



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:50 am GMT

PDB ID : 1G0I
Title : CRYSTAL STRUCTURE OF MJ0109 GENE PRODUCT INOSITOL MONOPHOSPHATASE-FRUCTOSE 1,6 BISPHTHATASE
Authors : Johnson, K.A.; Chen, L.; Yang, H.; Roberts, M.F.; Stec, B.
Deposited on : 2000-10-06
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

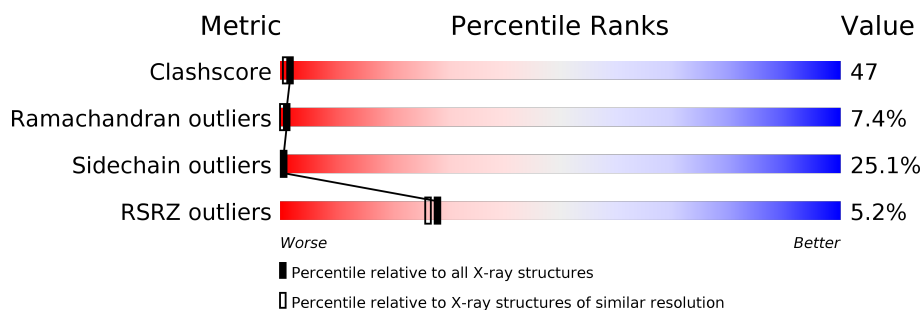
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	252	
1	B	252	

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
4	INS	B	294	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4124 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 INOSITOL MONOPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2018	1309	321	382	6			
1	B	252	Total	C	N	O	S	0	0	0
			2018	1309	321	382	6			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

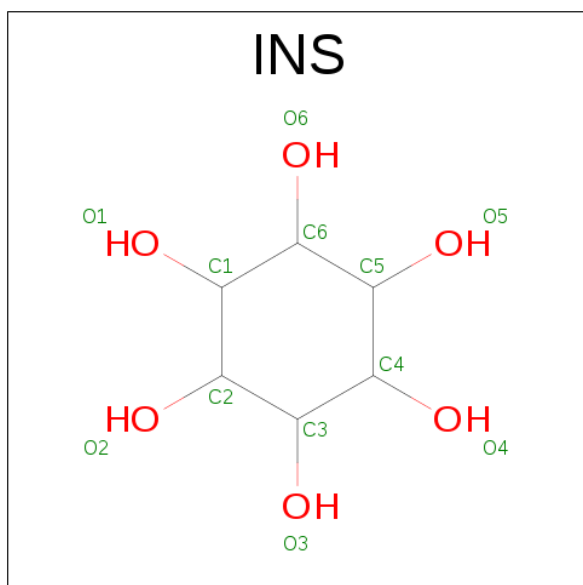
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mn	0	0
			3	3		
2	A	3	Total	Mn	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2,3,4,5,6-HEXAHYDROXY-CYCLOHEXANE (three-letter code: INS) (formula: C₆H₁₂O₆).



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

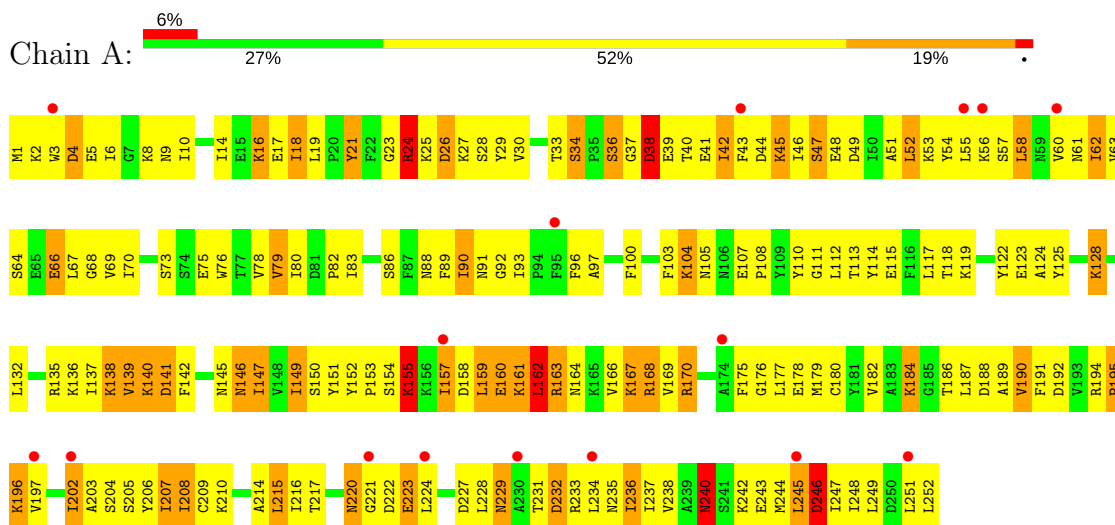
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	27	Total	O	0	0
			27	27		

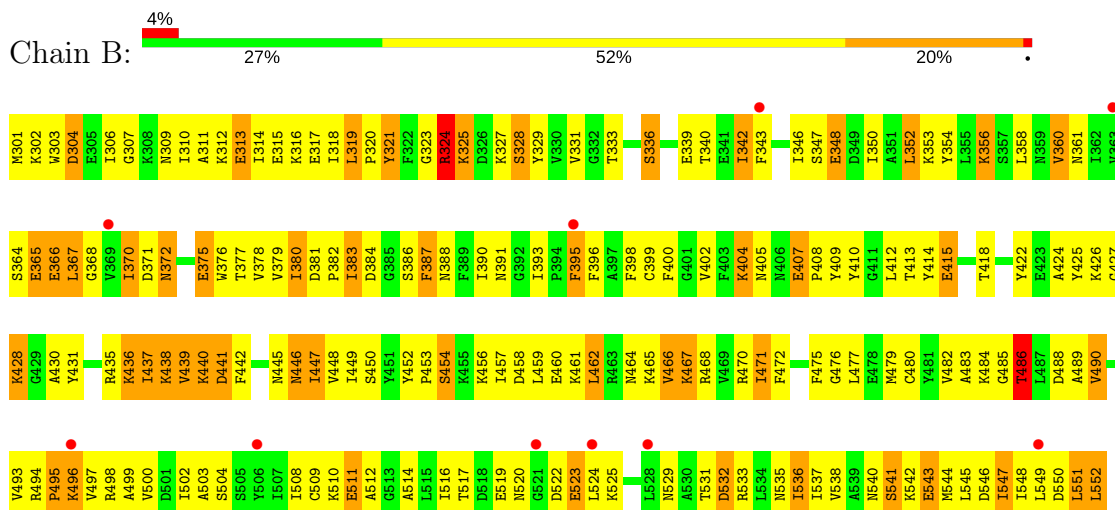
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: INOSITOL MONOPHOSPHATASE



• Molecule 1: INOSITOL MONOPHOSPHATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.02Å 78.45Å 130.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.40 47.80 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.5 (12.00-2.40) 88.8 (47.80-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.24Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.251 , 0.339 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 820.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4124	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: PO4, MN, INS

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	0.34	0/2058	0.89	4/2774 (0.1%)
1	B	0.30	0/2058	0.84	1/2774 (0.0%)
All	All	0.32	0/4116	0.87	5/5548 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLY	O-C-N	-10.99	105.12	122.70
1	A	221	GLY	CA-C-N	7.07	132.74	117.20
1	A	24	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	324	ARG	CD-NE-CZ	6.45	132.63	123.60
1	A	24	ARG	CD-NE-CZ	5.62	131.47	123.60

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	2018	0	2035	194	0
1	B	2018	0	2032	193	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	12	0	12	1	0
4	B	12	0	12	3	0
5	A	21	0	0	1	0
5	B	27	0	0	2	0
All	All	4124	0	4091	385	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 47.

All (385) 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:217:THR:HG21	1:A:245:LEU:HD21	1.35	1.01
1:B:454:SER:H	1:B:457:ILE:HG13	1.28	0.97
1:A:55:LEU:HD22	1:A:78:VAL:HG21	1.47	0.95
1:B:452:TYR:HB3	1:B:494:ARG:HE	1.33	0.93
1:A:63:VAL:HG22	1:A:69:VAL:HG22	1.49	0.92
1:A:168:ARG:HG2	4:A:594:INS:H6	1.50	0.91
1:A:217:THR:HG21	1:A:245:LEU:CD2	2.07	0.83
1:A:88:ASN:HB3	1:A:93:ILE:HB	1.65	0.79
1:B:375:GLU:HB3	1:B:405:ASN:OD1	1.83	0.78
1:B:400:PHE:HB3	1:B:412:LEU:HB3	1.66	0.78
1:A:227:ASP:O	1:A:228:LEU:HD23	1.83	0.78
1:A:179:MET:SD	1:A:202:ILE:HG22	2.24	0.78
1:A:55:LEU:HD11	1:A:100:PHE:HE1	1.49	0.78
1:A:162:LEU:O	1:A:166:VAL:HG23	1.84	0.77
1:A:186:THR:HG22	1:A:187:LEU:HD23	1.67	0.77
1:B:529:ASN:HD21	1:B:532:ASP:HB2	1.49	0.77
1:B:454:SER:HB2	1:B:493:VAL:HG23	1.67	0.77
1:B:517:THR:HG21	1:B:545:LEU:CD2	2.15	0.76
1:B:352:LEU:O	1:B:356:LYS:HB2	1.85	0.76
1:B:479:MET:SD	1:B:502:ILE:HG22	2.26	0.76
1:B:524:LEU:HD22	1:B:536:ILE:HD12	1.67	0.75
1:B:439:VAL:HG13	1:B:512:ALA:O	1.86	0.75
1:A:243:GLU:O	1:A:247:ILE:HG13	1.87	0.75
1:B:415:GLU:OE2	1:B:477:LEU:HD21	1.86	0.75
1:B:488:ASP:O	1:B:540:ASN:HB2	1.87	0.74
1:A:202:ILE:HG21	1:A:236:ILE:HD13	1.68	0.74
1:A:204:SER:O	1:A:208:ILE:HD12	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:OD1	1:A:194:ARG:HG3	1.89	0.73
1:B:447:ILE:HD13	1:B:447:ILE:H	1.50	0.73
1:A:18:ILE:HD13	1:A:83:ILE:HD11	1.69	0.73
1:A:188:ASP:O	1:A:240:ASN:HB2	1.88	0.72
1:A:28:SER:HB3	1:A:90:ILE:HD11	1.71	0.72
1:B:468:ARG:HG2	4:B:294:INS:H4	1.69	0.72
1:B:407:GLU:HG3	1:B:408:PRO:HD2	1.71	0.72
1:A:125:TYR:H	1:A:128:LYS:HG2	1.55	0.72
1:B:382:PRO:O	1:B:383:ILE:HD12	1.90	0.72
1:A:150:SER:HB2	1:A:170:ARG:O	1.90	0.71
1:A:97:ALA:HB2	1:A:177:LEU:HD13	1.72	0.70
1:B:457:ILE:HD11	1:B:493:VAL:HG21	1.72	0.70
1:A:62:ILE:HG23	1:A:70:ILE:HB	1.74	0.70
1:A:115:GLU:OE2	1:A:177:LEU:HD21	1.92	0.69
1:B:313:GLU:HG2	1:B:350:ILE:HG21	1.73	0.69
1:B:462:LEU:O	1:B:466:VAL:HG23	1.93	0.69
1:A:153:PRO:HB2	1:A:157:ILE:HG13	1.74	0.68
1:B:494:ARG:HH12	1:B:496:LYS:HG2	1.58	0.68
1:B:378:VAL:HG22	1:B:402:VAL:HG12	1.76	0.68
1:B:531:THR:HG22	1:B:532:ASP:H	1.57	0.68
1:A:104:LYS:O	1:A:107:GLU:HB3	1.93	0.68
1:B:402:VAL:HG22	1:B:410:TYR:O	1.94	0.68
1:A:139:VAL:HG22	1:A:140:LYS:H	1.58	0.67
1:A:30:VAL:HG21	1:A:39:GLU:OE1	1.94	0.67
1:B:517:THR:HG21	1:B:545:LEU:HD22	1.75	0.67
1:B:304:ASP:HB3	1:B:410:TYR:OH	1.96	0.66
1:A:34:SER:HA	5:A:612:HOH:O	1.96	0.66
1:A:196:LYS:HG3	1:A:233:ARG:NH2	2.11	0.66
1:B:509:CYS:HB3	1:B:514:ALA:HB3	1.78	0.66
1:B:435:ARG:HH21	1:B:437:ILE:HG22	1.61	0.65
1:A:147:ILE:HG22	1:A:149:ILE:HG22	1.77	0.65
1:A:206:TYR:CD1	1:A:216:ILE:HD13	2.30	0.65
1:B:424:ALA:HB2	1:B:430:ALA:HA	1.77	0.65
1:B:336:SER:HB2	1:B:533:ARG:NH2	2.12	0.65
1:B:497:VAL:HG11	1:B:536:ILE:HG22	1.78	0.65
1:B:340:THR:HG23	1:B:366:GLU:HG3	1.78	0.65
1:B:447:ILE:HD11	1:B:465:LYS:O	1.96	0.65
1:A:125:TYR:HD2	1:A:128:LYS:HD2	1.62	0.64
1:B:499:ALA:HB3	1:B:529:ASN:O	1.97	0.64
1:A:205:SER:O	1:A:209:CYS:HB2	1.98	0.64
1:A:1:MET:HE3	1:A:6:ILE:HG12	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:O	1:A:89:PHE:HB3	1.97	0.63
1:B:445:ASN:O	1:B:447:ILE:HD13	1.99	0.63
1:B:454:SER:N	1:B:457:ILE:HG13	2.07	0.63
1:A:48:GLU:HB2	1:A:82:PRO:HG2	1.80	0.63
1:A:243:GLU:O	1:A:246:ASP:HB2	1.99	0.62
1:B:365:GLU:H	1:B:500:VAL:HG21	1.65	0.62
1:B:495:PRO:HG3	1:B:535:ASN:HD21	1.65	0.62
1:A:75:GLU:HB3	1:A:105:ASN:ND2	2.15	0.61
1:B:410:TYR:HB2	1:B:425:TYR:CD1	2.34	0.61
1:B:380:ILE:HA	1:B:399:CYS:O	2.00	0.61
1:B:447:ILE:HA	1:B:488:ASP:OD1	2.00	0.61
1:B:447:ILE:HG12	1:B:467:LYS:H	1.65	0.61
1:A:149:ILE:HD11	1:A:191:PHE:HE1	1.65	0.60
1:A:111:GLY:O	1:A:123:GLU:HA	2.01	0.60
1:A:179:MET:HA	1:A:182:VAL:HG12	1.83	0.60
1:B:438:LYS:HG2	1:B:439:VAL:N	2.16	0.60
1:B:388:ASN:HA	1:B:393:ILE:HD12	1.84	0.60
1:B:517:THR:HG21	1:B:545:LEU:HD21	1.84	0.59
1:B:462:LEU:HD12	1:B:551:LEU:HD13	1.84	0.59
1:A:206:TYR:CD1	1:A:224:LEU:HD23	2.37	0.59
1:B:452:TYR:HB3	1:B:494:ARG:NE	2.12	0.59
1:A:229:ASN:H	1:A:229:ASN:HD22	1.47	0.59
1:A:122:TYR:CD2	1:A:180:CYS:HB3	2.38	0.59
1:A:140:LYS:HD3	1:A:188:ASP:OD1	2.02	0.59
1:A:42:ILE:O	1:A:46:ILE:HG12	2.02	0.59
1:B:445:ASN:O	1:B:467:LYS:HB2	2.03	0.59
1:B:509:CYS:HB2	1:B:516:ILE:HD11	1.85	0.59
1:B:552:LEU:O	1:B:552:LEU:HD12	2.03	0.58
1:B:544:MET:O	1:B:547:ILE:HB	2.02	0.58
1:A:55:LEU:CD1	1:A:80:ILE:HD11	2.33	0.58
1:B:462:LEU:HD12	1:B:551:LEU:CD1	2.33	0.58
1:A:125:TYR:HB2	1:A:128:LYS:HB3	1.85	0.58
1:B:312:LYS:O	1:B:315:GLU:HB3	2.03	0.58
1:B:343:PHE:CE2	1:B:390:ILE:HD13	2.38	0.58
1:B:364:SER:HB2	1:B:380:ILE:HD11	1.85	0.58
1:A:45:LYS:HG2	1:A:45:LYS:O	2.04	0.58
1:A:25:LYS:O	1:A:25:LYS:HG2	2.03	0.57
1:B:516:ILE:O	1:B:524:LEU:HB3	2.03	0.57
1:B:440:LYS:HD3	1:B:485:GLY:O	2.04	0.57
1:B:536:ILE:HG13	1:B:537:ILE:N	2.18	0.57
1:A:169:VAL:O	1:A:170:ARG:HG2	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:OD2	1:A:197:VAL:HG12	2.05	0.57
1:B:313:GLU:HG2	1:B:350:ILE:CG2	2.34	0.57
1:A:88:ASN:HA	1:A:93:ILE:HD12	1.87	0.56
1:B:435:ARG:NH2	1:B:437:ILE:HG22	2.20	0.56
1:B:395:PHE:CE1	1:B:477:LEU:HD23	2.39	0.56
1:B:480:CYS:O	1:B:483:ALA:HB3	2.05	0.56
1:B:364:SER:HB2	1:B:380:ILE:CD1	2.36	0.56
1:A:4:ASP:HB3	1:A:125:TYR:OH	2.05	0.56
1:B:447:ILE:O	1:B:467:LYS:HB3	2.05	0.56
1:A:14:ILE:HD12	1:A:47:SER:OG	2.05	0.56
1:B:504:SER:O	1:B:508:ILE:HG13	2.05	0.56
1:A:58:LEU:HB3	1:A:60:VAL:HG13	1.87	0.56
1:B:376:TRP:CD2	1:B:404:LYS:HG2	2.40	0.56
1:B:453:PRO:HA	1:B:493:VAL:HG22	1.87	0.56
1:B:497:VAL:HG11	1:B:536:ILE:CG2	2.36	0.56
1:B:535:ASN:HD22	1:B:535:ASN:N	2.04	0.56
1:B:402:VAL:HG23	1:B:409:TYR:HB3	1.86	0.55
1:A:110:TYR:O	1:A:207:ILE:HD13	2.07	0.55
1:A:224:LEU:HD22	1:A:236:ILE:HD12	1.88	0.55
1:B:454:SER:O	1:B:457:ILE:HB	2.07	0.55
1:A:112:LEU:HD12	1:A:113:THR:N	2.22	0.55
1:B:346:ILE:O	1:B:350:ILE:HD12	2.06	0.55
1:B:412:LEU:HD12	1:B:413:THR:H	1.71	0.55
1:A:186:THR:HG22	1:A:187:LEU:CD2	2.34	0.55
1:A:210:LYS:HG2	1:A:216:ILE:HD12	1.88	0.55
1:B:336:SER:CB	1:B:498:ARG:HD3	2.36	0.54
1:A:191:PHE:HB2	1:A:237:ILE:HG12	1.89	0.54
1:A:3:TRP:HA	1:A:6:ILE:HD12	1.89	0.54
1:B:412:LEU:HD12	1:B:413:THR:N	2.23	0.54
1:B:468:ARG:HG2	4:B:294:INS:H6	1.90	0.54
1:A:62:ILE:CG2	1:A:70:ILE:HB	2.38	0.54
1:A:229:ASN:N	1:A:229:ASN:HD22	2.04	0.54
1:B:361:ASN:HB2	1:B:377:THR:HB	1.89	0.54
1:B:495:PRO:CG	1:B:535:ASN:HD21	2.19	0.54
1:A:159:LEU:CD2	1:A:163:ARG:HH21	2.20	0.54
1:A:24:ARG:HH11	1:A:24:ARG:CB	2.21	0.54
1:B:376:TRP:CE3	1:B:404:LYS:HG2	2.44	0.53
1:B:452:TYR:O	1:B:494:ARG:HG2	2.08	0.53
1:A:246:ASP:O	1:A:249:LEU:HB2	2.08	0.53
1:A:2:LYS:HB2	1:A:5:GLU:OE1	2.07	0.53
1:B:303:TRP:HB2	5:B:627:HOH:O	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PHE:CE2	1:A:117:LEU:HD23	2.43	0.53
1:B:390:ILE:HG23	1:B:391:ASN:OD1	2.09	0.53
1:B:415:GLU:HG2	1:B:418:THR:HB	1.90	0.53
1:A:147:ILE:HD13	1:A:244:MET:SD	2.49	0.53
1:A:16:LYS:NZ	1:A:17:GLU:HG2	2.23	0.53
1:B:340:THR:CG2	1:B:366:GLU:HG3	2.38	0.53
1:A:100:PHE:HB3	1:A:112:LEU:HB3	1.91	0.52
1:A:162:LEU:HA	1:A:251:LEU:HD21	1.91	0.52
1:A:176:GLY:O	1:A:179:MET:HB2	2.09	0.52
1:A:231:THR:HG22	1:A:232:ASP:H	1.75	0.52
1:A:48:GLU:OE2	1:A:66:GLU:HB2	2.10	0.52
1:B:422:TYR:CD2	1:B:480:CYS:HB3	2.44	0.52
1:B:454:SER:HB2	1:B:493:VAL:CG2	2.39	0.52
1:B:413:THR:HG21	1:B:480:CYS:SG	2.50	0.52
1:B:318:ILE:O	1:B:321:TYR:HB2	2.10	0.52
1:B:468:ARG:CG	4:B:294:INS:H4	2.36	0.52
1:B:475:PHE:CE2	1:B:490:VAL:HG22	2.45	0.52
1:A:76:TRP:CH2	1:A:104:LYS:HD2	2.45	0.51
1:A:179:MET:HG2	1:A:238:VAL:HG21	1.92	0.51
1:A:28:SER:HG	1:A:43:PHE:HE2	1.58	0.51
1:A:47:SER:HB3	1:A:82:PRO:HB3	1.90	0.51
1:A:149:ILE:HG23	1:A:166:VAL:HG11	1.92	0.51
1:A:61:ASN:HB2	1:A:76:TRP:O	2.10	0.51
1:B:306:ILE:O	1:B:310:ILE:HG13	2.10	0.51
1:B:381:ASP:OD1	1:B:384:ASP:HA	2.09	0.51
1:A:125:TYR:N	1:A:128:LYS:HG2	2.24	0.51
1:B:342:ILE:HG13	1:B:342:ILE:O	2.10	0.51
1:A:190:VAL:O	1:A:190:VAL:HG13	2.11	0.51
1:A:41:GLU:O	1:A:44:ASP:HB2	2.11	0.51
1:A:45:LYS:O	1:A:49:ASP:HB2	2.10	0.51
1:A:69:VAL:O	1:A:69:VAL:HG12	2.11	0.51
1:B:447:ILE:CG1	1:B:466:VAL:HA	2.40	0.50
1:A:182:VAL:HG22	1:A:182:VAL:O	2.11	0.50
1:A:175:PHE:CE2	1:A:190:VAL:HG22	2.46	0.50
1:A:197:VAL:HG13	1:A:234:LEU:O	2.11	0.50
1:A:237:ILE:O	1:A:237:ILE:HG22	2.10	0.50
1:B:304:ASP:HB3	1:B:410:TYR:CZ	2.45	0.50
1:B:476:GLY:O	1:B:479:MET:HB2	2.12	0.50
1:A:124:ALA:CB	1:A:208:ILE:HA	2.40	0.50
1:B:314:ILE:O	1:B:318:ILE:HG13	2.11	0.50
1:B:449:ILE:HG22	1:B:489:ALA:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:O	1:A:21:TYR:HB2	2.12	0.50
1:A:222:ASP:O	1:A:223:GLU:O	2.30	0.50
1:A:6:ILE:O	1:A:10:ILE:HD12	2.12	0.50
1:B:395:PHE:CD1	1:B:477:LEU:HD23	2.47	0.50
1:B:524:LEU:CD2	1:B:536:ILE:HD12	2.38	0.50
1:A:194:ARG:NH1	1:A:196:LYS:HB2	2.27	0.49
1:A:152:TYR:OH	1:A:178:GLU:OE2	2.30	0.49
1:B:520:ASN:O	1:B:522:ASP:OD2	2.30	0.49
1:A:55:LEU:HD11	1:A:100:PHE:CE1	2.38	0.49
1:A:53:LYS:HE2	1:A:54:TYR:CE1	2.47	0.49
1:A:125:TYR:HB2	1:A:128:LYS:CG	2.42	0.49
1:B:468:ARG:HG3	1:B:468:ARG:HH11	1.78	0.49
1:B:360:VAL:HG12	1:B:376:TRP:O	2.12	0.49
1:B:311:ALA:HB1	1:B:414:TYR:CD1	2.48	0.49
1:B:547:ILE:O	1:B:551:LEU:HG	2.12	0.49
1:A:58:LEU:CB	1:A:60:VAL:HG13	2.43	0.49
1:A:179:MET:O	1:A:182:VAL:HG12	2.13	0.49
1:B:328:SER:HB3	1:B:390:ILE:HD11	1.95	0.49
1:A:4:ASP:O	1:A:8:LYS:HG3	2.13	0.48
1:B:410:TYR:HB2	1:B:425:TYR:CE1	2.48	0.48
1:A:103:PHE:CE2	1:A:108:PRO:HD3	2.48	0.48
1:A:48:GLU:CD	1:A:66:GLU:HB2	2.34	0.48
1:A:63:VAL:HB	1:A:79:VAL:HG12	1.95	0.48
1:B:408:PRO:O	1:B:426:LYS:HG3	2.13	0.48
1:A:149:ILE:HD11	1:A:191:PHE:CE1	2.45	0.48
1:A:24:ARG:HH11	1:A:24:ARG:HA	1.78	0.48
1:B:516:ILE:O	1:B:516:ILE:HG22	2.13	0.48
1:A:152:TYR:HB3	1:A:194:ARG:NE	2.28	0.48
1:B:496:LYS:HD3	1:B:496:LYS:HA	1.45	0.48
1:B:343:PHE:CD2	1:B:390:ILE:HD13	2.48	0.48
1:A:125:TYR:HB2	1:A:128:LYS:CB	2.44	0.48
1:A:154:SER:N	1:A:157:ILE:HG13	2.28	0.48
1:B:361:ASN:HB2	1:B:377:THR:CB	2.44	0.48
1:B:482:VAL:HG21	1:B:490:VAL:HG12	1.96	0.48
1:A:125:TYR:CD2	1:A:128:LYS:HD2	2.46	0.47
1:A:48:GLU:HB2	1:A:82:PRO:CG	2.43	0.47
1:A:202:ILE:HG21	1:A:236:ILE:CD1	2.39	0.47
1:B:440:LYS:HB2	1:B:485:GLY:HA2	1.95	0.47
1:A:248:ILE:O	1:A:252:LEU:HG	2.14	0.47
1:B:448:VAL:HG22	1:B:468:ARG:HB2	1.96	0.47
1:A:113:THR:HB	1:A:122:TYR:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:PHE:CZ	1:B:386:SER:HB3	2.50	0.47
1:B:458:ASP:CG	1:B:461:LYS:HB2	2.35	0.47
1:A:37:GLY:O	1:A:38:ASP:O	2.32	0.47
1:B:370:ILE:HG22	1:B:370:ILE:O	2.15	0.47
1:B:457:ILE:CD1	1:B:493:VAL:HG21	2.42	0.47
1:A:159:LEU:HB3	1:B:459:LEU:CD1	2.45	0.47
1:B:375:GLU:O	1:B:404:LYS:HA	2.15	0.46
1:A:63:VAL:HG13	1:A:69:VAL:CG2	2.46	0.46
1:B:383:ILE:HG22	1:B:383:ILE:O	2.15	0.46
1:B:449:ILE:HG13	1:B:466:VAL:CG1	2.46	0.46
1:A:184:LYS:O	1:A:184:LYS:HG3	2.15	0.46
1:A:160:GLU:O	1:A:164:ASN:HB2	2.15	0.46
1:A:60:VAL:HG21	1:A:78:VAL:HG23	1.97	0.46
1:B:447:ILE:HG12	1:B:466:VAL:HA	1.98	0.46
1:B:545:LEU:HD12	1:B:549:LEU:HG	1.98	0.46
1:B:510:LYS:HA	1:B:510:LYS:HD2	1.53	0.46
1:A:224:LEU:HD22	1:A:236:ILE:CD1	2.46	0.45
1:A:51:ALA:HB1	1:A:80:ILE:HD13	1.98	0.45
1:B:529:ASN:ND2	1:B:532:ASP:HB2	2.26	0.45
1:A:16:LYS:HZ3	1:A:17:GLU:HG2	1.80	0.45
1:A:216:ILE:HG22	1:A:224:LEU:CB	2.46	0.45
1:A:235:ASN:O	1:A:236:ILE:HB	2.16	0.45
1:A:24:ARG:NH1	1:A:26:ASP:OD2	2.50	0.45
1:A:151:TYR:OH	1:A:163:ARG:NH2	2.50	0.45
1:A:194:ARG:O	1:A:196:LYS:N	2.50	0.45
1:B:316:LYS:NZ	1:B:317:GLU:OE2	2.50	0.45
1:B:348:GLU:OE2	1:B:366:GLU:HB2	2.16	0.45
1:B:440:LYS:HB3	1:B:440:LYS:HE3	1.51	0.45
1:A:23:GLY:O	1:A:25:LYS:N	2.50	0.45
1:A:62:ILE:HD11	1:A:80:ILE:HD12	1.99	0.45
1:A:216:ILE:HG22	1:A:224:LEU:HB3	1.99	0.45
1:B:312:LYS:HB3	1:B:312:LYS:HE3	1.68	0.45
1:B:542:LYS:O	1:B:545:LEU:HB3	2.17	0.45
1:B:352:LEU:HD21	1:B:367:LEU:HD13	1.99	0.45
1:A:188:ASP:O	1:A:189:ALA:HB2	2.17	0.45
1:A:202:ILE:HD13	1:A:224:LEU:HD21	1.98	0.44
1:A:55:LEU:HD12	1:A:80:ILE:HD11	1.99	0.44
1:A:147:ILE:CG2	1:A:149:ILE:HG22	2.46	0.44
1:A:166:VAL:HG12	1:A:167:LYS:N	2.32	0.44
1:A:182:VAL:HG21	1:A:189:ALA:HA	1.99	0.44
1:A:246:ASP:O	1:A:249:LEU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:HH11	1:A:24:ARG:CA	2.29	0.44
1:B:361:ASN:HB2	1:B:377:THR:CG2	2.47	0.44
1:A:167:LYS:O	1:A:168:ARG:HG3	2.17	0.44
1:B:303:TRP:HA	1:B:306:ILE:HD12	2.00	0.44
1:A:91:ASN:HB3	1:B:486:THR:HG23	1.98	0.44
1:B:519:GLU:HG3	1:B:520:ASN:H	1.83	0.44
1:A:112:LEU:HD12	1:A:113:THR:H	1.81	0.44
1:A:40:THR:HG23	1:A:66:GLU:HG3	1.98	0.44
1:A:90:ILE:HG23	1:A:91:ASN:OD1	2.18	0.44
1:B:319:LEU:N	1:B:320:PRO:HD2	2.32	0.44
1:A:28:SER:OG	1:A:29:TYR:N	2.51	0.44
1:A:63:VAL:HG13	1:A:69:VAL:HG23	1.99	0.44
1:B:383:ILE:N	5:B:644:HOH:O	2.50	0.44
1:B:311:ALA:HB2	1:B:398:PHE:CD2	2.52	0.44
1:A:196:LYS:HG3	1:A:233:ARG:HH21	1.80	0.44
1:B:342:ILE:HG13	1:B:346:ILE:HD12	2.00	0.44
1:B:470:ARG:HD2	1:B:472:PHE:CZ	2.53	0.44
1:A:154:SER:OG	1:A:155:LYS:N	2.50	0.44
1:A:207:ILE:O	1:A:210:LYS:N	2.49	0.44
1:B:448:VAL:N	1:B:488:ASP:OD1	2.50	0.44
1:A:140:LYS:NZ	1:A:188:ASP:OD1	2.50	0.44
1:A:28:SER:CB	1:A:90:ILE:HD11	2.45	0.44
1:B:324:ARG:HH11	1:B:324:ARG:HG2	1.83	0.44
1:B:531:THR:O	1:B:532:ASP:O	2.35	0.44
1:A:136:LYS:HG2	1:A:138:LYS:HE3	2.00	0.44
1:A:179:MET:HA	1:A:182:VAL:CG1	2.48	0.44
1:A:244:MET:HG3	1:A:248:ILE:CD1	2.47	0.44
1:A:30:VAL:HA	1:A:41:GLU:HG2	2.00	0.43
1:B:303:TRP:CE3	1:B:306:ILE:HD13	2.53	0.43
1:B:448:VAL:O	1:B:448:VAL:HG12	2.17	0.43
1:B:537:ILE:O	1:B:537:ILE:HG22	2.17	0.43
1:A:30:VAL:HG11	1:A:39:GLU:OE1	2.18	0.43
1:B:367:LEU:HD23	1:B:368:GLY:O	2.18	0.43
1:B:441:ASP:OD2	1:B:441:ASP:N	2.49	0.43
1:A:139:VAL:HG13	1:A:140:LYS:N	2.33	0.43
1:A:55:LEU:HD13	1:A:78:VAL:HG11	2.01	0.43
1:A:68:GLY:O	1:A:69:VAL:HG23	2.19	0.43
1:B:372:ASN:HD22	1:B:372:ASN:HA	1.65	0.43
1:A:186:THR:C	1:A:187:LEU:HD23	2.39	0.43
1:A:41:GLU:O	1:A:44:ASP:N	2.49	0.43
1:B:446:ASN:O	1:B:448:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:O	1:A:146:ASN:HB2	2.19	0.43
1:A:52:LEU:N	1:A:52:LEU:HD23	2.33	0.43
1:A:125:TYR:HB2	1:A:128:LYS:HD2	2.00	0.43
1:A:220:ASN:ND2	1:A:220:ASN:H	2.16	0.43
1:A:47:SER:HB3	1:A:82:PRO:CB	2.49	0.43
1:B:306:ILE:HG22	1:B:307:GLY:N	2.33	0.43
1:B:544:MET:O	1:B:548:ILE:HD12	2.19	0.43
1:A:245:LEU:HD12	1:A:249:LEU:HG	2.01	0.43
1:B:460:GLU:O	1:B:464:ASN:ND2	2.52	0.43
1:B:480:CYS:HA	1:B:483:ALA:CB	2.49	0.43
1:B:361:ASN:ND2	1:B:377:THR:HG22	2.34	0.42
1:B:402:VAL:CG2	1:B:410:TYR:HB3	2.49	0.42
1:B:496:LYS:HA	1:B:533:ARG:HD3	2.00	0.42
1:A:161:LYS:HB3	1:A:251:LEU:HG	2.01	0.42
1:B:498:ARG:NH2	3:B:593:PO4:O1	2.52	0.42
1:A:64:SER:HA	1:A:80:ILE:O	2.19	0.42
1:A:159:LEU:HD23	1:A:163:ARG:HH21	1.83	0.42
1:B:323:GLY:O	1:B:325:LYS:N	2.49	0.42
1:B:495:PRO:HD3	1:B:535:ASN:HD21	1.83	0.42
1:A:118:THR:O	1:A:118:THR:HG22	2.20	0.42
1:A:141:ASP:OD2	1:A:141:ASP:N	2.50	0.42
1:A:215:LEU:N	1:A:215:LEU:HD23	2.34	0.42
1:A:58:LEU:HD23	1:A:58:LEU:N	2.34	0.42
1:B:447:ILE:HG13	1:B:466:VAL:HA	2.00	0.42
1:B:449:ILE:CG2	1:B:489:ALA:HB3	2.49	0.42
1:B:361:ASN:HB2	1:B:377:THR:HG22	2.01	0.42
1:A:97:ALA:HB2	1:A:177:LEU:CD1	2.45	0.42
1:B:303:TRP:O	1:B:306:ILE:HB	2.20	0.42
1:B:319:LEU:O	1:B:321:TYR:N	2.50	0.42
1:B:543:GLU:O	1:B:546:ASP:HB2	2.19	0.42
1:A:3:TRP:CH2	1:A:58:LEU:HD12	2.55	0.42
1:A:97:ALA:HB1	1:A:114:TYR:O	2.19	0.42
1:A:132:LEU:HB2	1:A:137:ILE:HG21	2.01	0.42
1:A:244:MET:O	1:A:248:ILE:HD12	2.20	0.42
1:A:36:SER:OG	1:A:233:ARG:NH1	2.53	0.42
1:B:431:TYR:HD1	1:B:436:LYS:HA	1.85	0.42
1:B:439:VAL:HG11	1:B:514:ALA:N	2.34	0.42
1:A:170:ARG:HH11	1:A:170:ARG:HG2	1.85	0.41
1:B:353:LYS:HE2	1:B:354:TYR:HE1	1.84	0.41
1:B:471:ILE:HG21	1:B:471:ILE:HD13	1.88	0.41
1:B:425:TYR:O	1:B:511:GLU:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:SER:HB3	1:B:367:LEU:HD22	2.02	0.41
1:B:509:CYS:HB3	1:B:514:ALA:CB	2.49	0.41
1:A:214:ALA:C	1:A:215:LEU:HD23	2.41	0.41
1:B:388:ASN:O	1:B:393:ILE:N	2.50	0.41
1:A:207:ILE:HG22	1:A:208:ILE:N	2.36	0.41
1:B:496:LYS:O	1:B:533:ARG:HD3	2.21	0.41
1:A:52:LEU:HD11	1:A:67:LEU:HD23	2.03	0.41
1:B:387:PHE:O	1:B:390:ILE:HG22	2.20	0.41
1:A:195:PRO:HD3	1:A:235:ASN:HD21	1.86	0.41
1:A:14:ILE:HG23	1:A:47:SER:OG	2.20	0.41
1:B:324:ARG:NH1	1:B:324:ARG:HA	2.36	0.41
1:A:160:GLU:OE2	1:A:161:LYS:HG3	2.21	0.41
1:B:379:VAL:CG1	1:B:500:VAL:HA	2.51	0.41
1:B:468:ARG:NH1	1:B:468:ARG:HG3	2.36	0.41
1:A:149:ILE:HG23	1:A:166:VAL:CG1	2.50	0.41
1:A:124:ALA:HB3	1:A:208:ILE:HA	2.03	0.41
1:B:380:ILE:HG22	1:B:400:PHE:HD1	1.86	0.40
1:B:435:ARG:HH21	1:B:437:ILE:CG2	2.31	0.40
1:B:476:GLY:O	1:B:479:MET:N	2.51	0.40
1:B:479:MET:HG2	1:B:538:VAL:HG21	2.03	0.40
1:B:523:GLU:O	1:B:525:LYS:HG2	2.20	0.40
1:B:541:SER:OG	1:B:542:LYS:N	2.50	0.40
1:B:517:THR:CG2	1:B:545:LEU:HD22	2.48	0.40
1:B:367:LEU:HD11	1:B:370:ILE:HD11	2.03	0.40
1:A:4:ASP:HB2	1:A:110:TYR:OH	2.22	0.40
1:B:366:GLU:OE2	1:B:366:GLU:HA	2.22	0.40
1:B:378:VAL:HG12	1:B:380:ILE:HG23	2.03	0.40
1:B:431:TYR:CE1	1:B:436:LYS:HG3	2.57	0.40
1:A:113:THR:N	1:A:122:TYR:O	2.52	0.40
1:B:495:PRO:CD	1:B:535:ASN:HD21	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/252 (99%)	185 (74%)	44 (18%)	21 (8%)	1	0
1	B	250/252 (99%)	191 (76%)	43 (17%)	16 (6%)	1	0
All	All	500/504 (99%)	376 (75%)	87 (17%)	37 (7%)	1	0

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	38	ASP
1	A	146	ASN
1	A	203	ALA
1	A	223	GLU
1	B	428	LYS
1	B	532	ASP
1	A	42	ILE
1	A	142	PHE
1	A	195	PRO
1	A	207	ILE
1	A	208	ILE
1	B	365	GLU
1	B	471	ILE
1	B	495	PRO
1	A	139	VAL
1	A	190	VAL
1	A	236	ILE
1	B	321	TYR
1	B	324	ARG
1	B	387	PHE
1	B	446	ASN
1	B	503	ALA
1	B	511	GLU
1	B	442	PHE
1	A	162	LEU
1	A	168	ARG
1	A	240	ASN
1	B	370	ILE
1	A	155	LYS
1	A	158	ASP
1	A	246	ASP
1	B	427	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	486	THR
1	B	490	VAL
1	A	92	GLY
1	A	18	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/221 (100%)	169 (76%)	52 (24%)	1	1
1	B	221/221 (100%)	162 (73%)	59 (27%)	0	0
All	All	442/442 (100%)	331 (75%)	111 (25%)	0	0

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	9	ASN
1	A	16	LYS
1	A	19	LEU
1	A	21	TYR
1	A	24	ARG
1	A	26	ASP
1	A	27	LYS
1	A	33	THR
1	A	34	SER
1	A	36	SER
1	A	38	ASP
1	A	45	LYS
1	A	47	SER
1	A	52	LEU
1	A	56	LYS
1	A	57	SER
1	A	58	LEU
1	A	62	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	66	GLU
1	A	73	SER
1	A	79	VAL
1	A	90	ILE
1	A	104	LYS
1	A	119	LYS
1	A	128	LYS
1	A	135	ARG
1	A	138	LYS
1	A	140	LYS
1	A	141	ASP
1	A	147	ILE
1	A	149	ILE
1	A	155	LYS
1	A	157	ILE
1	A	159	LEU
1	A	160	GLU
1	A	161	LYS
1	A	162	LEU
1	A	163	ARG
1	A	167	LYS
1	A	170	ARG
1	A	184	LYS
1	A	196	LYS
1	A	202	ILE
1	A	215	LEU
1	A	220	ASN
1	A	229	ASN
1	A	232	ASP
1	A	240	ASN
1	A	242	LYS
1	A	245	LEU
1	A	246	ASP
1	B	301	MET
1	B	302	LYS
1	B	304	ASP
1	B	309	ASN
1	B	313	GLU
1	B	319	LEU
1	B	324	ARG
1	B	325	LYS
1	B	327	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	328	SER
1	B	329	TYR
1	B	331	VAL
1	B	333	THR
1	B	336	SER
1	B	339	GLU
1	B	342	ILE
1	B	347	SER
1	B	348	GLU
1	B	352	LEU
1	B	356	LYS
1	B	358	LEU
1	B	360	VAL
1	B	366	GLU
1	B	367	LEU
1	B	371	ASP
1	B	372	ASN
1	B	375	GLU
1	B	380	ILE
1	B	383	ILE
1	B	395	PHE
1	B	396	PHE
1	B	404	LYS
1	B	407	GLU
1	B	415	GLU
1	B	428	LYS
1	B	436	LYS
1	B	437	ILE
1	B	438	LYS
1	B	439	VAL
1	B	440	LYS
1	B	441	ASP
1	B	447	ILE
1	B	450	SER
1	B	454	SER
1	B	456	LYS
1	B	462	LEU
1	B	466	VAL
1	B	467	LYS
1	B	484	LYS
1	B	486	THR
1	B	496	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	523	GLU
1	B	536	ILE
1	B	541	SER
1	B	543	GLU
1	B	547	ILE
1	B	550	ASP
1	B	551	LEU
1	B	552	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	105	ASN
1	A	145	ASN
1	A	220	ASN
1	A	229	ASN
1	A	240	ASN
1	B	359	ASN
1	B	372	ASN
1	B	445	ASN
1	B	464	ASN
1	B	520	ASN
1	B	535	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	PO4	A	293	2	4,4,4	1.06	0	6,6,6	0.42	0
4	INS	A	594	-	12,12,12	1.41	3 (25%)	18,18,18	1.02	2 (11%)
4	INS	B	294	-	12,12,12	1.35	1 (8%)	18,18,18	1.46	3 (16%)
3	PO4	B	593	2	4,4,4	1.04	0	6,6,6	0.40	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	PO4	A	293	2	-	0/0/0/0	0/0/0/0
4	INS	A	594	-	-	0/0/24/24	0/1/1/1
4	INS	B	294	-	-	0/0/24/24	0/1/1/1
3	PO4	B	593	2	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	594	INS	C6-C1	2.08	1.57	1.52
4	A	594	INS	C2-C1	2.11	1.57	1.52
4	A	594	INS	O1-C1	3.10	1.50	1.43
4	B	294	INS	O1-C1	3.23	1.50	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	594	INS	C4-C3-C2	2.01	114.39	110.84
4	B	294	INS	C3-C2-C1	2.57	115.37	110.84
4	A	594	INS	O2-C2-C1	2.68	116.20	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	294	INS	C4-C3-C2	2.99	116.11	110.84
4	B	294	INS	O2-C2-C1	3.27	117.47	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	594	INS	1	0
4	B	294	INS	3	0
3	B	593	PO4	1	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	252/252 (100%)	0.36	16 (6%) 21 19	6, 48, 87, 120	0
1	B	252/252 (100%)	0.37	10 (3%) 39 38	12, 46, 85, 118	0
All	All	504/504 (100%)	0.36	26 (5%) 28 26	6, 47, 86, 120	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	LEU	6.5
1	A	230	ALA	6.0
1	A	197	VAL	4.8
1	B	549	LEU	4.7
1	A	245	LEU	3.9
1	A	251	LEU	3.3
1	A	234	LEU	3.0
1	A	95	PHE	3.0
1	B	496	LYS	2.9
1	A	55	LEU	2.8
1	A	56	LYS	2.7
1	A	43	PHE	2.7
1	B	521	GLY	2.6
1	B	506	TYR	2.5
1	B	524	LEU	2.4
1	B	528	LEU	2.4
1	A	3	TRP	2.4
1	B	395	PHE	2.4
1	B	369	VAL	2.3
1	A	174	ALA	2.3
1	B	343	PHE	2.2
1	A	202	ILE	2.2
1	A	60	VAL	2.1
1	A	221	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	157	ILE	2.1
1	B	363	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	INS	B	294	12/12	0.62	0.37	3.41	53,71,83,93	12
4	INS	A	594	12/12	0.76	0.36	1.95	50,82,94,101	12
3	PO4	B	593	5/5	0.93	0.13	-0.94	18,25,34,58	0
3	PO4	A	293	5/5	0.94	0.10	-1.42	29,40,49,67	0
2	MN	B	591	1/1	0.79	0.09	-2.25	38,38,38,38	0
2	MN	B	592	1/1	0.98	0.08	-2.36	45,45,45,45	0
2	MN	A	291	1/1	0.99	0.06	-2.54	36,36,36,36	0
2	MN	A	290	1/1	0.98	0.03	-2.65	39,39,39,39	0
2	MN	B	590	1/1	0.97	0.04	-2.83	19,19,19,19	0
2	MN	A	292	1/1	0.89	0.09	-	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.