Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:00 PM GMT

PDB ID	:	1DK4
Title	:	CRYSTAL STRUCTURE OF MJ0109 GENE PRODUCT INOSITOL MONOPHOSPHATASE
Authors	:	Stec, B.; Yang, H.; Johnson, K.A.; Chen, L.; Roberts, M.F.
Deposited on	:	1999-12-06
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

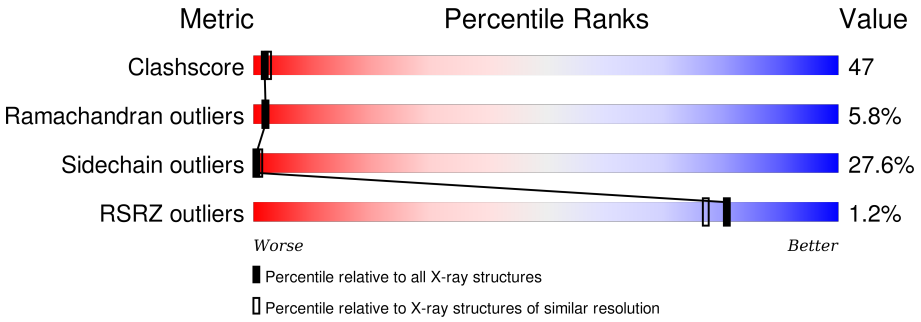
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	% 27% 52% 20%
1	B	252	% 24% 54% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4106 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.

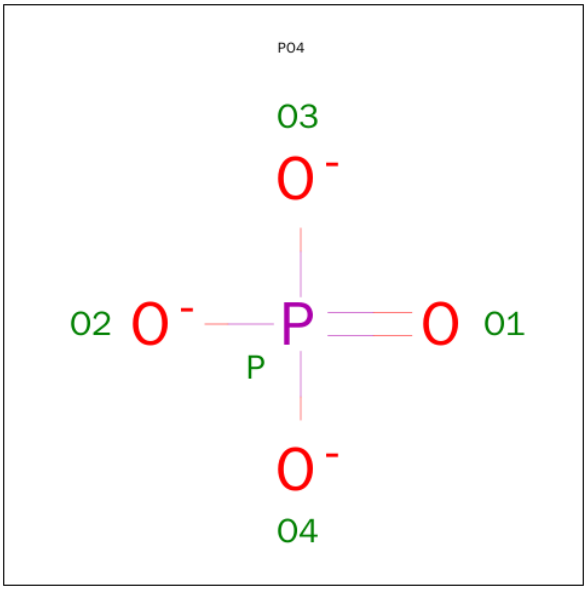
- Molecule 1 is a protein called INOSITOL MONOPHOSPHATASE.

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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

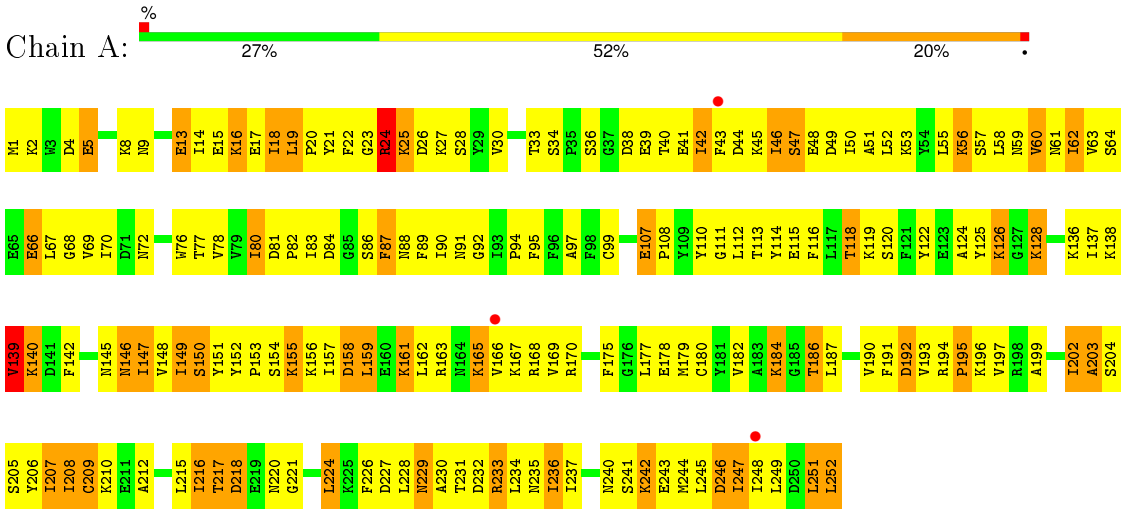
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	28	Total O 28 28	0	0
4	B	26	Total O 26 26	0	0

3 Residue-property plots (i)

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.

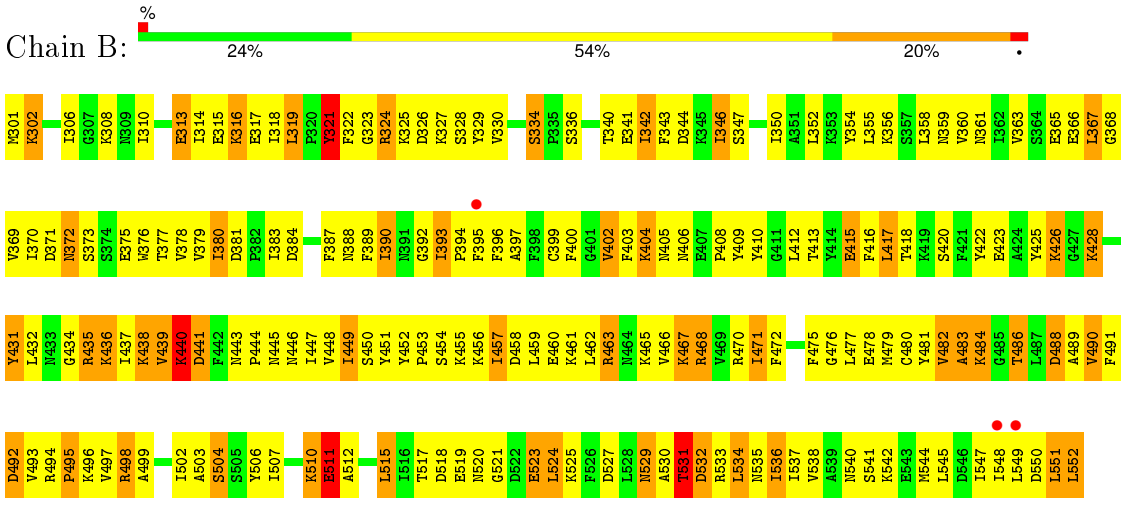
- Molecule 1: INOSITOL MONOPHOSPHATASE

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	68.87Å 78.43Å 129.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60 78.43 – 2.23	Depositor EDS
% Data completeness (in resolution range)	96.3 (12.00-2.60) 90.3 (78.43-2.23)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.22Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.242 , 0.331 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 1059.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 32145 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4106	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 5.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, PO4

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	0.85	0/2774
1	B	0.30	0/2058	0.85	1/2774 (0.0%)
All	All	0.32	0/4116	0.85	1/5548 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	468	ARG	CD-NE-CZ	5.06	130.68	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	190	0
1	B	2018	0	2032	199	0
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	0	0
4	A	28	0	0	4	0
4	B	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4106	0	4067	380	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 (380) 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:229:ASN:HD21	1:A:232:ASP:HB2	1.22	1.04
1:B:425:TYR:HB2	1:B:428:LYS:HD2	1.37	1.04
1:A:63:VAL:HG22	1:A:69:VAL:HG22	1.41	1.03
1:B:447:ILE:HG22	1:B:466:VAL:HG13	1.47	0.95
1:A:216:ILE:HG22	1:A:224:LEU:HB3	1.50	0.93
1:B:361:ASN:HB2	1:B:377:THR:HA	1.52	0.92
1:B:454:SER:H	1:B:457:ILE:HG12	1.36	0.88
1:A:61:ASN:HB3	1:A:77:THR:HG23	1.55	0.86
1:A:237:ILE:HD12	1:A:248:ILE:HG21	1.55	0.86
1:B:420:SER:HB3	1:B:432:LEU:HD11	1.57	0.85
1:B:363:VAL:HB	1:B:379:VAL:HG22	1.59	0.85
1:A:18:ILE:HG22	1:A:46:ILE:HD11	1.58	0.84
1:B:457:ILE:HD11	1:B:493:VAL:HG21	1.60	0.84
1:B:388:ASN:HA	1:B:393:ILE:HG13	1.60	0.83
1:B:448:VAL:HG22	1:B:468:ARG:HB2	1.60	0.82
1:B:352:LEU:HD21	1:B:367:LEU:HD13	1.62	0.82
1:B:334:SER:HB2	1:B:366:GLU:HA	1.62	0.80
1:A:217:THR:HG21	1:A:245:LEU:HD11	1.63	0.80
1:B:534:LEU:HD12	1:B:535:ASN:O	1.85	0.77
1:A:158:ASP:OD2	1:A:161:LYS:HD3	1.85	0.76
1:A:191:PHE:HB2	1:A:237:ILE:HD13	1.65	0.76
1:A:227:ASP:O	1:A:228:LEU:HD23	1.84	0.76
1:A:1:MET:HB2	1:A:5:GLU:OE1	1.86	0.76
1:B:479:MET:HG2	1:B:538:VAL:HG21	1.68	0.74
1:B:548:ILE:HA	1:B:551:LEU:HD11	1.69	0.74
1:B:431:TYR:HE1	1:B:436:LYS:HE3	1.52	0.74
1:A:149:ILE:HD11	1:A:162:LEU:HD21	1.69	0.73
1:A:90:ILE:HG23	1:A:91:ASN:OD1	1.88	0.73
1:B:341:GLU:O	1:B:344:ASP:HB2	1.88	0.73
1:B:302:LYS:O	1:B:306:ILE:HD12	1.88	0.72
1:A:60:VAL:HG21	1:A:78:VAL:HG23	1.71	0.72
1:B:488:ASP:O	1:B:540:ASN:HB2	1.90	0.72
1:B:402:VAL:HG13	1:B:410:TYR:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:SER:HB3	1:A:80:ILE:HG12	1.69	0.71
1:B:412:LEU:HD12	1:B:422:TYR:O	1.90	0.71
1:A:40:THR:OG1	1:A:66:GLU:HG3	1.90	0.71
1:B:495:PRO:HD3	1:B:535:ASN:HD21	1.55	0.71
1:A:151:TYR:HD1	1:A:153:PRO:HD3	1.56	0.71
1:A:47:SER:HB3	1:A:82:PRO:HB3	1.73	0.71
1:B:355:LEU:HD13	1:B:378:VAL:HG11	1.73	0.71
1:B:454:SER:N	1:B:457:ILE:HG12	2.05	0.70
1:A:87:PHE:O	1:A:90:ILE:HG22	1.90	0.70
1:A:81:ASP:HB3	1:A:99:CYS:HB2	1.72	0.70
1:A:138:LYS:HA	1:A:212:ALA:HB1	1.73	0.70
1:B:439:VAL:HG13	1:B:512:ALA:O	1.93	0.69
1:A:2:LYS:HG3	1:A:5:GLU:OE1	1.91	0.69
1:B:521:GLY:HA2	1:B:549:LEU:HD11	1.73	0.69
1:A:61:ASN:HB2	1:A:76:TRP:O	1.92	0.69
1:B:496:LYS:O	1:B:533:ARG:HD3	1.93	0.68
1:B:449:ILE:HG23	1:B:466:VAL:HG13	1.73	0.68
1:A:149:ILE:HD13	1:A:166:VAL:HG21	1.74	0.68
1:A:139:VAL:HG22	1:A:212:ALA:O	1.94	0.67
1:B:404:LYS:NZ	1:B:405:ASN:HD21	1.92	0.67
1:A:194:ARG:NH1	1:A:196:LYS:HB2	2.09	0.67
1:B:360:VAL:HB	1:B:376:TRP:O	1.93	0.67
1:A:229:ASN:ND2	1:A:232:ASP:HB2	2.04	0.67
1:A:248:ILE:O	1:A:252:LEU:HD23	1.95	0.66
1:A:153:PRO:HB2	1:A:157:ILE:HG13	1.78	0.66
1:A:152:TYR:O	1:A:194:ARG:HG2	1.95	0.66
1:A:179:MET:SD	1:A:202:ILE:HG22	2.36	0.66
1:A:115:GLU:OE2	1:A:177:LEU:HD11	1.96	0.66
1:B:452:TYR:O	1:B:492:ASP:HA	1.97	0.65
1:A:231:THR:HG22	1:A:232:ASP:H	1.61	0.65
1:A:169:VAL:O	1:A:170:ARG:HG2	1.96	0.65
1:B:388:ASN:HB3	1:B:393:ILE:HB	1.76	0.65
1:B:402:VAL:HG22	1:B:409:TYR:HB3	1.79	0.64
1:B:544:MET:O	1:B:547:ILE:HB	1.97	0.64
1:B:453:PRO:HA	1:B:493:VAL:HG22	1.79	0.64
1:B:412:LEU:HD12	1:B:413:THR:H	1.62	0.64
1:A:30:VAL:HG11	1:A:39:GLU:OE1	1.98	0.64
1:A:196:LYS:HA	1:A:233:ARG:HG2	1.79	0.63
1:A:30:VAL:HG21	1:A:39:GLU:OE1	1.98	0.63
1:A:15:GLU:HG3	1:A:116:PHE:HD2	1.63	0.63
1:B:403:PHE:HD2	1:B:408:PRO:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:O	1:A:56:LYS:HB2	1.99	0.62
1:B:517:THR:HG22	1:B:518:ASP:O	1.98	0.62
1:A:162:LEU:O	1:A:166:VAL:HG23	1.99	0.62
1:A:124:ALA:HB3	1:A:208:ILE:HA	1.80	0.62
1:A:182:VAL:HG21	1:A:190:VAL:HG12	1.82	0.61
1:B:494:ARG:HH11	1:B:496:LYS:HG3	1.65	0.61
1:B:470:ARG:O	1:B:471:ILE:HG13	2.00	0.61
1:B:450:SER:HA	1:B:470:ARG:O	2.00	0.61
1:B:404:LYS:HZ1	1:B:405:ASN:HD21	1.46	0.61
1:A:204:SER:O	1:A:208:ILE:HD12	2.00	0.61
1:A:206:TYR:CD1	1:A:216:ILE:HD13	2.35	0.61
1:A:48:GLU:OE2	1:A:66:GLU:HB2	2.00	0.60
1:A:86:SER:O	1:A:89:PHE:HB3	2.01	0.60
1:B:365:GLU:HG3	1:B:498:ARG:NH1	2.17	0.60
1:A:136:LYS:HE2	4:A:615:HOH:O	2.00	0.60
1:B:479:MET:O	1:B:482:VAL:HG23	2.01	0.60
1:B:479:MET:SD	1:B:502:ILE:HG22	2.41	0.60
1:B:428:LYS:HG2	1:B:428:LYS:O	1.99	0.59
1:B:496:LYS:HA	1:B:533:ARG:HD2	1.85	0.59
1:B:314:ILE:O	1:B:318:ILE:HG13	2.03	0.59
1:A:139:VAL:HG11	1:A:240:ASN:HA	1.85	0.59
1:A:148:VAL:HG22	1:A:168:ARG:HB3	1.84	0.59
1:A:148:VAL:HG22	1:A:168:ARG:CB	2.33	0.59
1:A:149:ILE:HG23	1:A:166:VAL:HG13	1.84	0.59
1:B:494:ARG:NH1	1:B:496:LYS:HG3	2.18	0.59
1:B:410:TYR:HB2	1:B:425:TYR:CE1	2.38	0.58
1:B:468:ARG:HG3	1:B:468:ARG:HH11	1.67	0.58
1:B:310:ILE:HG12	1:B:354:TYR:CD2	2.37	0.58
1:A:45:LYS:O	1:A:49:ASP:HB2	2.03	0.58
1:A:125:TYR:HB2	1:A:128:LYS:HG3	1.83	0.58
1:B:462:LEU:HD13	1:B:551:LEU:HD13	1.85	0.58
1:A:91:ASN:HB3	1:B:486:THR:CG2	2.33	0.58
1:B:531:THR:HG22	1:B:532:ASP:H	1.66	0.58
1:B:479:MET:CG	1:B:538:VAL:HG21	2.34	0.58
1:A:246:ASP:O	1:A:249:LEU:HB2	2.04	0.58
1:A:59:ASN:ND2	1:A:72:ASN:HB3	2.19	0.58
1:A:196:LYS:CA	1:A:233:ARG:HG2	2.34	0.58
1:A:25:LYS:O	1:A:25:LYS:HG3	2.03	0.58
1:A:161:LYS:HB3	1:A:251:LEU:HD11	1.85	0.57
1:A:247:ILE:O	1:A:251:LEU:HD22	2.05	0.57
1:B:480:CYS:O	1:B:483:ALA:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:HG2	1:A:167:LYS:O	2.04	0.57
1:B:503:ALA:O	1:B:506:TYR:HB3	2.04	0.57
1:A:124:ALA:HB3	1:A:208:ILE:HG13	1.86	0.57
1:A:186:THR:O	1:A:187:LEU:HD23	2.05	0.57
1:B:495:PRO:O	1:B:533:ARG:HB3	2.05	0.57
1:A:111:GLY:O	1:A:208:ILE:HD11	2.04	0.56
1:A:161:LYS:O	1:A:165:LYS:HG2	2.05	0.56
1:B:507:ILE:O	1:B:511:GLU:HB2	2.06	0.56
1:B:449:ILE:H	1:B:466:VAL:CG1	2.19	0.56
1:B:470:ARG:HD2	1:B:472:PHE:CZ	2.39	0.56
1:A:180:CYS:O	1:A:184:LYS:HG2	2.05	0.56
1:B:544:MET:HG3	1:B:548:ILE:CD1	2.35	0.56
1:B:344:ASP:HA	1:B:383:ILE:HD12	1.87	0.56
1:B:475:PHE:CD1	1:B:497:VAL:HG21	2.40	0.56
1:A:83:ILE:HG21	1:A:86:SER:HA	1.88	0.56
1:B:431:TYR:CE1	1:B:436:LYS:HE3	2.36	0.56
1:A:112:LEU:HD12	1:A:113:THR:H	1.68	0.56
1:B:431:TYR:HB3	1:B:434:GLY:O	2.05	0.55
1:A:42:ILE:O	1:A:46:ILE:HG23	2.05	0.55
1:B:388:ASN:CB	1:B:393:ILE:HB	2.37	0.55
1:B:475:PHE:CE2	1:B:490:VAL:HG22	2.41	0.55
1:B:548:ILE:HA	1:B:551:LEU:CD1	2.37	0.54
1:A:243:GLU:O	1:A:247:ILE:HG12	2.07	0.54
1:B:340:THR:OG1	1:B:366:GLU:HB3	2.08	0.54
1:A:91:ASN:HB3	1:B:486:THR:HG23	1.88	0.54
1:A:153:PRO:HA	1:A:193:VAL:HG13	1.90	0.54
1:A:142:PHE:CE2	1:A:244:MET:HB2	2.43	0.54
1:A:159:LEU:HD22	1:B:459:LEU:HB3	1.91	0.53
1:A:60:VAL:HG23	1:A:61:ASN:O	2.08	0.53
1:B:457:ILE:CD1	1:B:493:VAL:HG21	2.35	0.53
1:A:175:PHE:HE2	1:A:191:PHE:O	1.92	0.53
1:A:55:LEU:HA	1:A:58:LEU:HD12	1.89	0.53
1:B:552:LEU:HD23	1:B:552:LEU:OXT	2.08	0.53
1:B:365:GLU:HG3	1:B:498:ARG:HH12	1.74	0.53
1:A:23:GLY:HA2	1:A:92:GLY:H	1.73	0.53
1:B:306:ILE:O	1:B:310:ILE:HG13	2.09	0.53
1:B:318:ILE:O	1:B:321:TYR:HB2	2.08	0.53
1:B:315:GLU:HG3	1:B:416:PHE:HD2	1.73	0.53
1:B:313:GLU:OE2	1:B:350:ILE:HG12	2.09	0.53
1:B:408:PRO:HB3	1:B:507:ILE:HG12	1.90	0.52
1:B:451:TYR:HD1	1:B:453:PRO:HD3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:O	1:A:146:ASN:HB2	2.09	0.52
1:B:380:ILE:HA	1:B:399:CYS:O	2.09	0.52
1:A:112:LEU:HD12	1:A:113:THR:N	2.25	0.52
1:A:177:LEU:HG	1:A:177:LEU:O	2.09	0.52
1:A:175:PHE:CZ	1:A:190:VAL:HG22	2.45	0.52
1:B:352:LEU:O	1:B:356:LYS:HB2	2.10	0.52
1:B:308:LYS:HE3	1:B:423:GLU:OE1	2.09	0.52
1:A:194:ARG:O	1:A:194:ARG:HG3	2.10	0.52
1:B:548:ILE:HD12	1:B:548:ILE:H	1.74	0.52
1:B:497:VAL:HG11	1:B:536:ILE:HG21	1.91	0.52
1:B:523:GLU:O	1:B:525:LYS:HG3	2.10	0.52
1:A:175:PHE:CE2	1:A:192:ASP:HB2	2.45	0.52
1:B:380:ILE:HG22	1:B:399:CYS:O	2.10	0.52
1:A:175:PHE:HE2	1:A:192:ASP:HB2	1.75	0.51
1:A:81:ASP:CB	1:A:99:CYS:HB2	2.41	0.51
1:A:218:ASP:HB3	1:A:224:LEU:HA	1.91	0.51
1:B:497:VAL:HG11	1:B:536:ILE:CG2	2.40	0.51
1:B:524:LEU:CD2	1:B:536:ILE:HD12	2.40	0.51
1:A:94:PRO:HD3	1:B:481:TYR:OH	2.10	0.51
1:B:449:ILE:HG23	1:B:466:VAL:CG1	2.38	0.51
1:A:194:ARG:HG3	1:A:194:ARG:HH11	1.73	0.51
1:B:545:LEU:O	1:B:549:LEU:HB2	2.10	0.51
1:B:524:LEU:HD22	1:B:536:ILE:HD12	1.92	0.51
1:B:499:ALA:HB3	1:B:529:ASN:O	2.11	0.51
1:A:70:ILE:O	1:A:70:ILE:HG22	2.11	0.51
1:A:226:PHE:HD1	1:A:227:ASP:O	1.94	0.51
1:B:426:LYS:HB3	1:B:426:LYS:NZ	2.19	0.51
1:A:224:LEU:HD22	1:A:236:ILE:HD12	1.92	0.50
1:A:108:PRO:HG2	1:A:126:LYS:NZ	2.26	0.50
1:B:518:ASP:CA	1:B:524:LEU:HD12	2.41	0.50
1:A:13:GLU:O	1:A:16:LYS:HB3	2.11	0.50
1:A:248:ILE:HG23	1:A:252:LEU:HD23	1.92	0.50
1:B:352:LEU:CD2	1:B:367:LEU:HD13	2.37	0.50
1:A:149:ILE:HG23	1:A:166:VAL:CG1	2.41	0.50
1:B:317:GLU:HG3	1:B:350:ILE:HD11	1.93	0.50
1:B:313:GLU:HG3	1:B:354:TYR:OH	2.12	0.50
1:A:205:SER:O	1:A:209:CYS:HB2	2.12	0.50
1:A:28:SER:OG	1:A:41:GLU:OE1	2.29	0.50
1:B:440:LYS:O	1:B:441:ASP:HB3	2.12	0.49
1:A:41:GLU:O	1:A:44:ASP:HB2	2.11	0.49
1:A:66:GLU:HB3	4:A:612:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:HB2	1:A:82:PRO:HG3	1.93	0.49
1:A:125:TYR:CB	1:A:128:LYS:HG3	2.42	0.49
1:A:235:ASN:O	1:A:236:ILE:HB	2.12	0.49
1:B:343:PHE:HD1	1:B:383:ILE:HD13	1.76	0.49
1:B:494:ARG:HH11	1:B:494:ARG:HG3	1.78	0.49
1:B:422:TYR:CD2	1:B:480:CYS:HB3	2.48	0.49
1:B:441:ASP:O	1:B:441:ASP:OD2	2.30	0.49
1:B:537:ILE:O	1:B:537:ILE:HG22	2.11	0.49
1:B:517:THR:O	1:B:537:ILE:HB	2.12	0.48
1:A:153:PRO:CB	1:A:157:ILE:HG13	2.43	0.48
1:B:336:SER:CB	1:B:498:ARG:HD3	2.43	0.48
1:B:412:LEU:HD12	1:B:413:THR:N	2.27	0.48
1:A:113:THR:HG21	1:A:180:CYS:SG	2.52	0.48
1:B:381:ASP:OD1	1:B:384:ASP:HA	2.13	0.48
1:A:242:LYS:O	1:A:242:LYS:HE3	2.12	0.48
1:B:544:MET:HG3	1:B:548:ILE:HD11	1.95	0.48
1:A:244:MET:HE3	1:A:244:MET:O	2.12	0.48
1:B:529:ASN:HD22	1:B:529:ASN:H	1.62	0.48
1:B:518:ASP:N	1:B:524:LEU:HD12	2.29	0.48
1:B:322:PHE:CE2	1:B:392:GLY:HA2	2.48	0.48
1:B:431:TYR:HA	1:B:437:ILE:H	1.79	0.48
1:A:246:ASP:HA	1:A:249:LEU:HD12	1.95	0.48
1:B:425:TYR:HD2	1:B:428:LYS:HE2	1.77	0.48
1:A:149:ILE:HD13	1:A:166:VAL:CG2	2.44	0.48
1:A:210:LYS:HG3	1:A:216:ILE:HD12	1.95	0.48
1:A:152:TYR:OH	1:A:178:GLU:OE2	2.32	0.47
1:A:191:PHE:O	1:A:192:ASP:HB2	2.13	0.47
1:B:494:ARG:O	1:B:494:ARG:HG3	2.14	0.47
1:B:479:MET:HA	1:B:482:VAL:HG23	1.96	0.47
1:A:137:ILE:HD12	1:A:184:LYS:HB3	1.97	0.47
1:A:186:THR:HG22	1:A:187:LEU:CD2	2.44	0.47
1:B:440:LYS:HB3	1:B:441:ASP:H	1.38	0.47
1:A:33:THR:O	1:A:33:THR:HG23	2.14	0.47
1:B:431:TYR:CD1	1:B:436:LYS:HG3	2.50	0.47
1:A:48:GLU:HB2	1:A:82:PRO:CG	2.44	0.47
1:B:384:ASP:OD2	1:B:476:GLY:HA3	2.15	0.47
1:A:18:ILE:HD12	1:A:89:PHE:CZ	2.49	0.47
1:B:471:ILE:O	1:B:471:ILE:HG22	2.13	0.47
1:A:124:ALA:CB	1:A:208:ILE:HA	2.44	0.47
1:A:22:PHE:CZ	1:A:92:GLY:HA2	2.50	0.47
1:B:535:ASN:O	1:B:536:ILE:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:CE	1:A:17:GLU:HG2	2.44	0.47
1:B:369:VAL:O	1:B:369:VAL:HG12	2.14	0.47
1:B:368:GLY:HA2	1:B:530:ALA:HB2	1.97	0.47
1:A:68:GLY:HA2	1:A:230:ALA:CB	2.45	0.46
1:A:190:VAL:O	1:A:190:VAL:HG13	2.15	0.46
1:A:97:ALA:HB1	1:A:114:TYR:O	2.15	0.46
1:B:497:VAL:HG12	1:B:534:LEU:O	2.16	0.46
1:A:28:SER:OG	1:A:43:PHE:HE2	1.97	0.46
1:B:395:PHE:CD1	1:B:477:LEU:HD23	2.50	0.46
1:A:170:ARG:HG2	1:A:170:ARG:HH11	1.80	0.46
1:A:146:ASN:HA	1:A:167:LYS:HD3	1.98	0.46
1:B:449:ILE:HD12	1:B:491:PHE:HE1	1.81	0.46
1:B:518:ASP:HA	1:B:524:LEU:HD12	1.97	0.46
1:A:22:PHE:CE2	1:A:92:GLY:HA2	2.51	0.46
1:A:14:ILE:HD12	1:A:47:SER:OG	2.16	0.46
1:B:376:TRP:CZ2	1:B:404:LYS:HD2	2.51	0.46
1:B:400:PHE:HB3	1:B:412:LEU:HB3	1.98	0.46
1:A:23:GLY:O	1:A:25:LYS:N	2.49	0.46
1:A:163:ARG:NH2	1:B:463:ARG:HH21	2.14	0.45
1:B:313:GLU:OE2	1:B:350:ILE:HG23	2.15	0.45
1:A:115:GLU:OE1	1:A:118:THR:OG1	2.30	0.45
1:B:545:LEU:HG	1:B:549:LEU:HD12	1.99	0.45
1:A:193:VAL:HA	1:A:235:ASN:HD22	1.80	0.45
1:A:237:ILE:O	1:A:237:ILE:HG22	2.17	0.45
1:B:329:TYR:CZ	1:B:342:ILE:HD13	2.51	0.45
1:A:192:ASP:OD2	1:A:194:ARG:NH1	2.50	0.45
1:B:336:SER:OG	1:B:533:ARG:NH2	2.50	0.45
1:A:157:ILE:O	1:A:159:LEU:N	2.50	0.45
1:A:207:ILE:O	1:A:210:LYS:N	2.50	0.45
1:A:196:LYS:O	1:A:233:ARG:NH2	2.50	0.45
1:A:237:ILE:HD12	1:A:248:ILE:CG2	2.35	0.45
1:B:495:PRO:HD3	1:B:535:ASN:ND2	2.29	0.45
1:A:246:ASP:O	1:A:249:LEU:N	2.50	0.45
1:A:229:ASN:ND2	1:A:231:THR:O	2.50	0.45
1:A:62:ILE:O	1:A:63:VAL:HG23	2.16	0.45
1:B:318:ILE:O	1:B:389:PHE:HZ	2.00	0.45
1:B:511:GLU:HA	1:B:511:GLU:OE1	2.16	0.45
1:A:244:MET:HA	1:A:247:ILE:HG13	1.98	0.45
1:B:437:ILE:HB	1:B:484:LYS:HA	1.98	0.45
1:B:478:GLU:O	1:B:481:TYR:HB2	2.17	0.45
1:B:319:LEU:HD23	1:B:319:LEU:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ILE:HG22	1:B:548:ILE:N	2.32	0.45
1:B:490:VAL:O	1:B:490:VAL:HG13	2.17	0.45
1:A:24:ARG:NH2	1:A:26:ASP:OD2	2.50	0.45
1:B:425:TYR:O	1:B:511:GLU:HG3	2.16	0.45
1:A:243:GLU:OE2	1:A:243:GLU:N	2.50	0.45
1:B:420:SER:HB3	1:B:432:LEU:CD1	2.38	0.44
1:A:140:LYS:O	1:A:240:ASN:ND2	2.50	0.44
1:A:199:ALA:HB2	4:A:607:HOH:O	2.17	0.44
1:B:451:TYR:OH	1:B:463:ARG:NH2	2.50	0.44
1:B:448:VAL:O	1:B:448:VAL:HG12	2.17	0.44
1:A:247:ILE:H	1:A:247:ILE:HG12	1.42	0.44
1:B:510:LYS:HA	1:B:510:LYS:CE	2.46	0.44
1:A:149:ILE:HG13	1:A:151:TYR:HD2	1.83	0.44
1:B:438:LYS:HG2	1:B:439:VAL:N	2.27	0.44
1:B:541:SER:OG	1:B:542:LYS:N	2.50	0.44
1:A:43:PHE:HE1	1:A:86:SER:HG	1.65	0.44
1:A:114:TYR:HD2	1:A:120:SER:O	2.00	0.44
1:A:4:ASP:HA	1:A:110:TYR:CE1	2.51	0.44
1:A:194:ARG:O	1:A:196:LYS:N	2.50	0.44
1:A:83:ILE:CG2	1:A:86:SER:HA	2.48	0.44
1:B:529:ASN:HD22	1:B:529:ASN:N	2.14	0.44
1:A:19:LEU:N	1:A:20:PRO:HD2	2.33	0.44
1:B:390:ILE:HD12	1:B:390:ILE:O	2.17	0.44
1:A:147:ILE:HG13	1:A:244:MET:SD	2.57	0.44
1:B:437:ILE:CD1	1:B:483:ALA:HB1	2.48	0.44
1:B:443:ASN:OD1	1:B:444:PRO:HD2	2.18	0.44
1:A:175:PHE:O	1:A:178:GLU:N	2.50	0.43
1:A:248:ILE:HG23	1:A:252:LEU:CD2	2.48	0.43
1:A:16:LYS:HE2	1:A:17:GLU:HG2	2.00	0.43
1:A:161:LYS:HB3	1:A:251:LEU:CD1	2.47	0.43
1:B:324:ARG:HH11	1:B:324:ARG:HG2	1.82	0.43
1:B:449:ILE:HD12	1:B:491:PHE:CE1	2.53	0.43
1:A:95:PHE:HE2	1:B:395:PHE:HD2	1.66	0.43
1:B:324:ARG:NH2	1:B:326:ASP:OD1	2.51	0.43
1:A:155:LYS:CD	1:A:155:LYS:H	2.30	0.43
1:A:217:THR:O	1:A:237:ILE:N	2.51	0.43
1:B:445:ASN:O	1:B:467:LYS:HB3	2.18	0.43
1:A:203:ALA:O	1:A:206:TYR:HB3	2.19	0.43
1:A:18:ILE:CG2	1:A:46:ILE:HD11	2.41	0.43
1:B:415:GLU:OE2	1:B:477:LEU:HD21	2.19	0.43
1:B:494:ARG:NH1	1:B:494:ARG:HG3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:TYR:CE1	1:B:436:LYS:HG3	2.53	0.43
1:A:67:LEU:N	4:A:612:HOH:O	2.51	0.43
1:B:544:MET:O	1:B:548:ILE:HD12	2.19	0.42
1:A:88:ASN:OD1	1:B:470:ARG:NH2	2.50	0.42
1:B:390:ILE:HA	1:B:390:ILE:HD13	1.91	0.42
1:B:396:PHE:O	1:B:397:ALA:HB2	2.20	0.42
1:A:107:GLU:HA	1:A:108:PRO:HD2	1.68	0.42
1:B:355:LEU:CD1	1:B:378:VAL:HG11	2.46	0.42
1:A:122:TYR:OH	1:A:184:LYS:HD3	2.19	0.42
1:B:316:LYS:HE3	1:B:317:GLU:OE2	2.19	0.42
1:A:48:GLU:O	1:A:51:ALA:N	2.53	0.42
1:A:242:LYS:HD2	1:A:242:LYS:HA	1.61	0.42
1:A:149:ILE:CD1	1:A:166:VAL:HG21	2.47	0.42
1:A:87:PHE:HA	1:A:90:ILE:HG22	2.01	0.42
1:A:191:PHE:CB	1:A:237:ILE:HD13	2.42	0.42
1:B:450:SER:O	1:B:490:VAL:HA	2.19	0.42
1:B:519:GLU:HG2	1:B:520:ASN:ND2	2.35	0.42
1:B:388:ASN:ND2	1:B:472:PHE:O	2.50	0.42
1:B:484:LYS:HD2	1:B:486:THR:OG1	2.20	0.42
1:B:372:ASN:HD22	1:B:372:ASN:HA	1.38	0.42
1:A:95:PHE:CE1	1:B:394:PRO:HD2	2.55	0.42
1:B:400:PHE:C	1:B:504:SER:HB2	2.40	0.41
1:B:521:GLY:CA	1:B:549:LEU:HD11	2.48	0.41
1:B:324:ARG:HA	1:B:324:ARG:NH1	2.36	0.41
1:B:458:ASP:OD2	1:B:461:LYS:HB2	2.20	0.41
1:A:193:VAL:O	1:A:195:PRO:HD3	2.20	0.41
1:B:454:SER:O	1:B:457:ILE:HB	2.20	0.41
1:B:488:ASP:O	1:B:489:ALA:HB2	2.20	0.41
1:B:417:LEU:HD22	1:B:417:LEU:HA	1.83	0.41
1:A:148:VAL:HG22	1:A:168:ARG:HB2	2.02	0.41
1:B:342:ILE:O	1:B:346:ILE:HB	2.21	0.41
1:B:323:GLY:O	1:B:325:LYS:N	2.50	0.41
1:B:449:ILE:HG12	1:B:466:VAL:HG11	2.03	0.41
1:A:207:ILE:O	1:A:210:LYS:HB2	2.21	0.41
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.86	0.41
1:A:138:LYS:HZ3	1:A:212:ALA:HA	1.84	0.41
1:B:435:ARG:HB3	1:B:435:ARG:HE	1.44	0.41
1:A:150:SER:O	1:A:151:TYR:HB3	2.21	0.41
1:A:196:LYS:C	1:A:233:ARG:HG2	2.41	0.41
1:B:396:PHE:O	1:B:477:LEU:HD22	2.20	0.41
1:B:321:TYR:HB3	1:B:389:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ILE:HD13	1:B:457:ILE:N	2.35	0.41
1:A:208:ILE:HG22	1:A:209:CYS:N	2.34	0.41
1:A:23:GLY:HA2	1:A:92:GLY:N	2.36	0.41
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.68	0.41
1:B:358:LEU:HD23	1:B:358:LEU:N	2.35	0.41
1:B:547:ILE:O	1:B:551:LEU:HG	2.21	0.41
1:A:138:LYS:NZ	1:A:212:ALA:HA	2.36	0.41
1:B:515:LEU:HD23	1:B:515:LEU:N	2.36	0.41
1:A:206:TYR:CE1	1:A:216:ILE:HG21	2.56	0.40
1:A:175:PHE:O	1:A:178:GLU:HB2	2.22	0.40
1:B:395:PHE:CG	1:B:472:PHE:HB3	2.56	0.40
1:B:495:PRO:CD	1:B:535:ASN:HD21	2.27	0.40
1:A:52:LEU:HD11	1:A:67:LEU:HD22	2.04	0.40
1:A:84:ASP:N	1:A:97:ALA:O	2.51	0.40
1:B:462:LEU:HD21	1:B:491:PHE:HZ	1.87	0.40
1:A:163:ARG:HH22	1:B:463:ARG:HH21	1.68	0.40
1:B:431:TYR:HD1	1:B:436:LYS:HA	1.86	0.40
1:A:139:VAL:HG12	1:A:240:ASN:HB2	2.03	0.40
1:B:467:LYS:O	1:B:467:LYS:HG3	2.21	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	250/252 (99%)	183 (73%)	52 (21%)	15 (6%)	2 2
1	B	250/252 (99%)	194 (78%)	42 (17%)	14 (6%)	2 2
All	All	500/504 (99%)	377 (75%)	94 (19%)	29 (6%)	2 2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	139	VAL
1	A	146	ASN
1	A	192	ASP
1	A	207	ILE
1	A	208	ILE
1	A	220	ASN
1	A	236	ILE
1	B	439	VAL
1	B	441	ASP
1	B	490	VAL
1	A	24	ARG
1	A	158	ASP
1	A	216	ILE
1	B	321	TYR
1	B	446	ASN
1	B	495	PRO
1	B	531	THR
1	A	203	ALA
1	B	387	PHE
1	B	511	GLU
1	B	523	GLU
1	A	195	PRO
1	B	483	ALA
1	A	87	PHE
1	B	440	LYS
1	B	471	ILE
1	B	536	ILE
1	A	221	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	221/221 (100%)	163 (74%)	58 (26%)	0 1
1	B	221/221 (100%)	157 (71%)	64 (29%)	0 1
All	All	442/442 (100%)	320 (72%)	122 (28%)	0 1

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	8	LYS
1	A	9	ASN
1	A	13	GLU
1	A	16	LYS
1	A	18	ILE
1	A	19	LEU
1	A	21	TYR
1	A	24	ARG
1	A	25	LYS
1	A	27	LYS
1	A	34	SER
1	A	36	SER
1	A	42	ILE
1	A	46	ILE
1	A	47	SER
1	A	50	ILE
1	A	53	LYS
1	A	56	LYS
1	A	57	SER
1	A	60	VAL
1	A	62	ILE
1	A	66	GLU
1	A	80	ILE
1	A	107	GLU
1	A	118	THR
1	A	119	LYS
1	A	126	LYS
1	A	128	LYS
1	A	139	VAL
1	A	140	LYS
1	A	147	ILE
1	A	149	ILE
1	A	150	SER
1	A	154	SER
1	A	155	LYS
1	A	156	LYS
1	A	159	LEU
1	A	161	LYS
1	A	165	LYS
1	A	184	LYS
1	A	186	THR

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Mol	Chain	Res	Type
1	A	197	VAL
1	A	202	ILE
1	A	209	CYS
1	A	215	LEU
1	A	217	THR
1	A	218	ASP
1	A	224	LEU
1	A	229	ASN
1	A	233	ARG
1	A	234	LEU
1	A	241	SER
1	A	242	LYS
1	A	246	ASP
1	A	247	ILE
1	A	251	LEU
1	A	252	LEU
1	B	301	MET
1	B	302	LYS
1	B	313	GLU
1	B	316	LYS
1	B	319	LEU
1	B	321	TYR
1	B	324	ARG
1	B	327	LYS
1	B	328	SER
1	B	330	VAL
1	B	334	SER
1	B	342	ILE
1	B	346	ILE
1	B	347	SER
1	B	359	ASN
1	B	367	LEU
1	B	370	ILE
1	B	371	ASP
1	B	372	ASN
1	B	373	SER
1	B	375	GLU
1	B	380	ILE
1	B	390	ILE
1	B	393	ILE
1	B	402	VAL
1	B	404	LYS

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Mol	Chain	Res	Type
1	B	406	ASN
1	B	415	GLU
1	B	417	LEU
1	B	418	THR
1	B	426	LYS
1	B	428	LYS
1	B	431	TYR
1	B	435	ARG
1	B	436	LYS
1	B	438	LYS
1	B	440	LYS
1	B	449	ILE
1	B	455	LYS
1	B	456	LYS
1	B	457	ILE
1	B	460	GLU
1	B	463	ARG
1	B	465	LYS
1	B	467	LYS
1	B	482	VAL
1	B	484	LYS
1	B	486	THR
1	B	488	ASP
1	B	492	ASP
1	B	498	ARG
1	B	504	SER
1	B	510	LYS
1	B	511	GLU
1	B	515	LEU
1	B	524	LEU
1	B	527	ASP
1	B	529	ASN
1	B	531	THR
1	B	532	ASP
1	B	534	LEU
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	105	ASN
1	A	229	ASN
1	A	235	ASN
1	B	372	ASN
1	B	405	ASN
1	B	433	ASN
1	B	445	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 8 ligands modelled in this entry, 6 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	PO4	A	293	2	4,4,4	0.82	0	6,6,6	0.27	0
3	PO4	B	593	2	4,4,4	0.84	0	6,6,6	0.27	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
3	PO4	B	593	2	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	252/252 (100%)	-0.12	3 (1%)	81	77	13, 46, 95, 133	0
1	B	252/252 (100%)	0.01	3 (1%)	81	77	10, 48, 89, 106	0
All	All	504/504 (100%)	-0.06	6 (1%)	81	77	10, 47, 92, 133	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	PHE	4.6
1	B	549	LEU	3.9
1	B	395	PHE	3.2
1	A	166	VAL	2.6
1	A	248	ILE	2.4
1	B	548	ILE	2.4

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, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PO4	A	293	5/5	0.90	0.16	0.60	31,33,57,65	0
2	ZN	B	592	1/1	0.98	0.14	-0.45	46,46,46,46	0
3	PO4	B	593	5/5	0.94	0.14	-0.94	24,25,37,41	0
2	ZN	A	291	1/1	0.93	0.08	-1.50	42,42,42,42	0
2	ZN	A	290	1/1	0.97	0.07	-2.15	34,34,34,34	0
2	ZN	B	590	1/1	0.98	0.04	-3.69	35,35,35,35	0
2	ZN	B	591	1/1	0.98	0.04	-4.58	27,27,27,27	0
2	ZN	A	292	1/1	0.86	0.11	-	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.