Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 09:13 pm GMT

PDB ID	:	2XQ2
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:

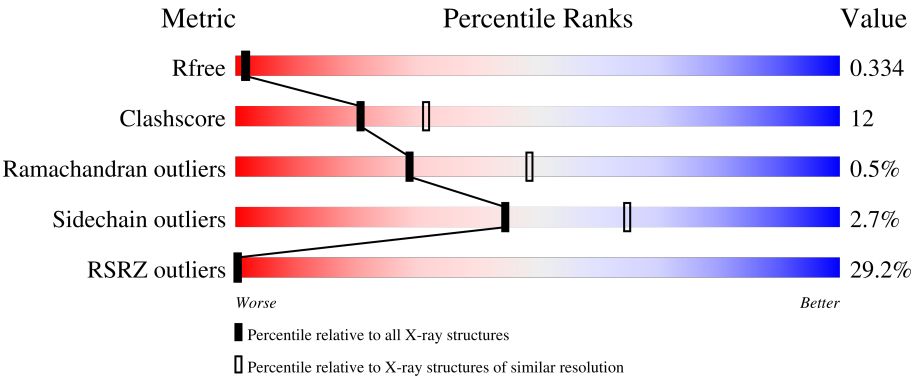
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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 <=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	18% 69% 21% • 9%
2	B	593	33% 72% 16% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	1574	-	-	-	X
3	PEG	A	1575	-	-	-	X
3	PEG	A	1576	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	538	4107	2762	612	711	22	0	0	0

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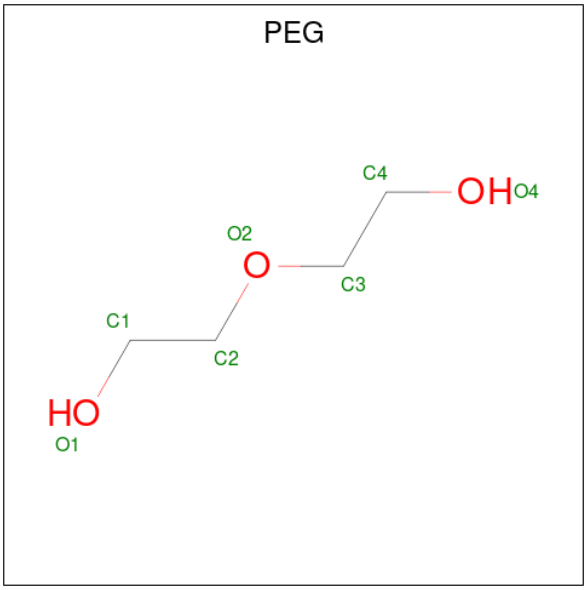
Chain	Residue	Modelled	Actual	Comment	Reference
B	589	HIS	-	expression tag	UNP P96169
B	590	HIS	-	expression tag	UNP P96169
B	591	HIS	-	expression tag	UNP P96169
B	592	HIS	-	expression tag	UNP P96169
B	593	HIS	-	expression tag	UNP P96169

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: 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.

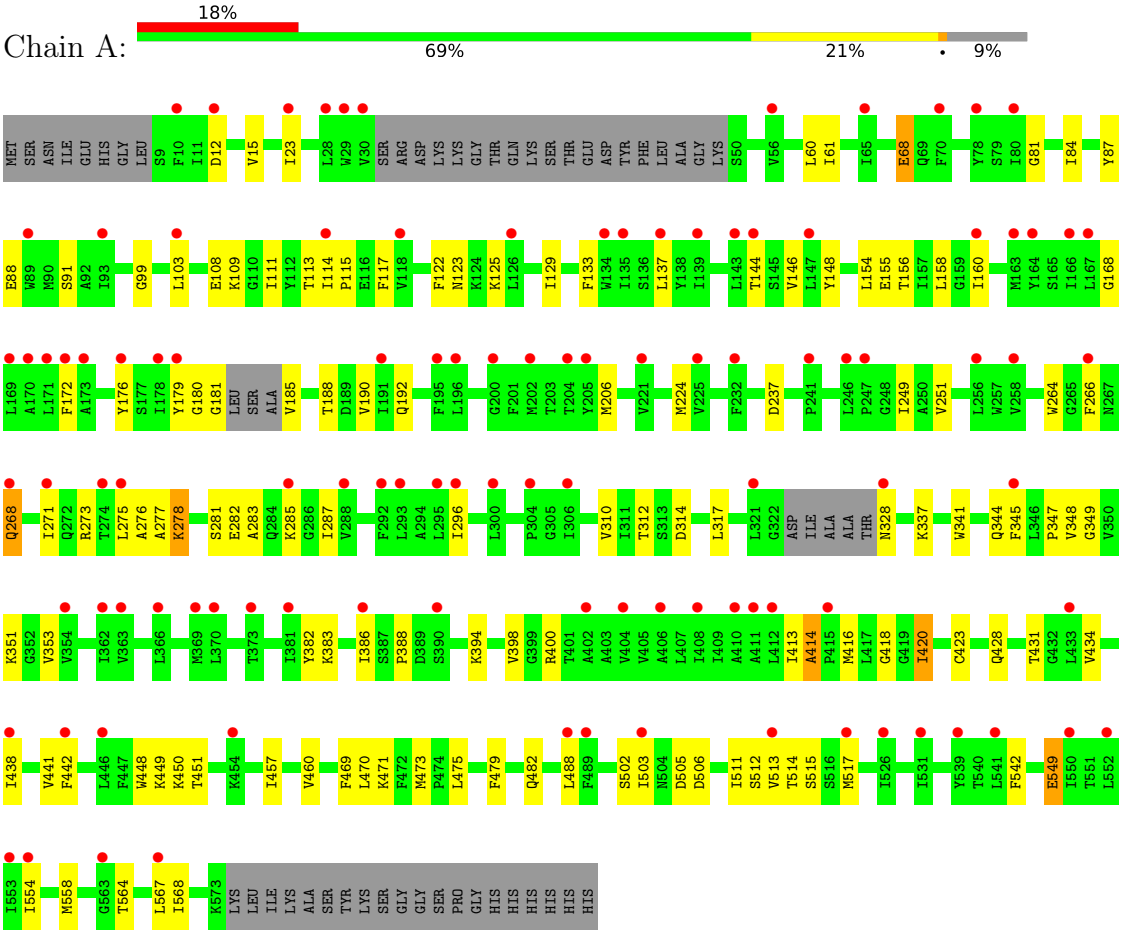
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0

3 Residue-property plots (i)

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.

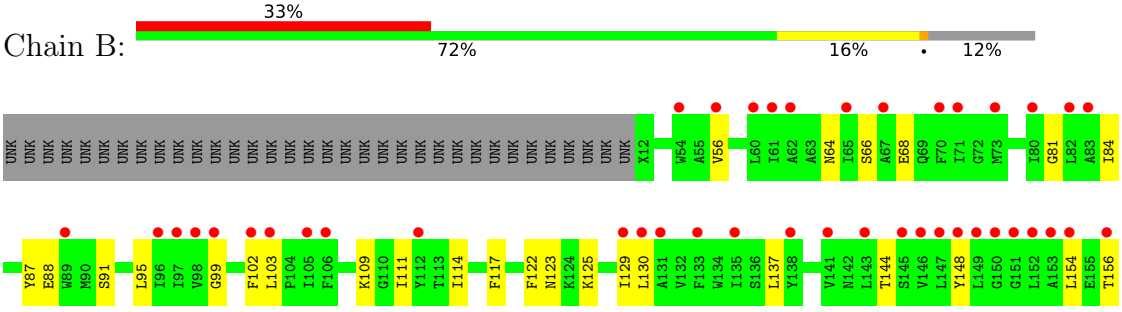
• Molecule 1: SODIUM/GLUCOSE COTRANSPORTER

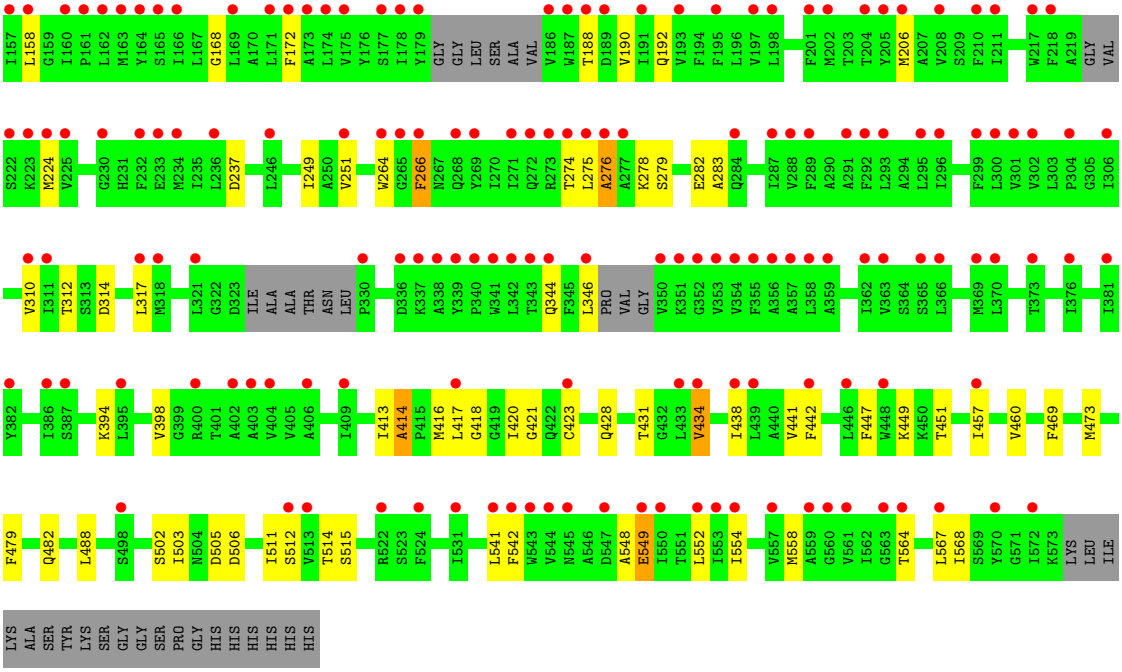
Chain A:



• Molecule 2: SODIUM/GLUCOSE COTRANSPORTER

Chain B:




I157 L158 G159 I160 P161 L162 M163 Y164 S165 I166 L167 G168 L169 A170 L171 F172 A173 L174 V175 Y176 S177 I178 Y179 GLY GLY LEU SER ALA VAL V186 W187 T188 D189 V190 I191 Q192 V193 F194 F195 L196 V197 L198 F201 M202 T203 T204 Y205 M206 A207 V208 S209 F210 I211 W217 F218 A219 GLY VAL
S222 K223 M224 V225 G230 H231 F232 E233 M234 I235 L236 D237 L246 I249 A250 V251 W264 G265 F266 N267 Q268 Y269 I270 I271 Q272 R273 T274 L275 A276 A277 K278 S279 E282 A283 Q284 I287 V288 P289 A290 A291 F292 L293 A294 L296 I296 P299 L300 V301 V302 L303 P304 G305 I306
V310 T311 T312 S313 D314 L317 M318 L321 G322 D323 ILE ALA ALA THR ASN LEU P330 D336 K337 A338 Y339 P340 W341 L342 T343 Q344 F345 L346 PRO VAL GLY V350 K351 G352 V353 V354 F355 A356 A357 L358 A359 I362 V363 S364 S365 L366 M369 L370 T373 I378 I381
Y382 I386 S387 K394 L395 V398 G399 R400 T401 A402 A403 V404 V405 A406 I409 I413 A414 P415 M416 L417 G418 G419 I420 G421 Q422 C423 Q428 T431 G432 L433 V434 I438 L439 A440 V441 F442 L446 F447 W448 K449 K450 T451 I457 V460 F469 M473
F479 Q482 L488 S498 S502 I503 N504 D505 D506 I511 S512 V513 T514 S515 R522 S523 F524 I531 L541 F542 W543 V544 N545 A546 D547 A548 E549 I550 T551 L552 I553 I554 V557 M558 A559 G560 V561 I562 G563 T564 L567 I568 S569 Y570 G571 I572 K573 LYS LEU ILE
LYS ALA SER TYR LYS SER GLY GLY SER PRO GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (68.01-2.73) 96.5 (68.01-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.251 , 0.274 0.287 , 0.334	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)	0.24 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/4210	0.72	2/5741 (0.0%)
2	B	0.46	0/3973	0.70	2/5413 (0.0%)
All	All	0.48	0/8183	0.71	4/11154 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	276	ALA	CB-CA-C	7.57	121.45	110.10
2	B	266	PHE	N-CA-C	6.79	129.35	111.00
1	A	268	GLN	CB-CA-C	5.43	121.26	110.40
1	A	348	VAL	N-CA-C	5.06	124.67	111.00

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	122	0
2	B	3957	0	4022	89	0
3	A	21	0	30	0	0
4	A	5	0	0	0	0
All	All	8090	0	8304	201	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 12.

All (201) 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
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
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:108:GLU:HB2	1:A:517:MET:HE1	1.52	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:NE2	1:A:428:GLN:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185:VAL:HG12	1:A:185:VAL:O	1.93	0.68
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: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
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:HB2	1:A:517:MET:CE	2.27	0.63
2:B:417:LEU:O	2:B:420:ILE:HG23	1.99	0.62
1:A:275:LEU:C	1:A:275:LEU:HD23	2.19	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:275:LEU:C	1:A:277:ALA:H	2.03	0.61
1:A:206:MET:SD	1:A:345:PHE:HD2	2.24	0.61
1:A:266:PHE:CZ	1:A:442:PHE:HB3	2.35	0.61
1:A:449:LYS:HE2	1:A:506:ASP:CG	2.21	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
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
2:B:449:LYS:HE2	2:B:506:ASP:CG	2.23	0.58
1:A:434:VAL:HG12	1:A:438:ILE:CD1	2.32	0.58
2:B:275:LEU:C	2:B:275:LEU:HD23	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:176:TYR:C	1:A:180:GLY:HA3	2.26	0.55
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
2:B:168:GLY:O	2:B:172:PHE:CG	2.61	0.54
1:A:108:GLU:CB	1:A:517:MET:HE1	2.34	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: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:108:GLU:CB	1:A:517:MET:CE	2.90	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
1:A:87:TYR:CZ	1:A:428:GLN:HG3	2.55	0.41
1:A:450:LYS:HZ1	2:B:449:LYS:HG3	1.84	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
1:A:275:LEU:C	1:A:275:LEU:CD2	2.89	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%)	25	44
2	B	496/593 (84%)	469 (95%)	25 (5%)	2 (0%)	34	55
All	All	1026/1186 (86%)	974 (95%)	47 (5%)	5 (0%)	29	48

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%)	421 (97%)	13 (3%)	41	61
2	B	410/436 (94%)	400 (98%)	10 (2%)	49	68
All	All	844/914 (92%)	821 (97%)	23 (3%)	44	65

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	23	ILE
1	A	68	GLU
1	A	237	ASP
1	A	249	ILE
1	A	251	VAL
1	A	296	ILE
1	A	312	THR
1	A	420	ILE
1	A	441	VAL
1	A	460	VAL
1	A	549	GLU
1	A	567	LEU
2	B	237	ASP
2	B	249	ILE
2	B	251	VAL
2	B	279	SER
2	B	312	THR
2	B	434	VAL
2	B	441	VAL
2	B	460	VAL
2	B	549	GLU
2	B	567	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	268	GLN
1	A	422	GLN
1	A	428	GLN
1	A	525	ASN
2	B	245	ASN
2	B	422	GLN
2	B	428	GLN
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 monosaccharides 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	1576	-	6,6,6	0.52	0	5,5,5	0.94	0
3	PEG	A	1575	-	6,6,6	0.56	0	5,5,5	0.73	0
3	PEG	A	1574	-	6,6,6	0.64	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	1576	-	-	2/4/4/4	-
3	PEG	A	1575	-	-	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, 95^{th} 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%)	1.22	107 (19%)	1	1	44, 88, 129, 164	0
2	B	506/593 (85%)	2.02	198 (39%)	0	0	67, 131, 188, 241	0
All	All	1044/1186 (88%)	1.61	305 (29%)	0	0	44, 104, 174, 241	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	353	VAL	13.3
2	B	354	VAL	9.7
2	B	218	PHE	9.7
2	B	154	LEU	8.9
2	B	179	TYR	8.9
2	B	339	TYR	8.3
2	B	395	LEU	8.3
2	B	175	VAL	8.2
2	B	217	TRP	8.2
2	B	189	ASP	8.0
2	B	160	ILE	8.0
2	B	195	PHE	7.7
2	B	161	PRO	7.5
2	B	187	TRP	7.5
2	B	158	LEU	7.4
2	B	276	ALA	7.4
2	B	60	LEU	7.4
2	B	318	MET	7.3
2	B	340	PRO	7.3
2	B	233	GLU	7.2
2	B	222	SER	6.8
2	B	317	LEU	6.8
2	B	274	THR	6.8
2	B	198	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
2	B	202	MET	6.7
2	B	404	VAL	6.6
2	B	166	ILE	6.5
2	B	211	ILE	6.5
2	B	358	LEU	6.4
2	B	350	VAL	6.4
2	B	173	ALA	6.3
2	B	169	LEU	6.3
2	B	232	PHE	6.3
2	B	567	LEU	6.2
2	B	177	SER	6.1
2	B	205	TYR	6.1
2	B	103	LEU	6.0
2	B	550	ILE	5.8
2	B	149	LEU	5.7
2	B	311	ILE	5.5
2	B	356	ALA	5.4
2	B	150	GLY	5.4
2	B	373	THR	5.3
1	A	166	ILE	5.3
2	B	162	LEU	5.3
2	B	272	GLN	5.2
2	B	225	VAL	5.2
2	B	133	PHE	5.2
2	B	352	GLY	5.2
1	A	10	PHE	5.1
2	B	82	LEU	5.0
2	B	343	THR	5.0
2	B	554	ILE	5.0
1	A	164	TYR	5.0
1	A	147	LEU	4.9
2	B	547	ASP	4.9
2	B	201	PHE	4.9
2	B	56	VAL	4.9
2	B	266	PHE	4.9
2	B	355	PHE	4.9
2	B	553	ILE	4.8
2	B	549	GLU	4.8
2	B	369	MET	4.8
2	B	197	VAL	4.8
2	B	552	LEU	4.7
2	B	359	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	351	LYS	4.7
2	B	174	LEU	4.7
2	B	366	LEU	4.6
1	A	176	TYR	4.6
2	B	300	LEU	4.6
1	A	345	PHE	4.5
2	B	210	PHE	4.5
2	B	376	ILE	4.5
2	B	102	PHE	4.4
2	B	156	THR	4.3
2	B	400	ARG	4.3
2	B	560	GLY	4.3
2	B	164	TYR	4.3
1	A	12	ASP	4.2
2	B	273	ARG	4.2
1	A	366	LEU	4.2
1	A	531	ILE	4.1
1	A	442	PHE	4.1
2	B	288	VAL	4.1
1	A	370	LEU	4.1
1	A	172	PHE	4.1
1	A	170	ALA	4.1
2	B	146	VAL	4.0
1	A	321	LEU	4.0
2	B	362	ILE	4.0
2	B	191	ILE	4.0
1	A	563	GLY	3.9
2	B	71	ILE	3.9
2	B	186	VAL	3.9
2	B	341	TRP	3.9
2	B	271	ILE	3.9
1	A	363	VAL	3.9
2	B	143	LEU	3.9
2	B	264	TRP	3.9
2	B	157	ILE	3.9
2	B	65	ILE	3.9
2	B	363	VAL	3.9
1	A	135	ILE	3.8
2	B	208	VAL	3.8
2	B	321	LEU	3.8
1	A	143	LEU	3.8
2	B	265	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	541	LEU	3.7
1	A	526	ILE	3.7
1	A	169	LEU	3.7
2	B	382	TYR	3.7
1	A	167	LEU	3.6
2	B	289	PHE	3.6
2	B	172	PHE	3.6
2	B	302	VAL	3.6
2	B	570	TYR	3.6
2	B	70	PHE	3.6
2	B	151	GLY	3.6
2	B	346	LEU	3.6
1	A	369	MET	3.5
2	B	80	ILE	3.5
2	B	545	ASN	3.5
1	A	268	GLN	3.5
1	A	412	LEU	3.5
1	A	173	ALA	3.4
2	B	147	LEU	3.4
2	B	557	VAL	3.4
1	A	103	LEU	3.4
1	A	513	VAL	3.4
2	B	513	VAL	3.4
2	B	403	ALA	3.4
2	B	564	THR	3.4
2	B	148	TYR	3.3
2	B	188	THR	3.3
2	B	54	TRP	3.3
2	B	406	ALA	3.3
1	A	179	TYR	3.2
2	B	561	VAL	3.2
1	A	70	PHE	3.2
1	A	415	PRO	3.2
2	B	442	PHE	3.2
2	B	99	GLY	3.2
1	A	195	PHE	3.2
2	B	386	ILE	3.2
1	A	292	PHE	3.1
2	B	310	VAL	3.1
1	A	296	ILE	3.1
2	B	129	ILE	3.1
2	B	330	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	89	TRP	3.1
1	A	288	VAL	3.1
2	B	370	LEU	3.1
1	A	410	ALA	3.0
2	B	295	LEU	3.0
1	A	29	TRP	3.0
1	A	139	ILE	3.0
1	A	408	ILE	3.0
2	B	563	GLY	3.0
1	A	30	VAL	3.0
1	A	550	ILE	3.0
1	A	554	ILE	3.0
2	B	105	ILE	3.0
1	A	438	ILE	2.9
1	A	160	ILE	2.9
2	B	145	SER	2.9
2	B	409	ILE	2.9
2	B	152	LEU	2.9
1	A	274	THR	2.9
2	B	67	ALA	2.9
2	B	292	PHE	2.9
1	A	552	LEU	2.9
2	B	338	ALA	2.9
1	A	178	ILE	2.8
1	A	567	LEU	2.8
1	A	433	LEU	2.8
2	B	304	PRO	2.8
1	A	386	ILE	2.8
1	A	553	ILE	2.8
2	B	306	ILE	2.8
2	B	544	VAL	2.8
1	A	114	ILE	2.8
2	B	171	LEU	2.8
2	B	365	SER	2.8
2	B	423	CYS	2.8
2	B	417	LEU	2.7
2	B	165	SER	2.7
2	B	336	ASP	2.7
1	A	295	LEU	2.7
1	A	163	MET	2.7
2	B	234	MET	2.7
2	B	287	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	291	ALA	2.7
1	A	221	VAL	2.7
2	B	224	MET	2.7
1	A	362	ILE	2.7
2	B	381	ILE	2.7
1	A	402	ALA	2.7
1	A	411	ALA	2.7
2	B	251	VAL	2.7
2	B	275	LEU	2.7
2	B	402	ALA	2.7
1	A	293	LEU	2.7
1	A	65	ILE	2.7
2	B	153	ALA	2.6
1	A	258	VAL	2.6
1	A	78	TYR	2.6
1	A	381	ILE	2.6
2	B	284	GLN	2.6
2	B	299	PHE	2.6
2	B	135	ILE	2.6
2	B	268	GLN	2.6
1	A	390	SER	2.6
2	B	542	PHE	2.6
1	A	454	LYS	2.5
2	B	178	ILE	2.5
1	A	300	LEU	2.5
1	A	328	ASN	2.5
2	B	61	ILE	2.5
1	A	171	LEU	2.5
1	A	541	LEU	2.5
1	A	503	ILE	2.5
2	B	193	VAL	2.5
2	B	163	MET	2.5
1	A	200	GLY	2.5
2	B	559	ALA	2.5
1	A	89	TRP	2.5
1	A	517	MET	2.5
1	A	80	ILE	2.5
2	B	83	ALA	2.5
2	B	438	ILE	2.5
2	B	246	LEU	2.4
2	B	572	ILE	2.4
2	B	141	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	206	MET	2.4
2	B	223	LYS	2.4
2	B	277	ALA	2.4
2	B	512	SER	2.4
1	A	225	VAL	2.4
2	B	524	PHE	2.4
2	B	130	LEU	2.4
2	B	98	VAL	2.4
1	A	93	ILE	2.4
1	A	118	VAL	2.4
2	B	543	TRP	2.4
2	B	62	ALA	2.3
2	B	204	THR	2.3
2	B	344	GLN	2.3
1	A	196	LEU	2.3
2	B	387	SER	2.3
2	B	301	VAL	2.3
2	B	357	ALA	2.3
1	A	191	ILE	2.3
1	A	354	VAL	2.3
2	B	457	ILE	2.3
1	A	134	TRP	2.3
1	A	56	VAL	2.3
2	B	448	TRP	2.2
1	A	144	THR	2.2
2	B	498	SER	2.2
1	A	275	LEU	2.2
2	B	236	LEU	2.2
2	B	106	PHE	2.2
1	A	241	PRO	2.2
1	A	247	PRO	2.2
1	A	256	LEU	2.2
2	B	446	LEU	2.2
2	B	522	ARG	2.2
1	A	232	PHE	2.2
2	B	97	ILE	2.2
1	A	246	LEU	2.2
2	B	439	LEU	2.2
1	A	126	LEU	2.2
1	A	373	THR	2.2
2	B	434	VAL	2.2
1	A	28	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	342	LEU	2.2
1	A	406	ALA	2.2
2	B	296	ILE	2.2
1	A	488	LEU	2.2
1	A	306	ILE	2.1
1	A	285	LYS	2.1
1	A	23	ILE	2.1
1	A	404	VAL	2.1
1	A	539	TYR	2.1
2	B	138	TYR	2.1
1	A	304	PRO	2.1
1	A	202	MET	2.1
2	B	531	ILE	2.1
1	A	489	PHE	2.1
1	A	446	LEU	2.1
2	B	269	TYR	2.1
1	A	137	LEU	2.1
2	B	112	TYR	2.1
2	B	293	LEU	2.0
1	A	271	ILE	2.0
2	B	96	ILE	2.0
2	B	131	ALA	2.0
1	A	204	THR	2.0
2	B	73	MET	2.0
2	B	230	GLY	2.0
2	B	337	LYS	2.0
1	A	266	PHE	2.0
2	B	433	LEU	2.0
1	A	205	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 monosaccharides in this entry.

6.4 Ligands

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	A	1574	7/7	0.29	0.50	121,207,245,253	0
3	PEG	A	1575	7/7	0.42	0.46	55,128,205,249	0
3	PEG	A	1576	7/7	0.65	0.59	45,63,205,221	0

6.5 Other polymers

There are no such residues in this entry.