	UNP P96169

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Chain	Residue	Modelled	Actual	Comment	Reference
A	568	ILE	-	expression tag	UNP P96169
A	569	SER	-	expression tag	UNP P96169
A	570	TYR	-	expression tag	UNP P96169
A	571	GLY	-	expression tag	UNP P96169
A	572	ILE	-	expression tag	UNP P96169
A	573	LYS	-	expression tag	UNP P96169
A	574	LYS	-	expression tag	UNP P96169
A	575	LEU	-	expression tag	UNP P96169
A	576	ILE	-	expression tag	UNP P96169
A	577	LYS	-	expression tag	UNP P96169
A	578	ALA	-	expression tag	UNP P96169
A	579	SER	-	expression tag	UNP P96169
A	580	TYR	-	expression tag	UNP P96169
A	581	LYS	-	expression tag	UNP P96169
A	582	SER	-	expression tag	UNP P96169
A	583	GLY	-	expression tag	UNP P96169
A	584	GLY	-	expression tag	UNP P96169
A	585	SER	-	expression tag	UNP P96169
A	586	PRO	-	expression tag	UNP P96169
A	587	GLY	-	expression tag	UNP P96169
A	588	HIS	-	expression tag	UNP P96169
A	589	HIS	-	expression tag	UNP P96169
A	590	HIS	-	expression tag	UNP P96169
A	591	HIS	-	expression tag	UNP P96169
A	592	HIS	-	expression tag	UNP P96169
A	593	HIS	-	expression tag	UNP P96169

- Molecule 2 is a protein called SODIUM/GLUCOSE COTRANSPORTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			3957	2651	594	691	21			

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	ALA	LYS	engineered mutation	UNP P96169
B	411	ALA	CYS	engineered mutation	UNP P96169
B	423	CYS	ALA	engineered mutation	UNP P96169
B	544	VAL	-	expression tag	UNP P96169
B	545	ASN	-	expression tag	UNP P96169
B	546	ALA	-	expression tag	UNP P96169

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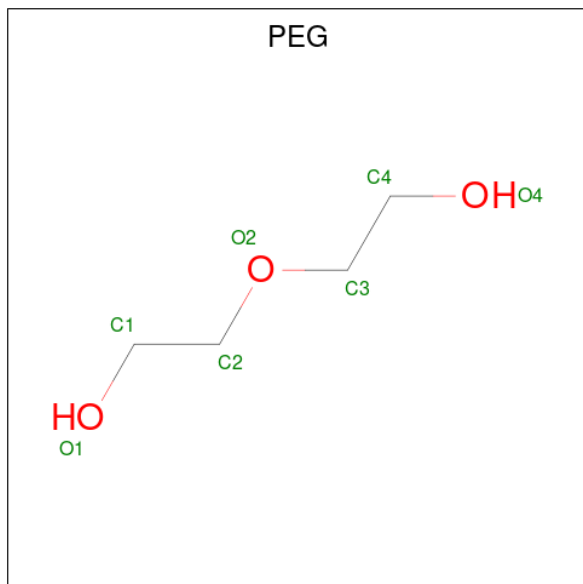
Chain	Residue	Modelled	Actual	Comment	Reference
B	547	ASP	-	expression tag	UNP P96169
B	548	ALA	-	expression tag	UNP P96169
B	549	GLU	-	expression tag	UNP P96169
B	550	ILE	-	expression tag	UNP P96169
B	551	THR	-	expression tag	UNP P96169
B	552	LEU	-	expression tag	UNP P96169
B	553	ILE	-	expression tag	UNP P96169
B	554	ILE	-	expression tag	UNP P96169
B	555	PHE	-	expression tag	UNP P96169
B	556	GLY	-	expression tag	UNP P96169
B	557	VAL	-	expression tag	UNP P96169
B	558	MET	-	expression tag	UNP P96169
B	559	ALA	-	expression tag	UNP P96169
B	560	GLY	-	expression tag	UNP P96169
B	561	VAL	-	expression tag	UNP P96169
B	562	ILE	-	expression tag	UNP P96169
B	563	GLY	-	expression tag	UNP P96169
B	564	THR	-	expression tag	UNP P96169
B	565	ILE	-	expression tag	UNP P96169
B	566	LEU	-	expression tag	UNP P96169
B	567	LEU	-	expression tag	UNP P96169
B	568	ILE	-	expression tag	UNP P96169
B	569	SER	-	expression tag	UNP P96169
B	570	TYR	-	expression tag	UNP P96169
B	571	GLY	-	expression tag	UNP P96169
B	572	ILE	-	expression tag	UNP P96169
B	573	LYS	-	expression tag	UNP P96169
B	574	LYS	-	expression tag	UNP P96169
B	575	LEU	-	expression tag	UNP P96169
B	576	ILE	-	expression tag	UNP P96169
B	577	LYS	-	expression tag	UNP P96169
B	578	ALA	-	expression tag	UNP P96169
B	579	SER	-	expression tag	UNP P96169
B	580	TYR	-	expression tag	UNP P96169
B	581	LYS	-	expression tag	UNP P96169
B	582	SER	-	expression tag	UNP P96169
B	583	GLY	-	expression tag	UNP P96169
B	584	GLY	-	expression tag	UNP P96169
B	585	SER	-	expression tag	UNP P96169
B	586	PRO	-	expression tag	UNP P96169
B	587	GLY	-	expression tag	UNP P96169
B	588	HIS	-	expression tag	UNP P96169

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Chain	Residue	Modelled	Actual	Comment	Reference
B	589	HIS	-	expression tag	UNP P96169
B	590	HIS	-	expression tag	UNP P96169
B	591	HIS	-	expression tag	UNP P96169
B	592	HIS	-	expression tag	UNP P96169
B	593	HIS	-	expression tag	UNP P96169

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0

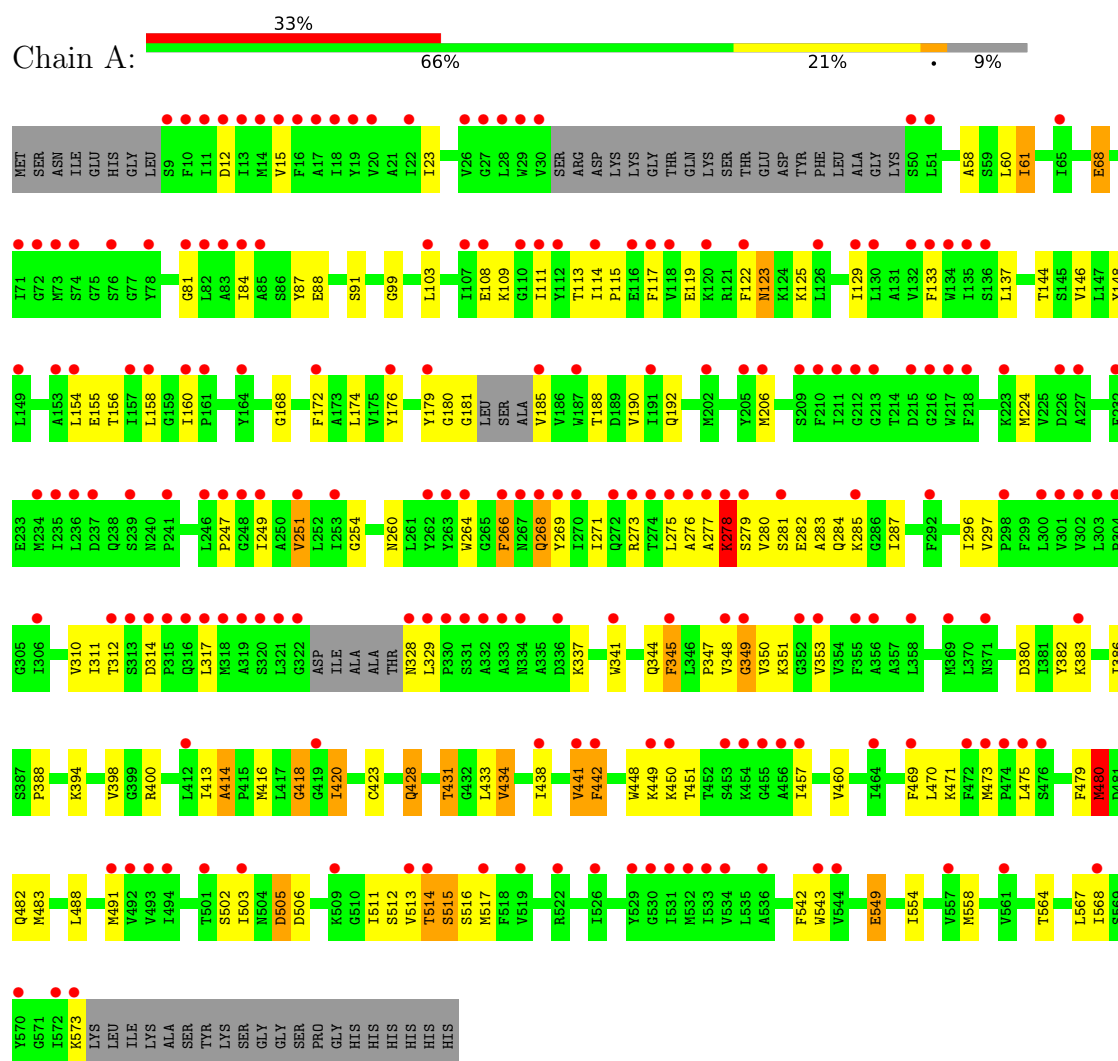
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0

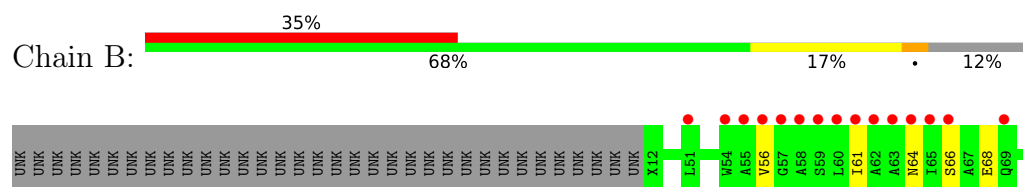
3 Residue-property plots

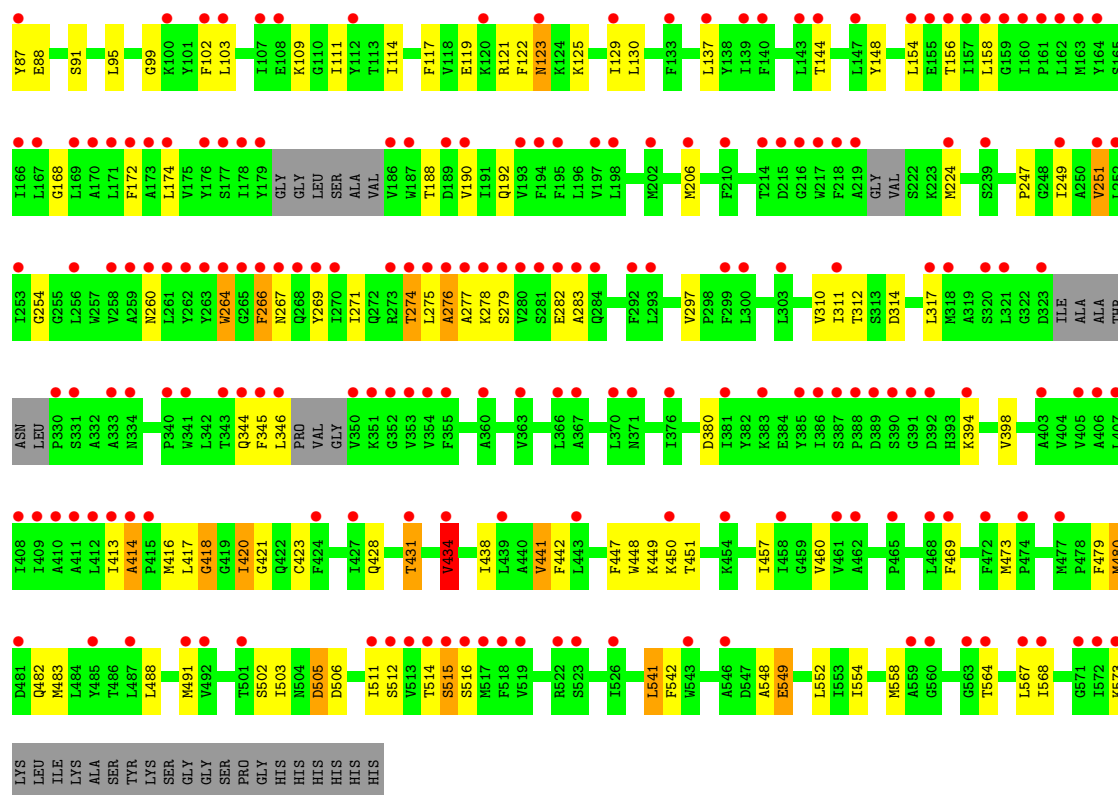
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: SODIUM/GLUCOSE COTRANSPORTER





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.30Å 112.68Å 238.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.01 – 2.73 68.01 – 2.73	Depositor EDS
% Data completeness (in resolution range)	(Not available) (68.01-2.73) 99.0 (68.01-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.251 , 0.274 0.288 , 0.339	Depositor DCC
R_{free} test set	3193 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8090	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: PEG

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	0.85	2/4210 (0.0%)	1.51	35/5741 (0.6%)
2	B	0.79	2/3973 (0.1%)	1.49	28/5413 (0.5%)
All	All	0.82	4/8183 (0.0%)	1.50	63/11154 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	121	ARG	C-N	5.97	1.42	1.33
2	B	266	PHE	CA-C	5.25	1.57	1.52
1	A	480	MET	SD-CE	-5.12	1.66	1.79
1	A	278	LYS	CA-C	5.12	1.59	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	VAL	N-CA-C	14.84	124.67	110.42
2	B	266	PHE	N-CA-C	12.99	129.35	112.72
2	B	345	PHE	CA-CB-CG	10.08	123.88	113.80
1	A	345	PHE	CA-CB-CG	10.02	123.81	113.80
1	A	269	TYR	N-CA-C	-9.89	99.94	112.90
2	B	420	ILE	N-CA-C	9.64	120.45	110.62
1	A	418	GLY	N-CA-C	9.12	123.67	112.73
2	B	264	TRP	N-CA-C	8.82	122.17	111.40
2	B	418	GLY	N-CA-C	8.75	123.23	112.73
1	A	266	PHE	N-CA-C	8.35	124.04	112.93
2	B	515	SER	N-CA-C	7.87	122.46	112.86
2	B	269	TYR	N-CA-C	-7.83	102.64	112.90
1	A	434	VAL	CB-CA-C	7.34	117.53	110.63
1	A	431	THR	N-CA-C	-7.17	103.54	111.36
2	B	277	ALA	N-CA-C	7.07	119.07	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	GLY	CA-C-N	6.98	130.02	120.46
1	A	349	GLY	C-N-CA	6.98	130.02	120.46
2	B	431	THR	N-CA-C	-6.91	103.81	111.82
2	B	516	SER	N-CA-C	-6.86	106.80	114.62
1	A	442	PHE	CA-CB-CG	6.25	120.05	113.80
1	A	254	GLY	CA-C-N	6.00	127.69	120.13
1	A	254	GLY	C-N-CA	6.00	127.69	120.13
1	A	505	ASP	CA-CB-CG	5.93	118.53	112.60
2	B	297	VAL	CB-CA-C	-5.89	108.10	113.70
2	B	254	GLY	CA-C-N	5.66	127.26	120.13
2	B	254	GLY	C-N-CA	5.66	127.26	120.13
2	B	434	VAL	CB-CA-C	5.65	116.03	111.06
1	A	329	LEU	N-CA-C	5.58	116.72	109.64
2	B	276	ALA	CB-CA-C	5.54	121.45	110.42
1	A	297	VAL	CB-CA-C	-5.54	108.43	113.70
1	A	268	GLN	CB-CA-C	5.45	121.26	110.42
2	B	505	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	58	ALA	CA-C-N	5.41	127.53	120.28
1	A	58	ALA	C-N-CA	5.41	127.53	120.28
2	B	441	VAL	N-CA-CB	5.41	117.89	110.54
1	A	543	TRP	CA-C-N	5.41	127.37	120.56
1	A	543	TRP	C-N-CA	5.41	127.37	120.56
2	B	260	ASN	N-CA-C	5.39	116.97	111.14
1	A	433	LEU	N-CA-C	-5.37	106.00	112.54
1	A	516	SER	N-CA-C	-5.34	106.61	113.02
1	A	123	ASN	N-CA-C	5.33	116.25	108.14
1	A	284	GLN	CA-C-N	5.32	127.41	120.28
1	A	284	GLN	C-N-CA	5.32	127.41	120.28
1	A	428	GLN	N-CA-C	5.31	116.76	110.97
1	A	441	VAL	N-CA-CB	5.30	117.75	110.54
1	A	515	SER	N-CA-C	5.28	122.05	110.80
2	B	267	ASN	N-CA-CB	-5.23	102.43	110.01
2	B	269	TYR	CA-C-N	5.23	128.73	120.47
2	B	269	TYR	C-N-CA	5.23	128.73	120.47
2	B	541	LEU	N-CA-C	5.22	117.39	111.02
2	B	311	ILE	CA-C-N	5.20	127.51	120.38
2	B	311	ILE	C-N-CA	5.20	127.51	120.38
1	A	260	ASN	N-CA-C	5.15	116.98	111.36
1	A	514	THR	N-CA-C	5.15	116.67	108.79
2	B	274	THR	CB-CA-C	5.14	121.05	110.31
1	A	279	SER	N-CA-C	-5.09	102.25	110.14
2	B	123	ASN	N-CA-C	5.09	116.26	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	VAL	CA-C-N	5.02	127.32	120.54
1	A	280	VAL	C-N-CA	5.02	127.32	120.54
1	A	311	ILE	CA-C-N	5.01	127.24	120.38
1	A	311	ILE	C-N-CA	5.01	127.24	120.38
2	B	264	TRP	CA-C-N	5.00	125.51	120.00
2	B	264	TRP	C-N-CA	5.00	125.51	120.00

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	4107	0	4252	130	0
2	B	3957	0	4022	96	0
3	A	21	0	30	0	0
4	A	5	0	0	0	0
All	All	8090	0	8304	215	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 13.

All (215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:CG2	1:A:115:PRO:HD3	1.82	1.09
1:A:502:SER:O	2:B:515:SER:HB2	1.64	0.98
2:B:148:TYR:CD2	2:B:417:LEU:HD22	2.00	0.96
1:A:81:GLY:O	1:A:84:ILE:HG22	1.65	0.96
1:A:108:GLU:HB2	1:A:517:MET:HE1	1.44	0.96
2:B:81:GLY:O	2:B:84:ILE:HG22	1.65	0.95
2:B:148:TYR:CE1	2:B:418:GLY:HA2	2.02	0.95
1:A:114:ILE:HG23	1:A:115:PRO:HD3	1.47	0.94
2:B:541:LEU:HD11	2:B:548:ALA:HB3	1.52	0.91
2:B:114:ILE:HG13	2:B:266:PHE:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:O	1:A:416:MET:HG2	1.71	0.90
1:A:114:ILE:HG22	1:A:115:PRO:HD3	1.50	0.90
2:B:413:ILE:O	2:B:416:MET:HG2	1.72	0.89
1:A:114:ILE:HD11	1:A:442:PHE:CE2	2.09	0.86
1:A:264:TRP:HE3	1:A:268:GLN:OE1	1.59	0.86
2:B:417:LEU:O	2:B:417:LEU:HD23	1.75	0.85
1:A:122:PHE:HE1	1:A:451:THR:HG22	1.42	0.84
1:A:341:TRP:O	1:A:344:GLN:HG2	1.77	0.84
2:B:122:PHE:HE1	2:B:451:THR:HG22	1.42	0.84
2:B:541:LEU:HD23	2:B:552:LEU:HD22	1.62	0.82
2:B:541:LEU:HD11	2:B:548:ALA:CB	2.10	0.82
1:A:99:GLY:HA2	1:A:103:LEU:HD12	1.61	0.81
1:A:114:ILE:HD11	1:A:442:PHE:CZ	2.15	0.81
1:A:264:TRP:CE3	1:A:268:GLN:OE1	2.34	0.81
2:B:114:ILE:CD1	2:B:266:PHE:O	2.28	0.81
2:B:148:TYR:CD2	2:B:417:LEU:CD2	2.63	0.81
2:B:99:GLY:HA2	2:B:103:LEU:HD12	1.62	0.79
1:A:60:LEU:HD22	1:A:268:GLN:NE2	1.98	0.79
1:A:114:ILE:HG23	1:A:115:PRO:CD	2.11	0.79
1:A:108:GLU:OE1	1:A:517:MET:SD	2.40	0.78
1:A:428:GLN:HA	1:A:428:GLN:NE2	1.99	0.78
1:A:103:LEU:HD11	1:A:271:ILE:HD11	1.66	0.77
2:B:114:ILE:CG1	2:B:266:PHE:O	2.32	0.77
1:A:176:TYR:O	1:A:180:GLY:HA3	1.85	0.76
1:A:502:SER:O	2:B:515:SER:CB	2.33	0.76
1:A:114:ILE:CG2	1:A:115:PRO:CD	2.62	0.75
2:B:417:LEU:HD21	2:B:423:CYS:SG	2.28	0.73
1:A:503:ILE:HA	2:B:515:SER:OG	1.89	0.73
1:A:148:TYR:CE1	1:A:418:GLY:HA2	2.24	0.73
2:B:428:GLN:NE2	2:B:428:GLN:HA	2.02	0.73
1:A:434:VAL:HG12	1:A:438:ILE:HD12	1.71	0.72
1:A:206:MET:SD	1:A:345:PHE:CD2	2.86	0.69
1:A:266:PHE:CE1	1:A:442:PHE:HB3	2.27	0.69
1:A:283:ALA:O	1:A:287:ILE:HG12	1.94	0.68
2:B:148:TYR:CG	2:B:417:LEU:HD22	2.28	0.68
1:A:60:LEU:HD22	1:A:268:GLN:HE21	1.58	0.67
1:A:275:LEU:C	1:A:275:LEU:HD23	2.19	0.67
1:A:185:VAL:HG12	1:A:185:VAL:O	1.93	0.67
1:A:515:SER:HB2	2:B:502:SER:O	1.96	0.66
1:A:148:TYR:HE1	1:A:418:GLY:HA2	1.59	0.66
2:B:469:PHE:O	2:B:473:MET:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:C	1:A:277:ALA:H	2.03	0.66
1:A:449:LYS:HE2	1:A:506:ASP:CG	2.21	0.65
1:A:190:VAL:HG13	1:A:568:ILE:HD12	1.77	0.65
1:A:469:PHE:O	1:A:473:MET:HB2	1.97	0.64
1:A:108:GLU:CB	1:A:517:MET:HE1	2.22	0.63
2:B:449:LYS:HE2	2:B:506:ASP:CG	2.23	0.63
2:B:275:LEU:C	2:B:275:LEU:HD23	2.24	0.62
2:B:417:LEU:O	2:B:420:ILE:HG23	1.99	0.62
2:B:190:VAL:HG13	2:B:568:ILE:HD12	1.80	0.62
1:A:68:GLU:HG2	1:A:146:VAL:HG22	1.82	0.62
2:B:148:TYR:HE1	2:B:418:GLY:HA2	1.59	0.62
2:B:420:ILE:HG13	2:B:421:GLY:N	2.14	0.62
1:A:206:MET:SD	1:A:345:PHE:HD2	2.24	0.61
2:B:448:TRP:CD1	2:B:451:THR:HG1	2.18	0.61
1:A:266:PHE:CZ	1:A:442:PHE:HB3	2.35	0.61
1:A:488:LEU:HD11	2:B:488:LEU:HD11	1.83	0.60
1:A:383:LYS:O	1:A:388:PRO:HA	2.02	0.60
1:A:176:TYR:C	1:A:180:GLY:HA3	2.26	0.60
1:A:448:TRP:CD1	1:A:451:THR:HG1	2.19	0.59
2:B:114:ILE:HD11	2:B:266:PHE:O	2.02	0.59
1:A:137:LEU:HD21	1:A:431:THR:HA	1.85	0.59
1:A:275:LEU:HD23	1:A:275:LEU:O	2.04	0.58
1:A:434:VAL:HG12	1:A:438:ILE:CD1	2.32	0.58
2:B:420:ILE:HD11	2:B:423:CYS:HA	1.86	0.58
2:B:102:PHE:HE1	2:B:266:PHE:CE2	2.23	0.57
1:A:413:ILE:HG23	1:A:416:MET:SD	2.44	0.57
1:A:15:VAL:CG1	1:A:353:VAL:HG22	2.35	0.56
1:A:449:LYS:HE2	1:A:506:ASP:OD2	2.05	0.56
2:B:251:VAL:HG23	2:B:480:MET:HE1	1.88	0.56
2:B:122:PHE:HE1	2:B:451:THR:CG2	2.16	0.56
1:A:512:SER:HB2	2:B:505:ASP:OD1	2.05	0.56
2:B:514:THR:HG22	2:B:515:SER:N	2.20	0.56
1:A:382:TYR:HA	1:A:386:ILE:HG12	1.87	0.56
1:A:224:MET:HB2	1:A:310:VAL:HG21	1.88	0.55
2:B:224:MET:HB2	2:B:310:VAL:HG21	1.87	0.55
2:B:449:LYS:HE2	2:B:506:ASP:OD2	2.06	0.55
1:A:314:ASP:HB3	1:A:317:LEU:HB2	1.89	0.55
1:A:282:GLU:O	1:A:285:LYS:HB2	2.06	0.54
1:A:103:LEU:HD11	1:A:271:ILE:CD1	2.36	0.54
1:A:168:GLY:O	1:A:172:PHE:CG	2.60	0.54
1:A:268:GLN:HG2	1:A:271:ILE:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:GLY:O	2:B:172:PHE:CG	2.61	0.54
2:B:420:ILE:CD1	2:B:423:CYS:HA	2.38	0.54
2:B:314:ASP:HB3	2:B:317:LEU:HB2	1.90	0.53
1:A:108:GLU:HB2	1:A:517:MET:CE	2.27	0.53
1:A:251:VAL:HG23	1:A:480:MET:HE1	1.89	0.53
1:A:281:SER:O	1:A:285:LYS:HG3	2.09	0.52
2:B:434:VAL:HG13	2:B:438:ILE:HD12	1.91	0.52
2:B:148:TYR:CZ	2:B:418:GLY:HA2	2.43	0.52
1:A:505:ASP:OD1	2:B:512:SER:HB2	2.09	0.52
1:A:87:TYR:OH	1:A:428:GLN:HG3	2.09	0.52
1:A:513:VAL:O	1:A:514:THR:OG1	2.26	0.52
1:A:122:PHE:CE1	1:A:451:THR:HG22	2.33	0.52
2:B:123:ASN:HD21	2:B:457:ILE:HD11	1.75	0.51
1:A:206:MET:CE	1:A:345:PHE:HD2	2.23	0.51
2:B:122:PHE:CE1	2:B:451:THR:HG22	2.33	0.51
2:B:87:TYR:OH	2:B:428:GLN:HG3	2.11	0.51
1:A:176:TYR:HA	1:A:180:GLY:HA3	1.93	0.51
2:B:137:LEU:HD21	2:B:431:THR:HA	1.92	0.51
2:B:111:ILE:HG21	2:B:117:PHE:HB2	1.92	0.51
2:B:541:LEU:CD1	2:B:548:ALA:HB3	2.33	0.51
1:A:479:PHE:O	1:A:482:GLN:HB2	2.12	0.51
1:A:113:THR:HG22	1:A:273:ARG:NH2	2.26	0.50
1:A:420:ILE:HD11	1:A:423:CYS:HA	1.93	0.50
1:A:449:LYS:NZ	1:A:506:ASP:OD2	2.44	0.50
1:A:564:THR:O	1:A:568:ILE:HG12	2.11	0.50
1:A:275:LEU:HG	1:A:283:ALA:CB	2.41	0.50
1:A:114:ILE:HG23	1:A:115:PRO:N	2.25	0.50
1:A:185:VAL:O	1:A:185:VAL:CG1	2.60	0.50
1:A:113:THR:CG2	1:A:273:ARG:HH21	2.24	0.49
1:A:434:VAL:CG1	1:A:438:ILE:CD1	2.90	0.49
2:B:168:GLY:O	2:B:172:PHE:CD2	2.66	0.49
2:B:438:ILE:HG22	2:B:442:PHE:CE2	2.48	0.49
2:B:479:PHE:HD1	2:B:483:MET:HE2	1.78	0.49
2:B:56:VAL:HG13	2:B:274:THR:HG22	1.95	0.49
2:B:154:LEU:HB3	2:B:158:LEU:HD12	1.95	0.49
1:A:449:LYS:CE	1:A:506:ASP:OD2	2.61	0.49
1:A:111:ILE:HG21	1:A:117:PHE:HB2	1.95	0.49
1:A:168:GLY:O	1:A:172:PHE:CD2	2.66	0.49
1:A:275:LEU:HG	1:A:283:ALA:HB3	1.94	0.48
1:A:154:LEU:HB3	1:A:158:LEU:HD12	1.95	0.48
2:B:564:THR:O	2:B:568:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PRO:HD2	2:B:480:MET:HE2	1.96	0.48
2:B:449:LYS:NZ	2:B:506:ASP:OD2	2.44	0.48
2:B:514:THR:CG2	2:B:515:SER:N	2.77	0.48
1:A:88:GLU:O	1:A:91:SER:HB2	2.14	0.47
2:B:542:PHE:HD2	2:B:549:GLU:HG3	1.79	0.47
2:B:420:ILE:HD11	2:B:423:CYS:CA	2.45	0.47
2:B:102:PHE:HE1	2:B:266:PHE:HE2	1.63	0.47
1:A:133:PHE:HB3	1:A:434:VAL:HG11	1.96	0.47
1:A:470:LEU:HB3	1:A:482:GLN:HG2	1.96	0.47
1:A:176:TYR:CA	1:A:180:GLY:HA3	2.44	0.47
2:B:88:GLU:O	2:B:91:SER:HB2	2.14	0.47
1:A:349:GLY:O	1:A:353:VAL:HG23	2.15	0.47
2:B:66:SER:HB3	2:B:68:GLU:OE1	2.15	0.47
1:A:206:MET:HE2	1:A:206:MET:HB3	1.88	0.47
2:B:275:LEU:HD23	2:B:275:LEU:O	2.14	0.47
2:B:102:PHE:CE1	2:B:266:PHE:CE2	3.03	0.47
1:A:394:LYS:O	1:A:398:VAL:HG23	2.14	0.47
1:A:268:GLN:HG2	1:A:271:ILE:N	2.30	0.46
2:B:449:LYS:CE	2:B:506:ASP:OD2	2.63	0.46
2:B:394:LYS:O	2:B:398:VAL:HG23	2.15	0.46
1:A:144:THR:HG23	1:A:414:ALA:HA	1.98	0.46
2:B:278:LYS:HG2	2:B:282:GLU:HG2	1.98	0.46
1:A:278:LYS:HG2	1:A:282:GLU:HG2	1.97	0.46
1:A:247:PRO:HD2	1:A:480:MET:HE2	1.96	0.46
2:B:554:ILE:O	2:B:558:MET:HG2	2.16	0.46
2:B:123:ASN:HD21	2:B:457:ILE:CD1	2.28	0.46
2:B:148:TYR:CE2	2:B:417:LEU:CD2	2.99	0.45
1:A:108:GLU:CB	1:A:517:MET:CE	2.90	0.45
1:A:156:THR:HG23	1:A:328:ASN:HB3	1.98	0.45
1:A:122:PHE:HE1	1:A:451:THR:CG2	2.19	0.45
1:A:515:SER:OG	2:B:503:ILE:HA	2.17	0.45
1:A:275:LEU:C	1:A:275:LEU:CD2	2.89	0.45
1:A:434:VAL:CG1	1:A:438:ILE:HD11	2.47	0.45
2:B:122:PHE:CE1	2:B:451:THR:CG2	2.98	0.45
1:A:206:MET:HE3	1:A:345:PHE:HD2	1.82	0.45
1:A:449:LYS:HG3	2:B:450:LYS:HZ1	1.82	0.44
2:B:417:LEU:HG	2:B:420:ILE:HG21	2.00	0.44
1:A:103:LEU:HD21	1:A:271:ILE:HG12	1.97	0.44
2:B:480:MET:HA	2:B:483:MET:HE3	2.00	0.44
1:A:347:PRO:O	1:A:351:LYS:HB2	2.18	0.44
1:A:473:MET:HB3	1:A:475:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:HD2	1:A:511:ILE:HG12	2.00	0.44
1:A:123:ASN:HD21	1:A:457:ILE:HD11	1.83	0.44
1:A:554:ILE:O	1:A:558:MET:HG2	2.18	0.44
1:A:188:THR:O	1:A:192:GLN:HB2	2.18	0.43
2:B:95:LEU:HD21	2:B:264:TRP:CE3	2.53	0.43
2:B:156:THR:O	2:B:344:GLN:OE1	2.36	0.43
1:A:514:THR:O	1:A:515:SER:HB3	2.19	0.43
1:A:122:PHE:CE1	1:A:451:THR:CG2	3.00	0.43
1:A:542:PHE:CD2	1:A:549:GLU:HG3	2.54	0.43
2:B:541:LEU:CD2	2:B:552:LEU:HD22	2.41	0.42
1:A:61:ILE:HD12	1:A:61:ILE:HA	1.95	0.42
1:A:155:GLU:OE1	1:A:337:LYS:NZ	2.52	0.42
2:B:188:THR:O	2:B:192:GLN:HB2	2.19	0.42
2:B:144:THR:HG23	2:B:414:ALA:HA	2.01	0.42
1:A:448:TRP:CZ3	2:B:447:PHE:O	2.73	0.42
1:A:160:ILE:H	1:A:160:ILE:HG13	1.71	0.42
1:A:420:ILE:CD1	1:A:423:CYS:HA	2.50	0.42
1:A:480:MET:HA	1:A:483:MET:HE2	2.01	0.42
1:A:514:THR:HG22	1:A:515:SER:N	2.35	0.42
2:B:541:LEU:HD11	2:B:548:ALA:HB1	1.95	0.42
1:A:275:LEU:C	1:A:277:ALA:N	2.71	0.41
1:A:450:LYS:HZ1	2:B:449:LYS:HG3	1.84	0.41
1:A:113:THR:CG2	1:A:273:ARG:NH2	2.82	0.41
2:B:64:ASN:HD21	2:B:264:TRP:HZ2	1.69	0.41
2:B:479:PHE:HA	2:B:482:GLN:NE2	2.35	0.41
2:B:479:PHE:CD1	2:B:483:MET:HE2	2.54	0.41
1:A:87:TYR:CZ	1:A:428:GLN:HG3	2.55	0.41
1:A:471:LYS:HG2	1:A:482:GLN:OE1	2.20	0.41
1:A:113:THR:HG22	1:A:273:ARG:HH21	1.86	0.41
1:A:179:TYR:CD2	1:A:179:TYR:N	2.89	0.41
1:A:181:GLY:HA2	1:A:400:ARG:HH12	1.86	0.41
1:A:268:GLN:NE2	1:A:271:ILE:HB	2.36	0.41
2:B:109:LYS:HD2	2:B:511:ILE:HG12	2.03	0.41
2:B:148:TYR:CE2	2:B:417:LEU:HD23	2.56	0.41
1:A:514:THR:CG2	1:A:515:SER:N	2.84	0.41
1:A:125:LYS:O	1:A:129:ILE:HG12	2.21	0.40
2:B:125:LYS:O	2:B:129:ILE:HG12	2.21	0.40
2:B:206:MET:HG3	2:B:346:LEU:HD23	2.02	0.40
2:B:275:LEU:HG	2:B:283:ALA:CB	2.51	0.40
2:B:417:LEU:O	2:B:417:LEU:CD2	2.59	0.40
2:B:130:LEU:HD22	2:B:438:ILE:HG12	2.03	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	530/593 (89%)	505 (95%)	22 (4%)	3 (1%)	21	36
2	B	496/593 (84%)	469 (95%)	25 (5%)	2 (0%)	30	47
All	All	1026/1186 (86%)	974 (95%)	47 (5%)	5 (0%)	24	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
2	B	276	ALA
1	A	276	ALA
1	A	414	ALA
2	B	414	ALA

5.3.2 Protein sidechains [i](#)

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	434/478 (91%)	414 (95%)	20 (5%)	24	43
2	B	410/436 (94%)	393 (96%)	17 (4%)	27	48
All	All	844/914 (92%)	807 (96%)	37 (4%)	25	45

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	23	ILE
1	A	61	ILE
1	A	68	GLU
1	A	119	GLU
1	A	174	LEU
1	A	249	ILE
1	A	251	VAL
1	A	296	ILE
1	A	312	THR
1	A	350	VAL
1	A	380	ASP
1	A	420	ILE
1	A	441	VAL
1	A	460	VAL
1	A	480	MET
1	A	491	MET
1	A	549	GLU
1	A	567	LEU
1	A	573	LYS
2	B	61	ILE
2	B	119	GLU
2	B	174	LEU
2	B	249	ILE
2	B	251	VAL
2	B	271	ILE
2	B	279	SER
2	B	312	THR
2	B	380	ASP
2	B	434	VAL
2	B	441	VAL
2	B	460	VAL
2	B	480	MET
2	B	491	MET
2	B	549	GLU
2	B	567	LEU
2	B	573	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	GLN
1	A	428	GLN

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Mol	Chain	Res	Type
1	A	504	ASN
1	A	525	ASN
2	B	245	ASN
2	B	284	GLN
2	B	422	GLN
2	B	428	GLN
2	B	504	ASN
2	B	525	ASN

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](#)

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	PEG	A	1575	-	6,6,6	0.57	0	5,5,5	0.72	0
3	PEG	A	1576	-	6,6,6	0.53	0	5,5,5	0.94	0
3	PEG	A	1574	-	6,6,6	0.65	0	5,5,5	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	1575	-	-	2/4/4/4	-
3	PEG	A	1576	-	-	2/4/4/4	-
3	PEG	A	1574	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1575	PEG	O1-C1-C2-O2
3	A	1576	PEG	O1-C1-C2-O2
3	A	1575	PEG	C1-C2-O2-C3
3	A	1574	PEG	O2-C3-C4-O4
3	A	1576	PEG	C1-C2-O2-C3
3	A	1574	PEG	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	27:UNK	C	51:LEU	N	23.43

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	538/593 (90%)	2.09	198 (36%) 1 1	44, 88, 129, 164	0
2	B	506/593 (85%)	2.49	209 (41%) 0 0	67, 131, 188, 241	0
All	All	1044/1186 (88%)	2.28	407 (38%) 1 0	44, 104, 174, 241	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	LEU	27.7
1	A	322	GLY	24.8
2	B	187	TRP	19.2
2	B	158	LEU	18.3
2	B	161	PRO	18.3
2	B	344	GLN	16.2
2	B	64	ASN	16.2
2	B	571	GLY	16.2
2	B	159	GLY	16.1
2	B	160	ILE	15.6
2	B	189	ASP	15.1
1	A	29	TRP	14.0
1	A	318	MET	14.0
2	B	351	LYS	13.6
1	A	320	SER	13.5
2	B	263	TYR	13.3
1	A	112	TYR	13.2
2	B	60	LEU	13.0
2	B	186	VAL	12.6
1	A	345	PHE	12.3
1	A	319	ALA	12.1
2	B	268	GLN	11.8
2	B	264	TRP	11.2
2	B	321	LEU	10.9

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Mol	Chain	Res	Type	RSRZ
2	B	350	VAL	10.8
2	B	62	ALA	10.7
1	A	329	LEU	10.5
1	A	210	PHE	10.4
1	A	474	PRO	10.3
2	B	267	ASN	10.2
2	B	63	ALA	9.9
1	A	28	LEU	9.8
1	A	533	ILE	9.7
2	B	279	SER	9.6
2	B	522	ARG	9.6
2	B	353	VAL	9.5
2	B	567	LEU	9.3
1	A	164	TYR	9.2
2	B	59	SER	9.2
1	A	328	ASN	9.1
1	A	273	ARG	9.1
1	A	276	ALA	8.6
2	B	274	THR	8.3
2	B	157	ILE	8.3
2	B	388	PRO	8.2
2	B	318	MET	8.2
2	B	55	ALA	8.1
2	B	345	PHE	8.0
2	B	280	VAL	7.9
2	B	262	TYR	7.7
1	A	269	TYR	7.7
1	A	10	PHE	7.7
2	B	265	GLY	7.6
2	B	341	TRP	7.6
1	A	134	TRP	7.5
2	B	176	TYR	7.4
1	A	274	THR	7.4
1	A	50	SER	7.4
2	B	273	ARG	7.3
2	B	261	LEU	7.2
2	B	317	LEU	7.2
2	B	275	LEU	7.2
2	B	61	ILE	7.1
1	A	341	TRP	7.1
1	A	543	TRP	7.1
1	A	442	PHE	7.1

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Mol	Chain	Res	Type	RSRZ
2	B	389	ASP	7.1
2	B	51	LEU	7.0
1	A	315	PRO	7.0
1	A	133	PHE	7.0
1	A	132	VAL	6.9
1	A	209	SER	6.9
2	B	156	THR	6.9
2	B	133	PHE	6.8
2	B	513	VAL	6.8
2	B	58	ALA	6.7
1	A	317	LEU	6.7
2	B	472	PHE	6.6
1	A	206	MET	6.6
2	B	202	MET	6.6
2	B	386	ILE	6.5
2	B	572	ILE	6.4
1	A	532	MET	6.3
1	A	530	GLY	6.3
1	A	573	LYS	6.3
1	A	11	ILE	6.2
2	B	65	ILE	6.2
2	B	278	LYS	6.2
2	B	563	GLY	6.1
2	B	270	ILE	6.0
1	A	348	VAL	6.0
2	B	266	PHE	6.0
2	B	198	LEU	6.0
1	A	268	GLN	5.9
1	A	472	PHE	5.9
2	B	564	THR	5.9
2	B	179	TYR	5.8
2	B	210	PHE	5.8
2	B	107	ILE	5.7
1	A	544	VAL	5.7
2	B	239	SER	5.7
1	A	217	TRP	5.7
2	B	407	LEU	5.6
2	B	461	VAL	5.6
1	A	161	PRO	5.6
1	A	248	GLY	5.6
2	B	346	LEU	5.5
1	A	205	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	517	MET	5.4
2	B	450	LYS	5.4
1	A	84	ILE	5.4
2	B	54	TRP	5.4
1	A	15	VAL	5.4
2	B	195	PHE	5.3
2	B	87	TYR	5.3
2	B	269	TYR	5.3
1	A	51	LEU	5.3
1	A	572	ILE	5.3
2	B	354	VAL	5.3
1	A	227	ALA	5.2
1	A	330	PRO	5.2
2	B	147	LEU	5.2
1	A	239	SER	5.2
2	B	190	VAL	5.2
1	A	277	ALA	5.2
2	B	411	ALA	5.2
1	A	473	MET	5.1
1	A	529	TYR	5.1
2	B	392	ASP	5.1
1	A	249	ILE	5.0
1	A	438	ILE	5.0
2	B	219	ALA	5.0
2	B	523	SER	5.0
2	B	394	LYS	5.0
2	B	573	LYS	4.9
1	A	503	ILE	4.9
1	A	82	LEU	4.9
1	A	333	ALA	4.8
1	A	9	SER	4.8
1	A	13	ILE	4.8
1	A	30	VAL	4.8
2	B	173	ALA	4.8
1	A	331	SER	4.8
1	A	262	TYR	4.8
1	A	272	GLN	4.8
2	B	164	TYR	4.7
1	A	302	VAL	4.7
2	B	363	VAL	4.7
2	B	352	GLY	4.7
2	B	155	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	340	PRO	4.7
1	A	110	GLY	4.6
1	A	267	ASN	4.6
1	A	285	LYS	4.6
1	A	130	LEU	4.6
1	A	16	PHE	4.6
1	A	266	PHE	4.6
2	B	390	SER	4.6
2	B	167	LEU	4.5
2	B	431	THR	4.5
2	B	462	ALA	4.5
2	B	311	ILE	4.5
2	B	408	ILE	4.5
2	B	258	VAL	4.5
2	B	526	ILE	4.5
1	A	83	ALA	4.5
1	A	353	VAL	4.5
1	A	441	VAL	4.4
2	B	465	PRO	4.4
2	B	560	GLY	4.4
1	A	476	SER	4.3
1	A	457	ILE	4.3
1	A	246	LEU	4.2
2	B	260	ASN	4.2
1	A	234	MET	4.2
2	B	143	LEU	4.2
1	A	536	ALA	4.2
1	A	135	ILE	4.2
1	A	355	PHE	4.2
1	A	14	MET	4.2
1	A	120	LYS	4.2
2	B	410	ALA	4.2
1	A	292	PHE	4.2
2	B	170	ALA	4.1
2	B	193	VAL	4.1
1	A	71	ILE	4.1
2	B	458	ILE	4.1
1	A	568	ILE	4.0
1	A	453	SER	4.0
1	A	19	TYR	4.0
1	A	263	TYR	4.0
1	A	456	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	349	GLY	3.9
1	A	450	LYS	3.9
2	B	343	THR	3.9
1	A	157	ILE	3.9
2	B	56	VAL	3.9
2	B	284	GLN	3.9
1	A	275	LEU	3.9
1	A	187	TRP	3.9
1	A	129	ILE	3.9
2	B	320	SER	3.8
1	A	561	VAL	3.8
1	A	18	ILE	3.8
2	B	292	PHE	3.8
2	B	519	VAL	3.8
1	A	226	ASP	3.8
2	B	323	ASP	3.8
1	A	454	LYS	3.8
1	A	493	VAL	3.8
1	A	126	LEU	3.8
2	B	367	ALA	3.8
1	A	419	GLY	3.8
2	B	251	VAL	3.8
2	B	206	MET	3.7
2	B	256	LEU	3.7
1	A	111	ILE	3.7
1	A	531	ILE	3.7
2	B	154	LEU	3.7
1	A	303	LEU	3.7
1	A	122	PHE	3.7
2	B	370	LEU	3.6
2	B	559	ALA	3.6
2	B	516	SER	3.6
1	A	237	ASP	3.6
1	A	513	VAL	3.6
1	A	103	LEU	3.6
1	A	519	VAL	3.6
2	B	103	LEU	3.6
2	B	144	THR	3.5
1	A	212	GLY	3.5
2	B	406	ALA	3.5
2	B	129	ILE	3.5
1	A	176	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	108	GLU	3.5
2	B	218	PHE	3.4
2	B	412	LEU	3.4
1	A	114	ILE	3.4
1	A	570	TYR	3.4
1	A	85	ALA	3.4
1	A	270	ILE	3.3
1	A	278	LYS	3.3
1	A	216	GLY	3.3
2	B	216	GLY	3.3
1	A	149	LEU	3.3
2	B	283	ALA	3.3
2	B	102	PHE	3.3
1	A	526	ILE	3.3
2	B	171	LEU	3.3
1	A	332	ALA	3.3
2	B	512	SER	3.3
2	B	385	TYR	3.3
1	A	383	LYS	3.3
2	B	427	ILE	3.2
1	A	241	PRO	3.2
2	B	276	ALA	3.2
1	A	185	VAL	3.2
2	B	518	PHE	3.2
1	A	492	VAL	3.2
1	A	371	ASN	3.2
1	A	17	ALA	3.2
2	B	139	ILE	3.2
2	B	174	LEU	3.1
2	B	252	LEU	3.1
2	B	413	ILE	3.1
2	B	546	ALA	3.1
2	B	568	ILE	3.1
2	B	468	LEU	3.1
1	A	236	LEU	3.1
2	B	414	ALA	3.1
1	A	235	ILE	3.0
2	B	405	VAL	3.0
2	B	178	ILE	3.0
2	B	477	MET	3.0
2	B	514	THR	3.0
2	B	163	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	166	ILE	3.0
2	B	214	THR	3.0
1	A	26	VAL	3.0
2	B	197	VAL	3.0
1	A	76	SER	3.0
2	B	69	GLN	3.0
2	B	511	ILE	3.0
1	A	358	LEU	2.9
1	A	247	PRO	2.9
1	A	298	PRO	2.9
2	B	331	SER	2.9
2	B	469	PHE	2.9
2	B	277	ALA	2.9
1	A	251	VAL	2.9
2	B	282	GLU	2.9
1	A	281	SER	2.9
1	A	27	GLY	2.9
2	B	487	LEU	2.9
1	A	116	GLU	2.8
2	B	177	SER	2.8
1	A	334	ASN	2.8
1	A	153	ALA	2.8
2	B	108	GLU	2.8
1	A	352	GLY	2.8
1	A	557	VAL	2.8
1	A	118	VAL	2.8
2	B	259	ALA	2.8
2	B	387	SER	2.7
1	A	455	GLY	2.7
2	B	57	GLY	2.7
1	A	12	ASP	2.7
2	B	333	ALA	2.7
1	A	469	PHE	2.7
2	B	424	PHE	2.7
2	B	439	LEU	2.7
1	A	72	GLY	2.7
1	A	314	ASP	2.7
1	A	412	LEU	2.7
2	B	443	LEU	2.7
1	A	356	ALA	2.7
2	B	434	VAL	2.7
2	B	376	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	301	VAL	2.7
1	A	449	LYS	2.7
1	A	191	ILE	2.6
1	A	211	ILE	2.6
2	B	366	LEU	2.6
1	A	136	SER	2.6
2	B	281	SER	2.6
1	A	316	GLN	2.6
1	A	509	LYS	2.6
1	A	218	PHE	2.6
1	A	74	SER	2.6
1	A	279	SER	2.6
1	A	65	ILE	2.6
2	B	100	LYS	2.6
2	B	334	ASN	2.6
1	A	312	THR	2.5
2	B	86	SER	2.5
1	A	73	MET	2.5
2	B	515	SER	2.5
2	B	492	VAL	2.5
2	B	217	TRP	2.5
1	A	179	TYR	2.5
2	B	381	ILE	2.5
2	B	409	ILE	2.5
1	A	517	MET	2.5
2	B	330	PRO	2.5
1	A	534	VAL	2.5
1	A	117	PHE	2.5
1	A	232	PHE	2.4
2	B	194	PHE	2.4
1	A	160	ILE	2.4
2	B	123	ASN	2.4
2	B	293	LEU	2.4
2	B	303	LEU	2.4
1	A	369	MET	2.4
2	B	391	GLY	2.4
1	A	20	VAL	2.4
1	A	475	LEU	2.3
1	A	22	ILE	2.3
1	A	107	ILE	2.3
1	A	494	ILE	2.3
2	B	224	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	336	ASP	2.3
2	B	120	LYS	2.3
1	A	81	GLY	2.3
2	B	355	PHE	2.3
2	B	137	LEU	2.3
1	A	491	MET	2.3
1	A	264	TRP	2.3
2	B	491	MET	2.3
2	B	371	ASN	2.3
1	A	213	GLY	2.3
1	A	154	LEU	2.3
2	B	474	PRO	2.3
1	A	306	ILE	2.2
1	A	202	MET	2.2
2	B	300	LEU	2.2
2	B	299	PHE	2.2
1	A	304	PRO	2.2
2	B	454	LYS	2.2
2	B	140	PHE	2.2
1	A	300	LEU	2.2
1	A	215	ASP	2.2
2	B	215	ASP	2.2
2	B	403	ALA	2.1
1	A	78	TYR	2.1
2	B	112	TYR	2.1
2	B	481	ASP	2.1
2	B	543	TRP	2.1
1	A	514	THR	2.1
1	A	223	LYS	2.1
2	B	169	LEU	2.1
2	B	172	PHE	2.1
1	A	522	ARG	2.1
2	B	501	THR	2.1
2	B	162	LEU	2.1
1	A	464	ILE	2.1
2	B	253	ILE	2.1
1	A	313	SER	2.0
2	B	66	SER	2.0
1	A	501	THR	2.0
2	B	415	PRO	2.0
1	A	158	LEU	2.0
1	A	253	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	172	PHE	2.0
2	B	360	ALA	2.0
2	B	383	LYS	2.0
2	B	249	ILE	2.0
2	B	485	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	A	1574	7/7	0.77	0.40	121,207,245,253	0
3	PEG	A	1575	7/7	0.80	0.30	55,128,205,249	0
3	PEG	A	1576	7/7	0.89	0.32	45,63,205,221	0

6.5 Other polymers [i](#)

There are no such residues in this entry.