



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 AM UTC

PDB ID : 3EN9 / pdb_00003en9
Title : Structure of the Methanococcus jannaschii KAE1-BUD32 fusion protein
Authors : Neculai, D.
Deposited on : 2008-09-25
Resolution : 2.67 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

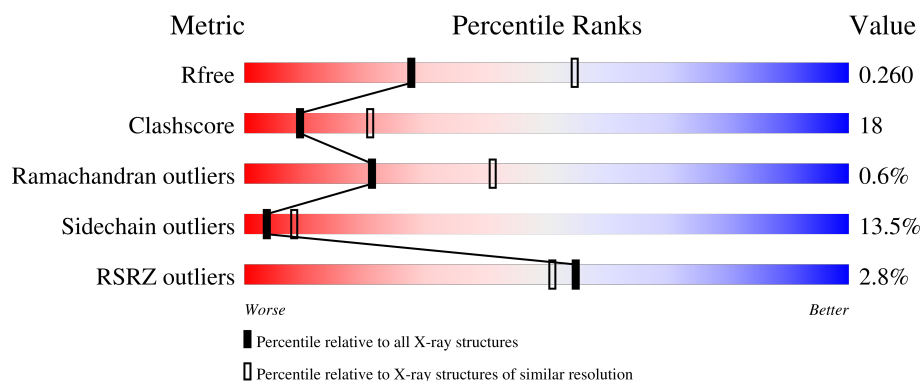
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

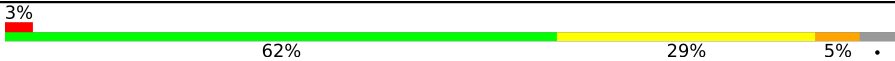
The reported resolution of this entry is 2.67 Å.

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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	540	
1	B	540	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8306 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 O-sialoglycoprotein endopeptidase/protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4130	2639	697	772	22			
1	B	511	Total	C	N	O	S	0	0	0
			4055	2591	681	762	21			

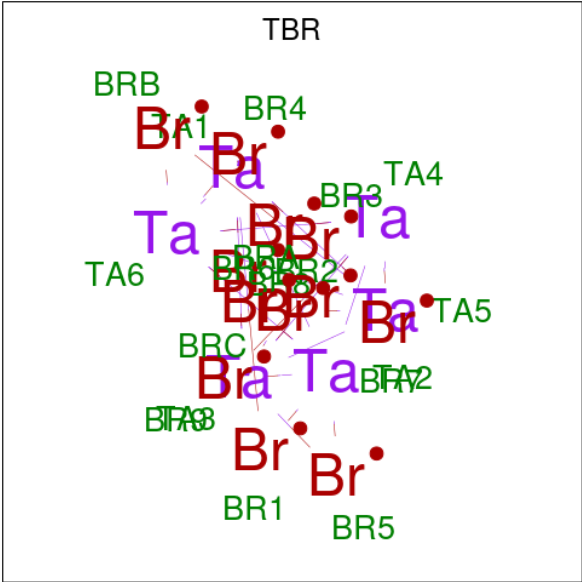
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q58530
A	-3	ALA	-	expression tag	UNP Q58530
A	-2	MET	-	expression tag	UNP Q58530
A	-1	ASP	-	expression tag	UNP Q58530
A	0	PRO	-	expression tag	UNP Q58530
B	-4	GLY	-	expression tag	UNP Q58530
B	-3	ALA	-	expression tag	UNP Q58530
B	-2	MET	-	expression tag	UNP Q58530
B	-1	ASP	-	expression tag	UNP Q58530
B	0	PRO	-	expression tag	UNP Q58530

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Br	Ta	0	0
			10	7	3		
3	B	1	Total	Br	Ta	0	0
			18	12	6		

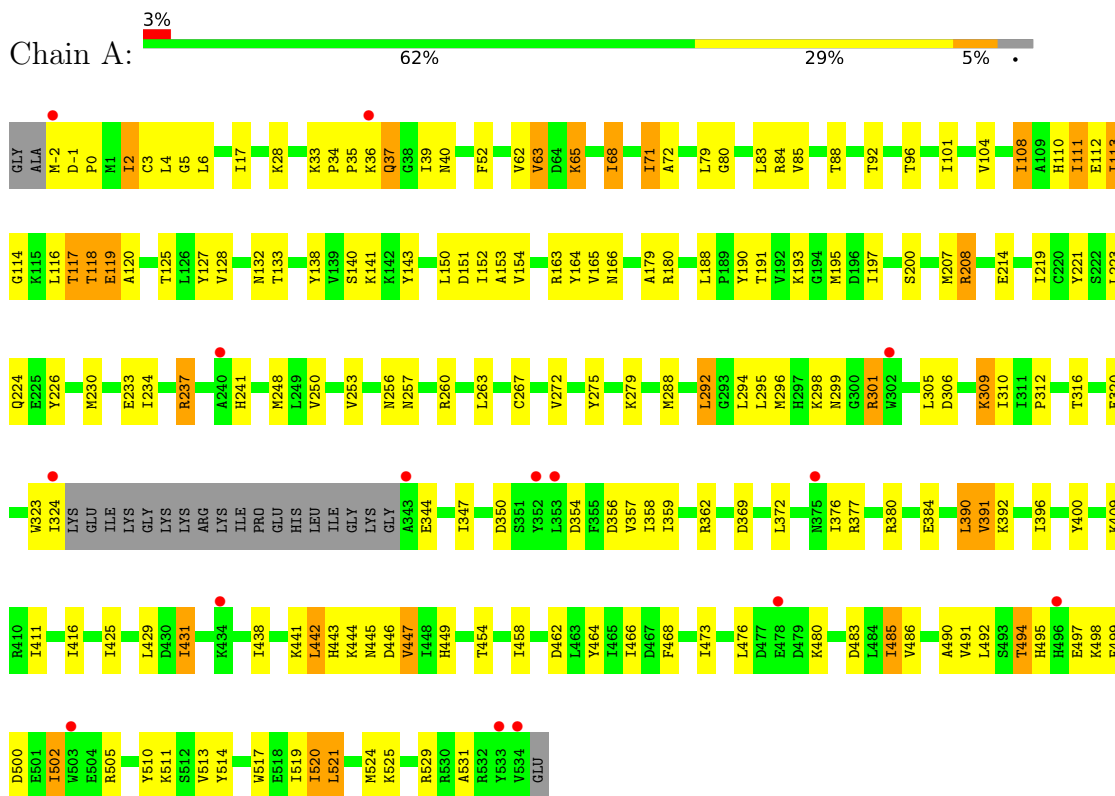
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	43	Total	O	0	0
			43	43		

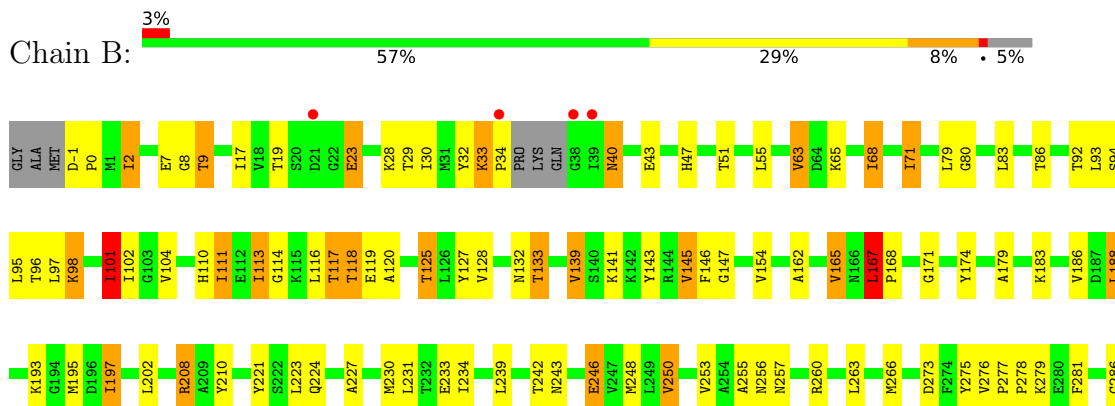
3 Residue-property plots

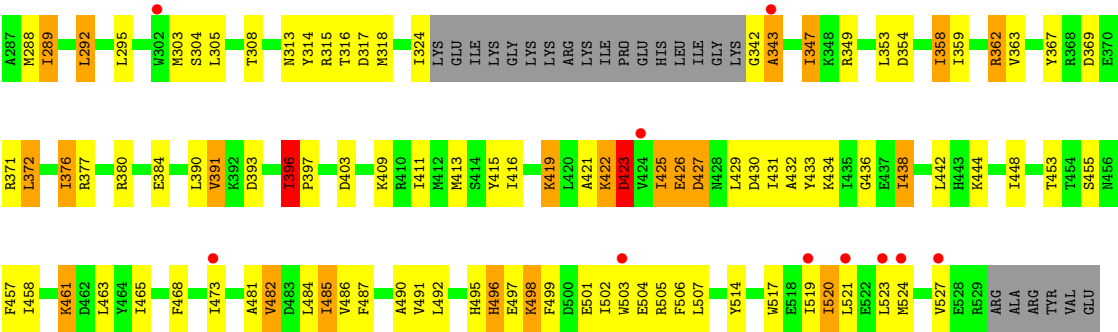
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: O-sialoglycoprotein endopeptidase/protein kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	148.73Å 148.73Å 136.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.29 – 2.67 65.29 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.29-2.67) 99.9 (65.29-2.67)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	55.01 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.202 , 0.264 0.202 , 0.260	Depositor DCC
R_{free} test set	2213 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8306	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: MG, TBR

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	0.54	0/4208	0.87	2/5681 (0.0%)
1	B	0.54	0/4130	0.88	8/5575 (0.1%)
All	All	0.54	0/8338	0.87	10/11256 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ASN	CA-C-N	6.63	126.87	119.32
1	B	40	ASN	C-N-CA	6.63	126.87	119.32
1	A	52	PHE	CA-C-N	-6.18	113.31	119.56
1	A	52	PHE	C-N-CA	-6.18	113.31	119.56
1	B	101	ILE	CB-CA-C	-5.70	102.15	110.81
1	B	167	LEU	CA-C-N	5.63	125.95	119.92
1	B	167	LEU	C-N-CA	5.63	125.95	119.92
1	B	396	ILE	CA-C-N	5.30	125.56	119.83
1	B	396	ILE	C-N-CA	5.30	125.56	119.83
1	B	233	GLU	N-CA-C	5.15	116.89	111.28

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	4130	0	4163	129	0
1	B	4055	0	4079	172	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	18	0	0	2	0
4	A	48	0	0	4	0
4	B	43	0	0	2	0
All	All	8306	0	8242	300	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 18.

All (300) 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:118:THR:HG22	1:A:120:ALA:H	1.33	0.93
1:B:71:ILE:HD11	1:B:101:ILE:HG23	1.51	0.93
1:B:114:GLY:O	1:B:118:THR:HB	1.71	0.90
1:B:30:ILE:HD13	1:B:55:LEU:HD21	1.53	0.90
1:A:128:VAL:HG23	1:A:253:VAL:HB	1.56	0.87
1:A:190:TYR:HA	1:A:230:MET:HE2	1.56	0.86
1:A:257:ASN:HD22	1:A:260:ARG:HH22	1.23	0.86
1:B:133:THR:HG21	1:B:154:VAL:H	1.41	0.85
1:A:257:ASN:ND2	1:A:260:ARG:HH22	1.74	0.84
1:B:257:ASN:HD22	1:B:260:ARG:HH21	1.26	0.83
1:B:118:THR:HG22	1:B:120:ALA:H	1.44	0.82
1:A:2:ILE:HD13	1:A:17:ILE:HG23	1.62	0.81
1:B:491:VAL:CG1	1:B:502:ILE:HD11	2.11	0.81
1:A:473:ILE:HD12	1:A:473:ILE:O	1.83	0.79
1:A:150:LEU:HD22	1:A:485:ILE:HD11	1.64	0.79
1:A:133:THR:HG21	1:A:154:VAL:H	1.50	0.77
1:B:118:THR:CG2	1:B:120:ALA:H	1.98	0.76
1:B:2:ILE:HD11	1:B:68:ILE:HG22	1.68	0.75
1:A:491:VAL:HG12	1:A:499:PHE:HD1	1.52	0.75
1:B:419:LYS:N	1:B:419:LYS:HD3	2.01	0.75
1:B:30:ILE:CD1	1:B:55:LEU:HD21	2.18	0.74
1:B:193:LYS:HD3	1:B:482:VAL:HG11	1.71	0.72
1:A:143:TYR:O	1:A:316:THR:HG23	1.90	0.72
1:B:377:ARG:HB3	1:B:409:LYS:HG2	1.71	0.71
1:A:113:ILE:O	1:A:117:THR:HB	1.90	0.71
1:B:119:GLU:HB2	1:B:275:TYR:CE1	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:CG2	1:B:154:VAL:H	2.02	0.71
1:B:342:GLY:HA2	1:B:343:ALA:O	1.90	0.71
1:A:118:THR:CG2	1:A:120:ALA:H	2.02	0.70
1:B:491:VAL:HG11	1:B:502:ILE:HD11	1.73	0.70
1:B:396:ILE:HB	1:B:438:ILE:HG22	1.73	0.69
1:B:491:VAL:HG13	1:B:502:ILE:HD11	1.75	0.69
1:B:257:ASN:ND2	1:B:260:ARG:HH21	1.89	0.68
1:A:164:TYR:CD2	1:A:207:MET:HE3	2.28	0.68
1:B:71:ILE:HD11	1:B:94:SER:HB2	1.75	0.68
1:B:376:ILE:HD13	1:B:380:ARG:CZ	2.23	0.68
1:A:110:HIS:HB3	1:A:250:VAL:HG11	1.75	0.68
1:A:104:VAL:HG13	1:A:292:LEU:HD13	1.76	0.67
1:B:257:ASN:HD22	1:B:260:ARG:NH2	1.92	0.67
1:A:2:ILE:HG13	1:A:68:ILE:HA	1.77	0.67
1:A:324:ILE:HD12	1:A:324:ILE:O	1.94	0.67
1:A:128:VAL:CG2	1:A:253:VAL:HB	2.25	0.67
1:A:296:MET:HB3	1:A:301:ARG:HD2	1.76	0.66
1:B:372:LEU:O	1:B:376:ILE:HG23	1.96	0.66
1:B:419:LYS:HD3	1:B:419:LYS:H	1.59	0.66
1:B:143:TYR:O	1:B:316:THR:HG23	1.97	0.64
1:A:-1:ASP:HB2	1:A:0:PRO:HD3	1.79	0.64
1:A:257:ASN:HD22	1:A:260:ARG:NH2	1.94	0.64
1:B:23:GLU:OE1	3:B:601:TBR:BR2	2.71	0.64
1:B:517:TRP:HE3	1:B:521:LEU:HD12	1.62	0.64
1:A:458:ILE:HG13	1:A:466:ILE:HD13	1.80	0.63
1:A:65:LYS:HG3	4:A:635:HOH:O	1.98	0.63
1:B:186:VAL:HG12	1:B:188:LEU:HD13	1.81	0.63
1:B:286:GLY:HA2	1:B:289:ILE:CD1	2.28	0.63
1:A:92:THR:O	1:A:96:THR:HG23	1.99	0.62
1:B:71:ILE:CD1	1:B:94:SER:HB2	2.29	0.62
1:B:132:ASN:O	1:B:133:THR:HG22	2.00	0.62
1:A:2:ILE:HD12	1:A:3:CYS:N	2.14	0.62
1:A:165:VAL:HG12	1:A:165:VAL:O	1.98	0.62
1:B:104:VAL:HG13	1:B:292:LEU:CD1	2.29	0.62
1:B:501:GLU:O	1:B:504:GLU:HB3	2.00	0.62
1:A:391:VAL:HG13	1:A:396:ILE:HB	1.80	0.61
1:A:305:LEU:HD21	4:A:633:HOH:O	1.99	0.61
1:B:2:ILE:HG22	1:B:19:THR:HG22	1.81	0.61
1:B:433:TYR:HB2	1:B:505:ARG:HB3	1.82	0.61
1:B:425:ILE:HG22	1:B:431:ILE:HG13	1.82	0.60
1:B:492:LEU:HD21	1:B:499:PHE:CD2	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:HG13	1:A:431:ILE:HG13	1.84	0.60
1:A:441:LYS:HG2	1:A:513:VAL:HG11	1.84	0.59
1:A:114:GLY:O	1:A:118:THR:HB	2.02	0.59
1:B:127:TYR:O	1:B:133:THR:HA	2.02	0.59
1:B:128:VAL:HG23	1:B:253:VAL:HB	1.83	0.59
1:B:7:GLU:OE2	1:B:9:THR:HB	2.03	0.58
1:A:377:ARG:HB3	1:A:409:LYS:HG2	1.85	0.58
1:B:23:GLU:OE1	3:B:601:TBR:BR1	2.77	0.58
1:A:409:LYS:HD2	1:A:409:LYS:N	2.18	0.58
1:A:429:LEU:HD11	1:A:498:LYS:HG2	1.84	0.58
1:A:4:LEU:C	1:A:4:LEU:HD23	2.29	0.57
1:B:425:ILE:HG22	1:B:431:ILE:CG1	2.34	0.57
1:B:110:HIS:HB3	1:B:250:VAL:HG11	1.87	0.57
1:A:111:ILE:HD11	1:A:143:TYR:OH	2.05	0.57
1:B:286:GLY:O	1:B:289:ILE:HD13	2.04	0.57
1:A:241:HIS:HE1	1:A:494:THR:HB	1.70	0.56
1:A:443:HIS:CG	1:A:480:LYS:HG2	2.40	0.56
1:A:310:ILE:HD12	1:A:312:PRO:HD3	1.85	0.56
1:B:396:ILE:HD11	1:B:465:ILE:CG2	2.36	0.56
1:B:117:THR:CG2	1:B:278:PRO:HD2	2.36	0.56
1:B:162:ALA:CB	1:B:171:GLY:HA3	2.36	0.56
1:A:214:GLU:HB2	1:A:219:ILE:HD11	1.89	0.55
1:B:111:ILE:HG21	1:B:125:THR:HG21	1.88	0.55
1:B:224:GLN:NE2	1:B:256:ASN:HD21	2.05	0.55
1:B:396:ILE:HD11	1:B:465:ILE:HG21	1.87	0.55
1:A:491:VAL:HG12	1:A:499:PHE:CD1	2.37	0.55
1:A:2:ILE:CD1	1:A:17:ILE:HG23	2.36	0.55
1:B:362:ARG:HH22	1:B:384:GLU:CD	2.15	0.55
1:A:511:LYS:HG3	1:A:517:TRP:CE2	2.42	0.55
1:B:227:ALA:HA	1:B:230:MET:HE3	1.87	0.55
1:A:113:ILE:HG12	1:A:288:MET:HB2	1.89	0.54
1:A:138:TYR:OH	1:A:324:ILE:HG12	2.07	0.54
1:A:224:GLN:NE2	1:A:256:ASN:HD21	2.05	0.54
1:B:315:ARG:HB2	1:B:318:MET:SD	2.47	0.54
1:A:309:LYS:HD3	1:A:309:LYS:O	2.07	0.54
1:A:390:LEU:HD22	1:A:390:LEU:O	2.06	0.54
1:A:359:ILE:HA	1:A:411:ILE:O	2.08	0.54
1:B:347:ILE:O	1:B:347:ILE:HG13	2.08	0.54
1:A:2:ILE:HD13	1:A:17:ILE:CG2	2.36	0.54
1:A:491:VAL:HG11	1:A:502:ILE:HG13	1.89	0.54
1:B:362:ARG:NH2	1:B:384:GLU:OE2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HD12	1:A:40:ASN:HB2	1.90	0.54
1:B:104:VAL:HG13	1:B:292:LEU:HD12	1.89	0.53
1:A:111:ILE:HD13	1:A:112:GLU:N	2.23	0.53
1:B:436:GLY:HA2	1:B:506:PHE:CE1	2.43	0.53
1:A:521:LEU:HD23	1:A:524:MET:HE2	1.91	0.53
1:A:127:TYR:O	1:A:133:THR:HA	2.09	0.53
1:B:444:LYS:HA	1:B:514:TYR:CE2	2.44	0.53
1:A:429:LEU:HB2	1:A:505:ARG:NH1	2.24	0.53
1:B:94:SER:CB	1:B:101:ILE:HG12	2.39	0.53
1:B:165:VAL:CG1	1:B:165:VAL:O	2.57	0.53
1:B:396:ILE:HB	1:B:438:ILE:CG2	2.39	0.53
1:A:2:ILE:HD12	1:A:2:ILE:C	2.34	0.52
1:B:139:VAL:HG21	1:B:146:PHE:HZ	1.74	0.52
1:B:421:ALA:C	1:B:423:ASP:H	2.17	0.52
1:B:92:THR:O	1:B:96:THR:HG23	2.09	0.52
1:B:279:LYS:NZ	1:B:279:LYS:HB3	2.25	0.52
1:A:391:VAL:CG1	1:A:396:ILE:HB	2.40	0.52
1:A:133:THR:CG2	1:A:154:VAL:H	2.19	0.52
1:B:2:ILE:HG13	1:B:68:ILE:HA	1.92	0.52
1:A:133:THR:HG23	1:A:153:ALA:HB1	1.92	0.52
1:B:485:ILE:HD13	1:B:527:VAL:HG11	1.90	0.52
1:B:68:ILE:HD11	1:B:97:LEU:CD1	2.41	0.51
1:A:132:ASN:O	1:A:133:THR:HG22	2.09	0.51
1:B:32:TYR:HB2	1:B:47:HIS:CG	2.45	0.51
1:B:396:ILE:HD12	1:B:438:ILE:HB	1.93	0.51
1:B:481:ALA:O	1:B:485:ILE:HG23	2.10	0.51
1:B:104:VAL:HG13	1:B:292:LEU:HD13	1.92	0.51
1:B:315:ARG:NH2	1:B:317:ASP:OD2	2.43	0.51
1:B:426:GLU:HB3	1:B:427:ASP:OD2	2.11	0.51
1:A:118:THR:HG23	1:A:119:GLU:N	2.26	0.51
1:B:94:SER:OG	1:B:101:ILE:HG12	2.11	0.51
1:B:113:ILE:HG12	1:B:288:MET:CB	2.41	0.51
1:B:33:LYS:HD2	1:B:33:LYS:O	2.11	0.50
1:B:482:VAL:O	1:B:486:VAL:HG23	2.11	0.50
1:B:32:TYR:HB2	1:B:47:HIS:CD2	2.47	0.50
1:B:227:ALA:HA	1:B:230:MET:CE	2.40	0.50
1:B:118:THR:HG22	1:B:120:ALA:N	2.21	0.50
1:B:17:ILE:HD13	1:B:63:VAL:CG2	2.42	0.49
1:B:30:ILE:HB	1:B:51:THR:HG21	1.93	0.49
1:B:202:LEU:HD22	1:B:230:MET:HE1	1.93	0.49
1:A:510:TYR:OH	1:A:520:ILE:HD11	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LYS:HD2	1:B:455:SER:HB3	1.94	0.49
1:A:165:VAL:O	1:A:166:ASN:HB2	2.12	0.49
1:B:391:VAL:C	1:B:393:ASP:H	2.19	0.49
1:A:141:LYS:HD2	1:A:141:LYS:N	2.26	0.49
1:B:416:ILE:N	1:B:416:ILE:HD12	2.28	0.49
1:A:324:ILE:HD12	1:A:324:ILE:C	2.37	0.48
1:B:17:ILE:HD13	1:B:63:VAL:HG21	1.95	0.48
1:B:145:VAL:HG23	1:B:147:GLY:H	1.78	0.48
1:A:113:ILE:HG12	1:A:288:MET:CB	2.44	0.48
1:B:162:ALA:HB1	1:B:171:GLY:HA3	1.95	0.48
1:B:503:TRP:O	1:B:507:LEU:HG	2.13	0.48
1:B:317:ASP:C	1:B:317:ASP:OD1	2.55	0.48
1:B:117:THR:O	1:B:117:THR:HG23	2.12	0.48
1:A:226:TYR:HB3	1:A:230:MET:HE3	1.96	0.48
1:A:118:THR:CG2	1:A:119:GLU:N	2.77	0.48
1:B:117:THR:HG23	1:B:278:PRO:HD2	1.96	0.48
1:B:246:GLU:HB3	1:B:273:ASP:HB2	1.95	0.48
1:B:197:ILE:HD13	1:B:234:ILE:HD13	1.96	0.48
1:B:8:GLY:HA3	1:B:86:THR:OG1	2.13	0.47
1:B:358:ILE:HG23	1:B:415:TYR:HB2	1.96	0.47
1:B:411:ILE:HG21	1:B:413:MET:HE2	1.96	0.47
1:A:80:GLY:O	1:A:84:ARG:HG3	2.14	0.47
1:B:391:VAL:HG22	1:B:396:ILE:CG2	2.45	0.47
1:A:71:ILE:O	1:A:71:ILE:HD13	2.15	0.47
1:A:114:GLY:HA3	1:A:248:MET:SD	2.55	0.47
1:B:425:ILE:HB	1:B:432:ALA:HB2	1.97	0.47
1:B:498:LYS:HB2	1:B:498:LYS:NZ	2.30	0.47
1:A:197:ILE:HG23	1:A:234:ILE:HG21	1.95	0.47
1:A:179:ALA:HB1	1:A:221:TYR:HA	1.97	0.47
1:B:28:LYS:HE2	1:B:30:ILE:HD11	1.96	0.47
1:B:193:LYS:HD3	1:B:482:VAL:CG1	2.44	0.47
1:B:304:SER:O	1:B:308:THR:HG23	2.15	0.47
1:A:425:ILE:O	1:A:429:LEU:HD13	2.15	0.47
1:B:113:ILE:HG12	1:B:288:MET:HB2	1.96	0.47
1:B:434:LYS:O	1:B:438:ILE:HG12	2.15	0.47
1:B:40:ASN:OD1	1:B:43:GLU:HB2	2.15	0.46
1:B:71:ILE:CD1	1:B:101:ILE:HG23	2.34	0.46
1:A:208:ARG:HA	1:A:208:ARG:HD3	1.61	0.46
1:A:299:ASN:ND2	1:A:323:TRP:HA	2.30	0.46
1:A:525:LYS:O	1:A:529:ARG:HG3	2.14	0.46
1:B:429:LEU:HD13	1:B:505:ARG:CZ	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LEU:O	1:B:527:VAL:HG23	2.15	0.46
1:A:442:LEU:HG	1:A:447:VAL:HG22	1.97	0.46
1:B:165:VAL:HG22	1:B:210:TYR:CE1	2.50	0.46
1:A:362:ARG:NH2	1:A:384:GLU:CD	2.73	0.46
1:B:367:TYR:CD1	1:B:367:TYR:C	2.94	0.46
1:A:37:GLN:NE2	1:A:163:ARG:HD3	2.30	0.46
1:B:279:LYS:HG2	4:B:634:HOH:O	2.15	0.46
1:B:353:LEU:O	1:B:354:ASP:HB2	2.16	0.46
1:B:197:ILE:HD11	1:B:231:LEU:HD23	1.98	0.45
1:B:519:ILE:O	1:B:523:LEU:HD23	2.16	0.45
1:A:28:LYS:HE2	1:A:28:LYS:HB3	1.63	0.45
1:A:294:LEU:O	1:A:298:LYS:HB2	2.16	0.45
1:B:139:VAL:CG2	1:B:146:PHE:HZ	2.28	0.45
1:A:444:LYS:HA	1:A:514:TYR:CE2	2.51	0.45
1:B:397:PRO:HB2	1:B:463:LEU:O	2.17	0.45
1:B:98:LYS:CD	1:B:98:LYS:O	2.65	0.45
1:A:5:GLY:HA2	1:A:72:ALA:O	2.15	0.45
1:A:140:SER:O	1:A:141:LYS:HB2	2.16	0.45
1:B:117:THR:HG21	1:B:278:PRO:HD2	1.97	0.45
1:A:-1:ASP:CB	1:A:0:PRO:HD3	2.46	0.45
1:A:392:LYS:NZ	1:A:400:TYR:HA	2.32	0.45
1:B:98:LYS:O	1:B:98:LYS:CG	2.64	0.45
1:B:457:PHE:HB3	1:B:463:LEU:HD22	1.99	0.45
1:A:416:ILE:HG12	1:A:464:TYR:CD1	2.51	0.44
1:B:128:VAL:HG12	1:B:133:THR:HB	1.98	0.44
1:A:519:ILE:HA	3:A:601:TBR:BR4	2.72	0.44
1:B:132:ASN:O	1:B:133:THR:CG2	2.65	0.44
1:A:33:LYS:HG2	1:B:403:ASP:HB2	2.00	0.44
1:B:114:GLY:HA3	1:B:248:MET:SD	2.58	0.44
1:A:132:ASN:O	1:A:133:THR:CG2	2.65	0.44
1:B:168:PRO:HB2	1:B:174:TYR:CE2	2.53	0.44
1:A:193:LYS:HB3	1:A:486:VAL:HG21	2.00	0.44
1:A:445:ASN:O	1:A:446:ASP:HB2	2.17	0.44
1:B:239:LEU:HD12	1:B:239:LEU:HA	1.82	0.44
1:A:138:TYR:CZ	1:A:324:ILE:HG12	2.53	0.43
1:A:165:VAL:O	1:A:165:VAL:CG1	2.65	0.43
1:B:71:ILE:HD13	1:B:101:ILE:HA	1.99	0.43
1:A:180:ARG:HG2	1:A:180:ARG:HH11	1.82	0.43
1:A:499:PHE:O	1:A:500:ASP:C	2.60	0.43
1:B:195:MET:HG3	4:B:603:HOH:O	2.17	0.43
1:B:110:HIS:HB3	1:B:250:VAL:CG1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:MET:HE3	1:B:524:MET:HB3	1.90	0.43
1:A:85:VAL:O	1:A:88:THR:HG22	2.19	0.43
1:B:495:HIS:O	1:B:496:HIS:C	2.61	0.43
1:A:39:ILE:HD12	1:A:39:ILE:C	2.44	0.43
1:A:138:TYR:OH	1:A:141:LYS:HA	2.19	0.43
1:B:113:ILE:O	1:B:117:THR:HB	2.18	0.43
1:B:120:ALA:HB2	1:B:275:TYR:CD2	2.54	0.43
1:A:34:PRO:HA	1:A:35:PRO:HD3	1.84	0.43
1:A:490:ALA:O	1:A:494:THR:HG23	2.19	0.43
1:A:120:ALA:HB2	1:A:275:TYR:CD2	2.54	0.43
1:B:-1:ASP:HA	1:B:0:PRO:HD3	1.67	0.43
1:B:33:LYS:HA	1:B:34:PRO:HD3	1.81	0.43
1:B:266:MET:HE3	1:B:266:MET:HB3	1.94	0.43
1:B:484:LEU:HD23	1:B:484:LEU:HA	1.91	0.43
1:B:487:PHE:O	1:B:490:ALA:HB3	2.18	0.43
1:B:276:VAL:HA	1:B:277:PRO:HD3	1.80	0.42
1:B:313:ASN:O	1:B:314:TYR:C	2.62	0.42
1:B:487:PHE:HE2	1:B:506:PHE:CD1	2.37	0.42
1:A:449:HIS:O	1:A:483:ASP:OD1	2.37	0.42
1:B:113:ILE:CD1	1:B:288:MET:HB3	2.50	0.42
1:B:165:VAL:O	1:B:165:VAL:HG13	2.19	0.42
1:A:2:ILE:CG1	1:A:68:ILE:HA	2.47	0.42
1:A:443:HIS:O	1:A:480:LYS:HE2	2.20	0.42
1:B:520:ILE:H	1:B:520:ILE:HG12	1.40	0.42
1:B:257:ASN:ND2	1:B:260:ARG:NH2	2.58	0.42
1:B:461:LYS:HE3	1:B:461:LYS:HB2	1.78	0.42
1:B:113:ILE:HD12	1:B:281:PHE:O	2.19	0.42
1:B:165:VAL:HG12	1:B:167:LEU:HD22	2.00	0.42
1:B:434:LYS:HB2	1:B:434:LYS:HE3	1.66	0.42
1:B:101:ILE:H	1:B:101:ILE:HG13	1.62	0.42
1:A:305:LEU:HD13	1:A:305:LEU:HA	1.91	0.42
1:B:421:ALA:C	1:B:423:ASP:N	2.78	0.42
1:B:102:ILE:HD12	1:B:303:MET:HG3	2.01	0.42
1:A:108:ILE:CG1	1:A:292:LEU:HD11	2.50	0.41
1:A:305:LEU:N	1:A:305:LEU:HD22	2.35	0.41
1:A:531:ALA:CB	4:A:640:HOH:O	2.67	0.41
1:B:369:ASP:OD1	1:B:371:ARG:HB2	2.20	0.41
1:B:463:LEU:HA	1:B:463:LEU:HD23	1.68	0.41
1:A:233:GLU:O	1:A:237:ARG:HG2	2.19	0.41
1:A:369:ASP:OD1	1:A:369:ASP:C	2.63	0.41
1:A:111:ILE:HD11	1:A:143:TYR:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG12	1:A:63:VAL:HG12	2.02	0.41
1:B:111:ILE:CG2	1:B:125:THR:HG21	2.49	0.41
1:B:461:LYS:HD3	1:B:461:LYS:C	2.45	0.41
1:A:241:HIS:CE1	1:A:494:THR:HB	2.53	0.41
1:B:202:LEU:HD22	1:B:230:MET:CE	2.51	0.41
1:B:442:LEU:HD23	1:B:442:LEU:HA	1.88	0.41
1:A:151:ASP:OD2	1:A:200:SER:HB2	2.19	0.41
1:A:350:ASP:HB3	1:A:357:VAL:HG22	2.03	0.41
1:B:253:VAL:C	1:B:255:ALA:H	2.27	0.41
1:B:253:VAL:C	1:B:255:ALA:N	2.79	0.41
1:A:195:MET:HE3	4:A:642:HOH:O	2.20	0.41
1:B:111:ILE:HG21	1:B:111:ILE:HD12	1.82	0.41
1:B:127:TYR:HA	1:B:250:VAL:O	2.21	0.41
1:B:133:THR:CG2	1:B:154:VAL:HG12	2.51	0.41
1:B:208:ARG:HD3	1:B:208:ARG:HA	1.74	0.41
1:A:151:ASP:OD1	1:A:152:ILE:N	2.53	0.40
1:B:242:THR:O	1:B:243:ASN:C	2.64	0.40
1:A:267:CYS:HB3	1:A:272:VAL:HG23	2.03	0.40
1:A:376:ILE:O	1:A:380:ARG:HG3	2.21	0.40
1:A:485:ILE:HG13	1:A:486:VAL:N	2.36	0.40
1:B:179:ALA:HB1	1:B:221:TYR:HA	2.03	0.40
1:B:429:LEU:O	1:B:430:ASP:C	2.65	0.40
1:A:344:GLU:O	1:A:344:GLU:HG2	2.22	0.40
1:A:429:LEU:HD22	1:A:429:LEU:H	1.86	0.40
1:A:454:THR:OG1	1:A:495:HIS:HE1	2.04	0.40
1:A:71:ILE:HD13	1:A:101:ILE:HG13	2.04	0.40
1:A:111:ILE:HD13	1:A:111:ILE:C	2.46	0.40
1:B:473:ILE:O	1:B:473:ILE:HD12	2.22	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	515/540 (95%)	480 (93%)	34 (7%)	1 (0%)	43	65
1	B	505/540 (94%)	467 (92%)	33 (6%)	5 (1%)	12	28
All	All	1020/1080 (94%)	947 (93%)	67 (7%)	6 (1%)	21	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	ALA
1	B	423	ASP
1	B	497	GLU
1	B	422	LYS
1	A	354	ASP
1	B	80	GLY

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	444/460 (96%)	392 (88%)	52 (12%)	5	12
1	B	436/460 (95%)	369 (85%)	67 (15%)	2	6
All	All	880/920 (96%)	761 (86%)	119 (14%)	4	8

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	MET
1	A	2	ILE
1	A	6	LEU
1	A	36	LYS
1	A	37	GLN
1	A	63	VAL
1	A	65	LYS
1	A	68	ILE
1	A	71	ILE
1	A	79	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	83	LEU
1	A	108	ILE
1	A	111	ILE
1	A	113	ILE
1	A	116	LEU
1	A	117	THR
1	A	118	THR
1	A	119	GLU
1	A	125	THR
1	A	188	LEU
1	A	191	THR
1	A	208	ARG
1	A	223	LEU
1	A	237	ARG
1	A	263	LEU
1	A	279	LYS
1	A	292	LEU
1	A	295	LEU
1	A	301	ARG
1	A	306	ASP
1	A	309	LYS
1	A	320	GLU
1	A	347	ILE
1	A	356	ASP
1	A	358	ILE
1	A	372	LEU
1	A	390	LEU
1	A	391	VAL
1	A	431	ILE
1	A	438	ILE
1	A	442	LEU
1	A	447	VAL
1	A	462	ASP
1	A	468	PHE
1	A	476	LEU
1	A	485	ILE
1	A	492	LEU
1	A	494	THR
1	A	497	GLU
1	A	502	ILE
1	A	520	ILE
1	A	521	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2	ILE
1	B	9	THR
1	B	23	GLU
1	B	29	THR
1	B	33	LYS
1	B	63	VAL
1	B	65	LYS
1	B	68	ILE
1	B	71	ILE
1	B	79	LEU
1	B	83	LEU
1	B	93	LEU
1	B	95	LEU
1	B	98	LYS
1	B	101	ILE
1	B	111	ILE
1	B	113	ILE
1	B	116	LEU
1	B	117	THR
1	B	118	THR
1	B	125	THR
1	B	133	THR
1	B	139	VAL
1	B	141	LYS
1	B	145	VAL
1	B	165	VAL
1	B	167	LEU
1	B	183	LYS
1	B	188	LEU
1	B	197	ILE
1	B	208	ARG
1	B	223	LEU
1	B	246	GLU
1	B	250	VAL
1	B	263	LEU
1	B	289	ILE
1	B	292	LEU
1	B	295	LEU
1	B	305	LEU
1	B	324	ILE
1	B	347	ILE
1	B	349	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	358	ILE
1	B	359	ILE
1	B	362	ARG
1	B	363	VAL
1	B	372	LEU
1	B	376	ILE
1	B	390	LEU
1	B	391	VAL
1	B	396	ILE
1	B	419	LYS
1	B	423	ASP
1	B	425	ILE
1	B	426	GLU
1	B	427	ASP
1	B	438	ILE
1	B	448	ILE
1	B	453	THR
1	B	458	ILE
1	B	461	LYS
1	B	468	PHE
1	B	482	VAL
1	B	485	ILE
1	B	496	HIS
1	B	498	LYS
1	B	520	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	132	ASN
1	A	156	ASN
1	A	160	GLN
1	A	224	GLN
1	A	241	HIS
1	A	257	ASN
1	A	299	ASN
1	A	495	HIS
1	A	496	HIS
1	B	27	ASN
1	B	224	GLN
1	B	257	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	270	GLN
1	B	299	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TBR	A	601	-	0,11,36	-	-	-		
3	TBR	B	601	-	0,36,36	-	-	-		

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	TBR	A	601	-	-	-	0/2/2/19

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TBR	1	0
3	B	601	TBR	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 ⓘ

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	519/540 (96%)	-0.14	15 (2%)	53 49	43, 64, 95, 147	0
1	B	511/540 (94%)	-0.02	14 (2%)	56 52	43, 66, 127, 167	0
All	All	1030/1080 (95%)	-0.08	29 (2%)	55 51	43, 65, 114, 167	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	TRP	4.0
1	A	352	TYR	3.6
1	B	523	LEU	3.5
1	B	503	TRP	3.2
1	B	38	GLY	3.2
1	A	36	LYS	3.1
1	A	353	LEU	3.0
1	A	434	LYS	3.0
1	A	533	TYR	3.0
1	A	240	ALA	3.0
1	B	521	LEU	2.9
1	A	324	ILE	2.9
1	A	503	TRP	2.8
1	B	343	ALA	2.8
1	A	534	VAL	2.7
1	A	343	ALA	2.6
1	A	-2	MET	2.5
1	B	424	VAL	2.5
1	B	34	PRO	2.4
1	B	21	ASP	2.3
1	B	527	VAL	2.3
1	B	39	ILE	2.2
1	B	519	ILE	2.2
1	A	478	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	302	TRP	2.1
1	B	524	MET	2.1
1	A	375	ASN	2.1
1	A	496	HIS	2.0
1	B	473	ILE	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(Å ²)	Q<0.9
2	MG	A	600	1/1	0.82	0.14	76,76,76,76	0
2	MG	B	600	1/1	0.82	0.10	77,77,77,77	0
3	TBR	A	601	10/18	0.93	0.09	91,113,178,192	10
3	TBR	B	601	18/18	0.98	0.05	57,65,71,75	18

6.5 Other polymers [i](#)

There are no such residues in this entry.