W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:54 PM GMT

PDB ID : 1G0I
Title : CRYSTAL STRUCTURE OF MJ0109 GENE PRODUCT INOSITOL MON
OPHOSPHATASE-FRUCTOSE1,6 BISPHOSPHATASE
Authors : Johnson, K.A.; Chen, L.; Yang, H.; Roberts, M.F.; Stec, B.
Deposited on : 2000-10-06
Resolution : 2.40 Å(reported)

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

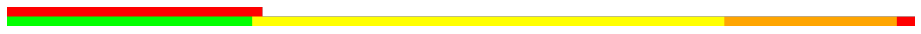|		
MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		47
Ramachandran outliers		7.4%
Sidechain outliers		25.1%
RSRZ outliers		32.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
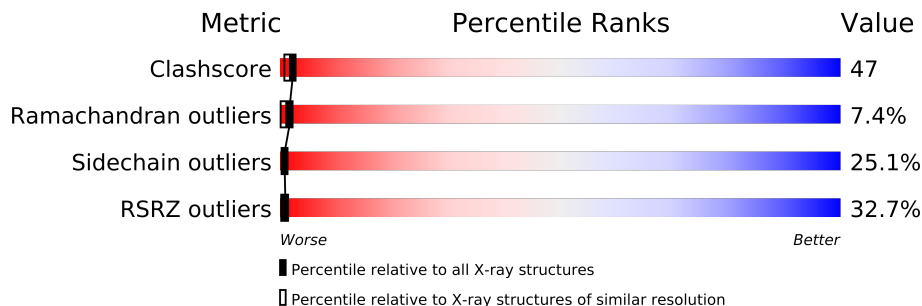
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	252	
1	B	252	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4124 atoms, of which 0 are hydrogen and 0 are deuterium.

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: O_4P).
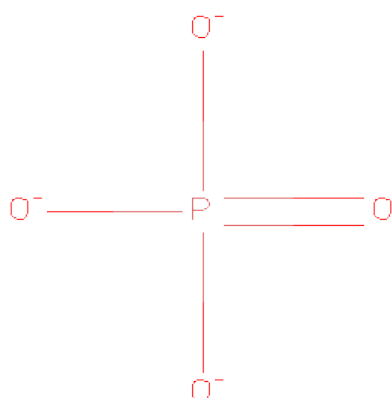
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0

- Molecule 4 is 1,2,3,4,5,6-HEXAHYDROXY-CYCLOHEXANE (three-letter code: INS) (formula: $C_6H_{12}O_6$).
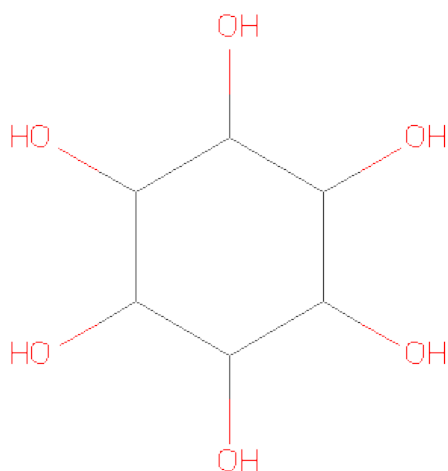
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 12	C 6	O 6	0	0
4	A	1	Total 12	C 6	O 6	0	0

- Molecule 5 is water.

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

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 errors 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

Chain A:

• Molecule 1: INOSITOL MONOPHOSPHATASE

Chain B:
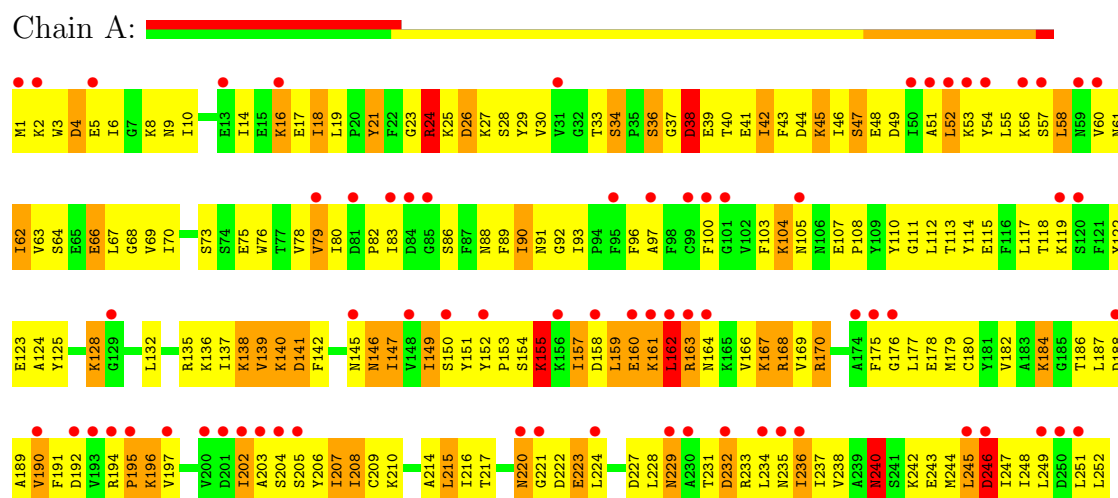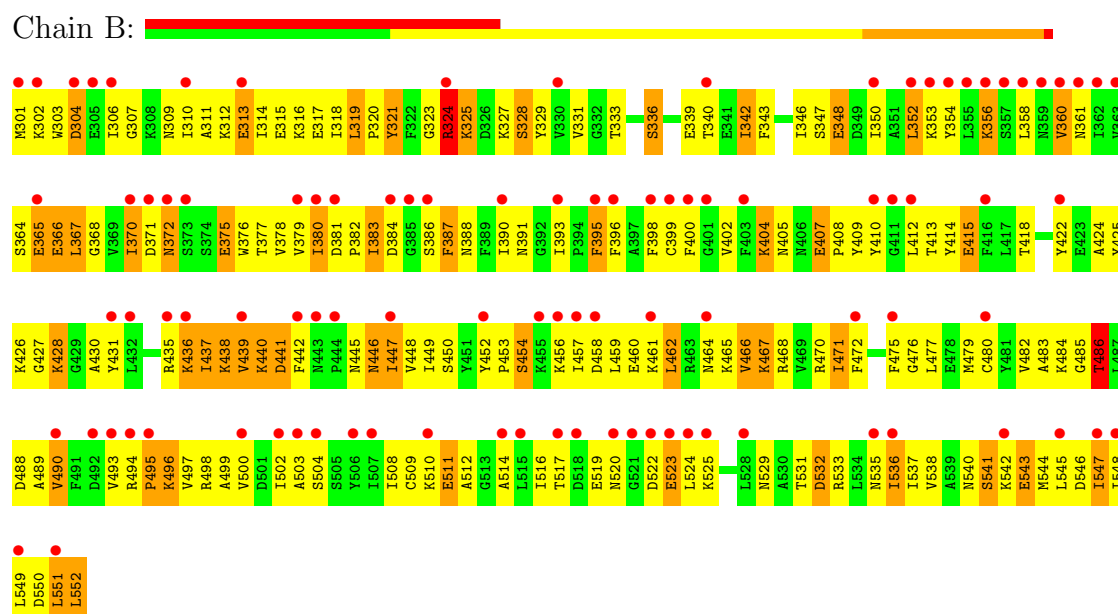
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	0.84 (at 2.24Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.251 , 0.339 0.262 , (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 , 822.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	1 of 30449 reflections (0.003%)	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.*

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[1]Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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 Close contacts (i)

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
2	B	3	0	0	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 47.

All (385) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:529:ASN:HD21	1:B:532:ASP:HB2	1.49	0.77
1:A:186:THR:HG22	1:A:187:LEU:HD23	1.67	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:447:ILE:HD13	1:B:447:ILE:H	1.50	0.73
1:A:192:ASP:OD1	1:A:194:ARG:HG3	1.89	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:B:494:ARG:HH12	1:B:496:LYS:HG2	1.58	0.68
1:A:153:PRO:HB2	1:A:157:ILE:HG13	1.74	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:B:509:CYS:HB3	1:B:514:ALA:HB3	1.78	0.66
1:A:196:LYS:HG3	1:A:233:ARG:NH2	2.11	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:447:ILE:HD11	1:B:465:LYS:O	1.96	0.65
1:B:340:THR:HG23	1:B:366:GLU:HG3	1.78	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
1:A:86:SER:O	1:A:89:PHE:HB3	1.97	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:410:TYR:HB2	1:B:425:TYR:CD1	2.34	0.61
1:A:75:GLU:HB3	1:A:105:ASN:ND2	2.15	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:179:MET:HA	1:A:182:VAL:HG12	1.83	0.60
1:A:111:GLY:O	1:A:123:GLU:HA	2.01	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:B:452:TYR:HB3	1:B:494:ARG:NE	2.12	0.59
1:A:206:TYR:CD1	1:A:224:LEU:HD23	2.37	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:B:509:CYS:HB2	1:B:516:ILE:HD11	1.85	0.59
1:B:445:ASN:O	1:B:467:LYS:HB2	2.03	0.59
1:A:42:ILE:O	1:A:46:ILE:HG12	2.02	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:364:SER:HB2	1:B:380:ILE:HD11	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:A:45:LYS:O	1:A:45:LYS:HG2	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:88:ASN:HA	1:A:93:ILE:HD12	1.87	0.56
1:B:395:PHE:CE1	1:B:477:LEU:HD23	2.39	0.56
1:B:435:ARG:NH2	1:B:437:ILE:HG22	2.20	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:B:453:PRO:HA	1:B:493:VAL:HG22	1.87	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: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:412:LEU:HD12	1:B:413:THR:H	1.71	0.55
1:B:346:ILE:O	1:B:350:ILE:HD12	2.06	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:3:TRP:HA	1:A:6:ILE:HD12	1.89	0.54
1:A:191:PHE:HB2	1:A:237:ILE:HG12	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:452:TYR:O	1:B:494:ARG:HG2	2.08	0.53
1:B:376:TRP:CE3	1:B:404:LYS:HG2	2.44	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:147:ILE:HD13	1:A:244:MET:SD	2.49	0.53
1:B:340:THR:CG2	1:B:366:GLU:HG3	2.38	0.53
1:A:16:LYS:NZ	1:A:17:GLU:HG2	2.23	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:48:GLU:OE2	1:A:66:GLU:HB2	2.10	0.52
1:A:231:THR:HG22	1:A:232:ASP:H	1.75	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:422:TYR:CD2	1:B:480:CYS:HB3	2.44	0.52
1:B:468:ARG:CG	4:B:294:INS:H4	2.36	0.52
1:B:318:ILE:O	1:B:321:TYR:HB2	2.10	0.52
1:B:475:PHE:CE2	1:B:490:VAL:HG22	2.45	0.52
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:76:TRP:CH2	1:A:104:LYS:HD2	2.45	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: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:A:182:VAL:HG22	1:A:182:VAL:O	2.11	0.50
1:B:476:GLY:O	1:B:479:MET:HB2	2.12	0.50
1:A:197:VAL:HG13	1:A:234:LEU:O	2.11	0.50
1:A:175:PHE:CE2	1:A:190:VAL:HG22	2.46	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
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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HH11	1:B:468:ARG:HG3	1.78	0.49
1:B:360:VAL:HG12	1:B:376:TRP:O	2.12	0.49
1:B:547:ILE:O	1:B:551:LEU:HG	2.12	0.49
1:B:311:ALA:HB1	1:B:414:TYR:CD1	2.48	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:B:410:TYR:HB2	1:B:425:TYR:CE1	2.48	0.48
1:A:4:ASP:O	1:A:8:LYS:HG3	2.13	0.48
1:A:63:VAL:HB	1:A:79:VAL:HG12	1.95	0.48
1:A:48:GLU:CD	1:A:66:GLU:HB2	2.34	0.48
1:A:103:PHE:CE2	1:A:108:PRO:HD3	2.48	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:B:516:ILE:O	1:B:516:ILE:HG22	2.13	0.48
1:A:24:ARG:HH11	1:A:24:ARG:HA	1.78	0.48
1:B:496:LYS:HD3	1:B:496:LYS:HA	1.45	0.48
1:A:152:TYR:HB3	1:A:194:ARG:NE	2.28	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
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:B:457:ILE:CD1	1:B:493:VAL:HG21	2.42	0.47
1:B:370:ILE:O	1:B:370:ILE:HG22	2.15	0.47
1:A:37:GLY:O	1:A:38:ASP:O	2.32	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:449:ILE:HG13	1:B:466:VAL:CG1	2.46	0.46
1:B:383:ILE:HG22	1:B:383:ILE:O	2.15	0.46
1:A:184:LYS:O	1:A:184:LYS:HG3	2.15	0.46
1:A:60:VAL:HG21	1:A:78:VAL:HG23	1.97	0.46
1:A:160:GLU:O	1:A:164:ASN:HB2	2.15	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: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:16:LYS:HZ3	1:A:17:GLU:HG2	1.80	0.45
1:A:194:ARG:O	1:A:196:LYS:N	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:151:TYR:OH	1:A:163:ARG:NH2	2.50	0.45
1:B:316:LYS:NZ	1:B:317:GLU:OE2	2.50	0.45
1:A:62:ILE:HD11	1:A:80:ILE:HD12	1.99	0.45
1:A:23:GLY:O	1:A:25:LYS:N	2.50	0.45
1:A:216:ILE:HG22	1:A:224:LEU:HB3	1.99	0.45
1:B:542:LYS:O	1:B:545:LEU:HB3	2.17	0.45
1:B:312:LYS:HB3	1:B:312:LYS:HE3	1.68	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:55:LEU:HD12	1:A:80:ILE:HD11	1.99	0.44
1:A:202:ILE:HD13	1:A:224:LEU:HD21	1.98	0.44
1:A:246:ASP:O	1:A:249:LEU:N	2.50	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:B:361:ASN:HB2	1:B:377:THR:CG2	2.47	0.44
1:A:24:ARG:HH11	1:A:24:ARG:CA	2.29	0.44
1:A:167:LYS:O	1:A:168:ARG:HG3	2.17	0.44
1:A:91:ASN:HB3	1:B:486:THR:HG23	1.98	0.44
1:B:303:TRP:HA	1:B:306:ILE:HD12	2.00	0.44
1:B:519:GLU:HG3	1:B:520:ASN:H	1.83	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:LEU:HD12	1:A:113:THR:H	1.81	0.44
1:A:90:ILE:HG23	1:A:91:ASN:OD1	2.18	0.44
1:A:40:THR:HG23	1:A:66:GLU:HG3	1.98	0.44
1:B:319:LEU:N	1:B:320:PRO:HD2	2.32	0.44
1:A:63:VAL:HG13	1:A:69:VAL:HG23	1.99	0.44
1:A:28:SER:OG	1:A:29:TYR:N	2.51	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: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:154:SER:OG	1:A:155:LYS:N	2.50	0.44
1:A:140:LYS:NZ	1:A:188:ASP:OD1	2.50	0.44
1:B:531:THR:O	1:B:532:ASP:O	2.35	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:A:244:MET:HG3	1:A:248:ILE:CD1	2.47	0.44
1:A:179:MET:HA	1:A:182:VAL:CG1	2.48	0.44
1:A:136:LYS:HG2	1:A:138:LYS:HE3	2.00	0.44
1:B:537:ILE:O	1:B:537:ILE:HG22	2.17	0.43
1:B:448:VAL:O	1:B:448:VAL:HG12	2.17	0.43
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: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: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:A:139:VAL:HG13	1:A:140:LYS:N	2.33	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:B:446:ASN:O	1:B:448:VAL:HG23	2.19	0.43
1:A:41:GLU:O	1:A:44:ASP:N	2.49	0.43
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:47:SER:HB3	1:A:82:PRO:CB	2.49	0.43
1:A:220:ASN:ND2	1:A:220:ASN:H	2.16	0.43
1:B:544:MET:O	1:B:548:ILE:HD12	2.19	0.43
1:B:306:ILE:HG22	1:B:307:GLY:N	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:245:LEU:HD12	1:A:249:LEU:HG	2.01	0.43
1:B:480:CYS:HA	1:B:483:ALA:CB	2.49	0.43
1:B:460:GLU:O	1:B:464:ASN:ND2	2.52	0.43
1:B:496:LYS:HA	1:B:533:ARG:HD3	2.00	0.42
1:B:402:VAL:CG2	1:B:410:TYR:HB3	2.49	0.42
1:B:361:ASN:ND2	1:B:377:THR:HG22	2.34	0.42
1:B:498:ARG:NH2	3:B:593:PO4:O1	2.52	0.42
1:A:161:LYS:HB3	1:A:251:LEU:HG	2.01	0.42
1:A:64:SER:HA	1:A:80:ILE:O	2.19	0.42
1:B:495:PRO:HD3	1:B:535:ASN:HD21	1.83	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: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:A:215:LEU:N	1:A:215:LEU:HD23	2.34	0.42
1:A:141:ASP:OD2	1:A:141:ASP:N	2.50	0.42
1:A:118:THR:O	1:A:118:THR:HG22	2.20	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:244:MET:O	1:A:248:ILE:HD12	2.20	0.42
1:B:439:VAL:HG11	1:B:514:ALA:N	2.34	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:A:132:LEU:HB2	1:A:137:ILE:HG21	2.01	0.42
1:A:170:ARG:HG2	1:A:170:ARG:HH11	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
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:B:388:ASN:O	1:B:393:ILE:N	2.50	0.41
1:A:214:ALA:C	1:A:215:LEU:HD23	2.41	0.41
1:B:496:LYS:O	1:B:533:ARG:HD3	2.21	0.41
1:A:207:ILE:HG22	1:A:208:ILE:N	2.36	0.41
1:B:387:PHE:O	1:B:390:ILE:HG22	2.20	0.41
1:A:52:LEU:HD11	1:A:67:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:GLU:OE2	1:A:161:LYS:HG3	2.21	0.41
1:A:195:PRO:HD3	1:A:235:ASN:HD21	1.86	0.41
1:B:468:ARG:NH1	1:B:468:ARG:HG3	2.36	0.41
1:A:14:ILE:HG23	1:A:47:SER:OG	2.20	0.41
1:B:379:VAL:CG1	1:B:500:VAL:HA	2.51	0.41
1:B:324:ARG:NH1	1:B:324:ARG:HA	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: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:435:ARG:HH21	1:B:437:ILE:CG2	2.31	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:523:GLU:O	1:B:525:LYS:HG2	2.20	0.40
1:B:367:LEU:HD11	1:B:370:ILE:HD11	2.03	0.40
1:B:378:VAL:HG12	1:B:380:ILE:HG23	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: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%)	2	1
All	All	500/504 (99%)	376 (75%)	87 (17%)	37 (7%)	2	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
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%)	1	0
All	All	442/442 (100%)	331 (75%)	111 (25%)	1	1

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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	0.61	0	6,6,6	0.31	0
4	INS	A	594	-	12,12,12	1.34	2 (16%)	18,18,18	0.98	1 (5%)
4	INS	B	294	-	12,12,12	1.28	1 (8%)	18,18,18	1.40	3 (16%)
3	PO4	B	593	2	4,4,4	0.61	0	6,6,6	0.31	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	294	INS	O1-C1	3.07	1.50	1.43
4	A	594	INS	O1-C1	2.95	1.50	1.43
4	A	594	INS	C2-C1	2.01	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	294	INS	O2-C2-C1	3.18	117.47	110.35
4	B	294	INS	C4-C3-C2	2.86	116.11	110.82
4	A	594	INS	O2-C2-C1	2.61	116.20	110.35
4	B	294	INS	C3-C2-C1	2.46	115.37	110.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	1.70	70 (27%)	1	1	6, 48, 87, 120	0
1	B	252/252 (100%)	2.44	98 (38%)	1	0	12, 46, 85, 118	0
All	All	504/504 (100%)	2.07	168 (33%)	1	1	6, 47, 86, 120	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	ASP	21.8
1	B	456	LYS	20.8
1	B	354	TYR	18.6
1	B	372	ASN	18.1
1	B	356	LYS	17.0
1	A	192	ASP	15.2
1	A	251	LEU	13.9
1	A	161	LYS	13.3
1	B	371	ASP	13.2
1	B	357	SER	13.0
1	A	194	ARG	12.6
1	B	522	ASP	12.4
1	B	359	ASN	12.2
1	B	492	ASP	12.0
1	A	175	PHE	11.8
1	A	99	CYS	11.7
1	B	493	VAL	11.5
1	B	494	ARG	10.3
1	B	373	SER	10.1
1	A	249	LEU	10.0
1	B	521	GLY	10.0
1	A	84	ASP	9.5
1	B	523	GLU	9.3
1	B	411	GLY	9.2

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Mol	Chain	Res	Type	RSRZ
1	B	495	PRO	9.2
1	B	412	LEU	9.1
1	B	452	TYR	9.0
1	A	56	LYS	9.0
1	B	306	ILE	8.8
1	A	162	LEU	8.6
1	B	385	GLY	8.2
1	A	156	LYS	8.1
1	B	362	ILE	7.9
1	B	381	ASP	7.8
1	A	81	ASP	7.8
1	B	370	ILE	7.7
1	A	202	ILE	7.6
1	A	152	TYR	7.6
1	A	53	LYS	7.5
1	A	1	MET	7.3
1	A	101	GLY	7.1
1	A	245	LEU	7.1
1	A	164	ASN	7.0
1	B	455	LYS	6.8
1	A	193	VAL	6.4
1	B	549	LEU	6.4
1	B	461	LYS	6.3
1	B	457	ILE	6.3
1	B	524	LEU	6.2
1	B	439	VAL	6.0
1	B	301	MET	6.0
1	A	246	ASP	5.9
1	A	85	GLY	5.9
1	A	145	ASN	5.7
1	B	504	SER	5.6
1	A	204	SER	5.6
1	B	302	LYS	5.6
1	B	350	ILE	5.5
1	A	190	VAL	5.5
1	B	361	ASN	5.4
1	B	458	ASP	5.4
1	B	384	ASP	5.2
1	B	340	THR	5.1
1	B	353	LYS	5.1
1	A	236	ILE	4.9
1	B	410	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	514	ALA	4.8
1	A	54	TYR	4.7
1	B	520	ASN	4.7
1	B	518	ASP	4.7
1	B	500	VAL	4.7
1	A	2	LYS	4.7
1	A	203	ALA	4.6
1	A	176	GLY	4.5
1	A	57	SER	4.5
1	B	503	ALA	4.5
1	B	360	VAL	4.5
1	A	83	ILE	4.5
1	B	358	LEU	4.4
1	B	386	SER	4.4
1	A	197	VAL	4.4
1	B	480	CYS	4.3
1	A	235	ASN	4.3
1	B	475	PHE	4.2
1	B	363	VAL	4.2
1	B	304	ASP	4.1
1	A	160	GLU	4.0
1	B	352	LEU	3.9
1	B	507	ILE	3.9
1	A	234	LEU	3.9
1	A	60	VAL	3.9
1	B	422	TYR	3.9
1	B	443	ASN	3.8
1	A	232	ASP	3.8
1	B	547	ILE	3.8
1	A	129	GLY	3.7
1	B	313	GLU	3.7
1	A	195	PRO	3.7
1	B	525	LYS	3.6
1	B	305	GLU	3.6
1	A	5	GLU	3.6
1	B	545	LEU	3.5
1	B	542	LYS	3.5
1	B	399	CYS	3.5
1	A	52	LEU	3.4
1	A	174	ALA	3.4
1	B	447	ILE	3.4
1	A	50	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	59	ASN	3.2
1	A	224	LEU	3.0
1	B	535	ASN	3.0
1	B	517	THR	2.9
1	B	401	GLY	2.9
1	B	432	LEU	2.9
1	B	395	PHE	2.8
1	B	472	PHE	2.8
1	B	396	PHE	2.7
1	B	442	PHE	2.7
1	B	464	ASN	2.7
1	A	158	ASP	2.7
1	A	97	ALA	2.6
1	B	551	LEU	2.6
1	B	380	ILE	2.6
1	A	220	ASN	2.6
1	A	51	ALA	2.5
1	A	230	ALA	2.5
1	B	398	PHE	2.5
1	A	16	LYS	2.5
1	B	355	LEU	2.5
1	B	490	VAL	2.5
1	B	400	PHE	2.5
1	B	528	LEU	2.5
1	A	163	ARG	2.5
1	B	324	ARG	2.4
1	A	31	VAL	2.4
1	A	13	GLU	2.4
1	B	310	ILE	2.4
1	B	506	TYR	2.4
1	A	229	ASN	2.3
1	B	431	TYR	2.3
1	B	330	VAL	2.3
1	B	379	VAL	2.3
1	A	119	LYS	2.3
1	B	390	ILE	2.3
1	B	403	PHE	2.3
1	B	515	LEU	2.2
1	A	120	SER	2.2
1	A	205	SER	2.2
1	A	201	ASP	2.2
1	B	502	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	444	PRO	2.2
1	A	79	VAL	2.2
1	B	548	ILE	2.2
1	B	436	LYS	2.2
1	B	510	LYS	2.2
1	A	100	PHE	2.2
1	A	221	GLY	2.2
1	A	150	SER	2.1
1	A	148	VAL	2.1
1	A	95	PHE	2.1
1	B	393	ILE	2.1
1	B	536	ILE	2.1
1	A	188	ASP	2.1
1	B	416	PHE	2.1
1	A	200	VAL	2.0
1	A	105	ASN	2.0
1	B	435	ARG	2.0
1	B	365	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	INS	B	294	12/12	0.48	0.39	53,71,83,93	12
4	INS	A	594	12/12	0.35	0.04	50,82,94,101	12
3	PO4	B	593	5/5	0.18	-0.98	18,25,34,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	B	590	1/1	0.18	-1.06	19,19,19,19	0
3	PO4	A	293	5/5	0.14	-1.07	29,40,49,67	0
2	MN	A	291	1/1	0.07	-1.14	36,36,36,36	0
2	MN	A	290	1/1	0.15	-1.22	39,39,39,39	0
2	MN	B	591	1/1	0.12	-1.53	38,38,38,38	0
2	MN	A	292	1/1	0.06	-2.69	60,60,60,60	0
2	MN	B	592	1/1	0.05	-2.80	45,45,45,45	0

6.5　Other polymers　ⓘ

There are no such residues in this entry.