



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:46 PM GMT

PDB ID : 1H54  
Title : Maltose phosphorylase from Lactobacillus brevis  
Authors : Van Tilbeurgh, H.; Egloff, M.-P.  
Deposited on : 2001-05-18  
Resolution : 2.15 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

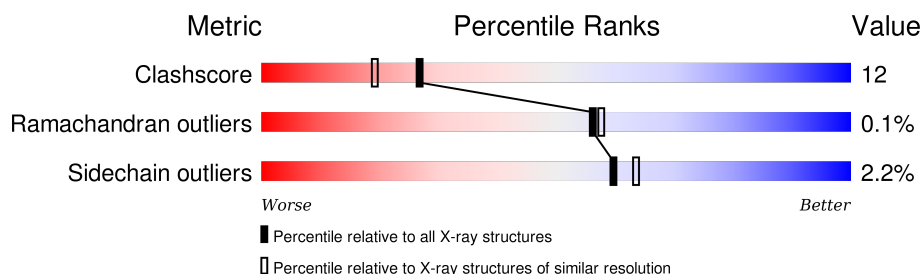
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	754	 76% 21% .
1	B	754	 79% 20% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13699 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.

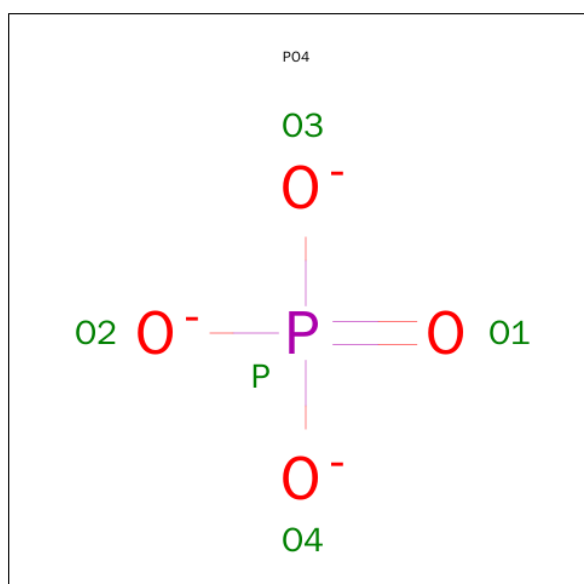
- Molecule 1 is a protein called MALTOSE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	753	Total	C	N	O	S	0	0	1
			6045	3843	1020	1165	17			
1	B	754	Total	C	N	O	S	0	0	0
			6055	3848	1020	1170	17			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	723	Total	O	0	0
			723	723		
4	B	869	Total	O	0	0
			869	869		



H679	
Y683	
H689	
H690	
Q695	
L696	
H697	
Y698	
A699	
P700	
F701	
T705	
W706	
Y709	
D742	
A754	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.75 Å   102.50 Å   114.00 Å 90.00°   111.30°   90.00°	Depositor
Resolution (Å)	29.10 – 2.15	Depositor
% Data completeness (in resolution range)	98.0 (29.10-2.15)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.186 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	0.33	0/6195	0.59	0/8419
1	B	0.34	0/6205	0.60	0/8432
All	All	0.33	0/12400	0.60	0/16851

There are no bond length outliers.

There are no bond angle outliers.

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	6045	0	5809	163	0
1	B	6055	0	5809	129	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	5	0	0	0	0
4	A	723	0	0	21	0
4	B	869	0	0	16	0
All	All	13699	0	11618	287	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.



All (287) 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:179:GLU:OE2	1:A:351:LYS:CE	1.88	1.20
1:A:179:GLU:OE2	1:A:351:LYS:HE3	1.55	1.06
1:A:179:GLU:OE2	1:A:351:LYS:CG	2.05	1.04
1:B:604:ILE:HD13	1:B:690:ARG:HH12	1.19	1.03
1:A:179:GLU:HA	1:A:179:GLU:OE1	1.53	1.03
1:A:128:ARG:HB2	1:A:131:VAL:HG23	1.51	0.93
1:A:426:ILE:HD13	1:A:467:ARG:NH1	1.84	0.92
1:B:604:ILE:HD13	1:B:690:ARG:NH1	1.83	0.92
1:A:420:GLU:HG2	1:B:419:TRP:HZ2	1.39	0.88
1:A:420:GLU:HB2	4:A:2441:HOH:O	1.76	0.85
1:A:179:GLU:OE2	1:A:351:LYS:HE2	1.75	0.85
1:A:657:LEU:HD12	1:A:662:TYR:HB2	1.56	0.85
1:A:341:ASN:ND2	1:A:360:THR:HG21	1.92	0.84
1:B:381:LEU:HD22	1:B:436:ILE:HD13	1.57	0.84
1:B:356:THR:HG23	4:B:2518:HOH:O	1.76	0.84
1:B:412:GLY:HA2	4:B:2561:HOH:O	1.75	0.84
1:A:673:THR:HG21	4:A:2674:HOH:O	1.79	0.81
1:B:361:GLU:HG3	1:B:432:ILE:HD13	1.65	0.79
1:B:207:PRO:HA	1:B:214:ARG:HD3	1.63	0.78
1:A:272:GLU:N	4:A:2337:HOH:O	2.16	0.78
1:A:247:LYS:HE2	4:A:2208:HOH:O	1.83	0.78
1:A:419:TRP:HZ2	1:B:420:GLU:HG2	1.49	0.78
1:A:179:GLU:OE2	1:A:351:LYS:HG3	1.83	0.77
1:A:341:ASN:HD22	1:A:342:ILE:H	1.30	0.77
1:B:320:GLN:HE21	1:B:656:ARG:HH12	1.32	0.76
1:A:341:ASN:HD21	1:A:360:THR:HG21	1.48	0.75
1:B:197:ASP:OD2	1:B:198:ARG:HG3	1.86	0.75
1:A:322:ILE:CD1	1:A:678:ALA:HB1	2.17	0.75
1:A:179:GLU:OE2	1:A:351:LYS:HG2	1.87	0.75
1:B:405:PHE:H	1:B:429:ASN:HD21	1.35	0.74
1:A:687:ALA:HA	1:A:700:PRO:HB3	1.69	0.74
1:A:405:PHE:H	1:A:429:ASN:HD21	1.37	0.73
1:B:325:ASN:HD22	1:B:678:ALA:HB3	1.52	0.73
1:B:613:LYS:HE2	4:B:2785:HOH:O	1.88	0.72
1:B:1:MET:HG2	1:B:661:ASN:O	1.89	0.72
1:A:272:GLU:HG2	4:A:2337:HOH:O	1.89	0.72
1:B:143:VAL:H	1:B:297:HIS:HD2	1.36	0.72
1:A:179:GLU:OE2	1:A:351:LYS:CD	2.36	0.72
1:A:467:ARG:NE	4:A:2469:HOH:O	2.23	0.71
1:B:608:THR:H	1:B:611:GLN:HE21	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:LYS:HE3	4:A:2651:HOH:O	1.89	0.71
1:B:494:ASN:HD22	1:B:499:ASN:HD21	1.39	0.70
1:A:613:LYS:HE2	4:A:2302:HOH:O	1.91	0.70
1:A:179:GLU:HB2	1:A:350:GLU:OE2	1.91	0.70
1:A:468:VAL:HG21	1:A:477:TYR:HB3	1.73	0.70
1:B:222:ARG:HG3	4:B:2351:HOH:O	1.92	0.69
1:A:394:ASN:HD21	1:A:414:GLU:H	1.39	0.69
1:A:162:GLU:OE2	1:A:247:LYS:HD3	1.92	0.68
1:B:705:THR:HG22	4:B:2835:HOH:O	1.93	0.68
1:A:236:ASN:ND2	1:A:238:LYS:H	1.91	0.68
1:A:320:GLN:HE21	1:A:656:ARG:HH12	1.39	0.68
1:A:344:PRO:HG2	1:A:353:GLY:HA2	1.76	0.68
1:A:363:PHE:CD1	1:A:629:LEU:HD13	2.29	0.67
1:A:566:VAL:HG13	1:A:621:PRO:O	1.94	0.67
1:B:330:PHE:HZ	1:B:371:ILE:HD12	1.57	0.67
1:A:658:ASP:OD2	1:A:671:HIS:HD2	1.78	0.67
1:B:478:MET:HB3	1:B:494:ASN:HD21	1.60	0.67
1:B:436:ILE:HD12	1:B:448:TYR:HE2	1.60	0.66
1:B:312:ILE:HB	1:B:319:GLN:HG2	1.77	0.66
1:A:179:GLU:CA	1:A:179:GLU:OE1	2.40	0.65
1:B:176:MET:SD	4:B:2281:HOH:O	2.54	0.65
1:A:207:PRO:HA	1:A:214:ARG:HD3	1.78	0.65
1:B:462:ARG:HD2	1:B:530:GLU:OE1	1.96	0.65
1:B:325:ASN:HD21	1:B:655:ALA:HA	1.62	0.64
1:B:176:MET:HB3	4:B:2284:HOH:O	1.97	0.64
1:B:427:HIS:HD2	1:B:431:ASP:OD2	1.80	0.64
1:B:705:THR:HG23	1:B:706:TRP:CD1	2.33	0.63
1:A:142:SER:HA	1:A:297:HIS:CD2	2.34	0.63
1:B:409:THR:HG21	4:B:2561:HOH:O	1.99	0.63
1:A:495:ASN:HD22	1:A:498:THR:H	1.47	0.62
1:B:325:ASN:HD22	1:B:678:ALA:CB	2.11	0.62
1:B:160:ASP:HB2	4:B:2244:HOH:O	2.00	0.62
1:A:196:ALA:HB1	1:A:229:ASN:HD21	1.65	0.61
1:B:604:ILE:HG21	1:B:690:ARG:NH1	2.15	0.61
1:B:105:LYS:HD3	1:B:106:ILE:N	2.16	0.60
1:A:1:MET:HG2	4:A:2663:HOH:O	2.02	0.59
1:B:157:ASN:ND2	1:B:159:SER:H	1.99	0.59
1:A:170:SER:CB	1:A:241:THR:HG22	2.32	0.59
1:B:436:ILE:HD11	4:B:2594:HOH:O	2.02	0.59
1:A:276:ALA:O	1:A:280:GLN:HG3	2.02	0.59
1:A:127:GLU:OE2	1:A:132:ARG:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASN:ND2	1:A:36:MET:H	2.00	0.59
1:B:361:GLU:CG	1:B:432:ILE:HD13	2.32	0.59
1:A:160:ASP:O	1:A:161:ALA:HB3	2.02	0.59
1:A:322:ILE:HD13	1:A:678:ALA:HB1	1.85	0.58
1:A:270:THR:CB	4:A:2337:HOH:O	2.50	0.58
1:A:426:ILE:HD13	1:A:467:ARG:HH12	1.67	0.58
1:A:143:VAL:H	1:A:297:HIS:HD2	1.52	0.58
1:B:325:ASN:ND2	1:B:678:ALA:CB	2.66	0.58
1:B:351:LYS:O	1:B:352:TYR:HB2	2.03	0.58
1:B:91:PRO:HG2	1:B:168:LYS:HB2	1.86	0.57
1:B:205:THR:O	1:B:214:ARG:HD2	2.05	0.57
1:A:495:ASN:ND2	1:A:498:THR:H	2.02	0.57
1:B:375:LYS:HE3	4:B:2526:HOH:O	2.04	0.57
1:B:319:GLN:HE21	1:B:319:GLN:CA	2.18	0.57
1:A:101:LEU:HD13	1:A:106:ILE:HD13	1.86	0.57
1:B:223:LEU:HD13	1:B:244:TYR:CE1	2.40	0.57
1:B:672:ILE:HA	1:B:675:MET:HG2	1.87	0.56
1:A:341:ASN:ND2	1:A:342:ILE:H	2.00	0.56
1:B:145:GLN:HE22	1:B:284:LYS:NZ	2.03	0.56
1:A:164:ASP:HB2	4:A:2208:HOH:O	2.04	0.56
1:A:697:HIS:HD2	1:A:742:ASP:OD1	1.89	0.56
1:A:205:THR:O	1:A:214:ARG:HD2	2.06	0.56
1:A:420:GLU:HG2	1:B:419:TRP:CZ2	2.30	0.56
1:A:206:THR:HB	1:A:207:PRO:HD2	1.86	0.56
1:A:308:SER:HB3	1:A:371:ILE:HB	1.88	0.56
1:A:166:THR:OG1	1:A:245:THR:HG22	2.05	0.56
1:B:597:LEU:HD12	1:B:634:HIS:CE1	2.41	0.56
1:A:333:TYR:CZ	1:A:380:LEU:HD13	2.41	0.56
1:A:31:LEU:HD11	1:A:120:LEU:HB2	1.87	0.56
1:B:697:HIS:HD2	1:B:742:ASP:OD1	1.88	0.55
1:B:274:LEU:HD23	1:B:274:LEU:C	2.27	0.55
1:A:299:ALA:O	1:A:303:GLN:HG3	2.05	0.55
1:B:224:VAL:HB	1:B:257:GLU:HB2	1.88	0.55
1:B:325:ASN:ND2	1:B:678:ALA:HB2	2.21	0.55
1:B:2:LYS:HE3	4:B:2006:HOH:O	2.05	0.55
1:B:620:GLU:HB3	1:B:621:PRO:HD3	1.88	0.55
1:B:597:LEU:HD12	1:B:634:HIS:HE1	1.72	0.54
1:A:170:SER:HB2	1:A:241:THR:HG22	1.90	0.54
1:B:33:ASN:ND2	1:B:36:MET:H	2.06	0.53
1:B:657:LEU:HD22	1:B:662:TYR:HB2	1.90	0.53
1:B:695:GLN:NE2	1:B:742:ASP:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:HD22	1:B:368:TYR:OH	2.08	0.53
1:B:654:THR:HG23	1:B:655:ALA:N	2.24	0.53
1:B:142:SER:HA	1:B:297:HIS:CD2	2.45	0.52
1:A:145:GLN:HE22	1:A:284:LYS:NZ	2.08	0.52
1:A:224:VAL:HB	1:A:257:GLU:HB2	1.91	0.52
1:B:428:ARG:O	1:B:432:ILE:HG12	2.10	0.52
1:B:612:LYS:HE3	1:B:640:ASP:OD2	2.09	0.52
1:A:604:ILE:HG21	1:A:690:ARG:HH12	1.73	0.52
1:B:363:PHE:CD1	1:B:629:LEU:HD22	2.44	0.52
1:A:179:GLU:CG	1:A:351:LYS:HG2	2.38	0.52
1:A:142:SER:HA	1:A:297:HIS:HD2	1.73	0.52
1:B:495:ASN:HD22	1:B:498:THR:H	1.58	0.51
1:A:510:LEU:HD13	1:A:535:GLN:HG2	1.92	0.51
1:A:179:GLU:CD	1:A:351:LYS:HG2	2.30	0.51
1:A:270:THR:HB	4:A:2337:HOH:O	2.09	0.51
1:A:39:ARG:NE	1:A:51:LEU:HB3	2.26	0.51
1:B:427:HIS:CD2	1:B:431:ASP:OD2	2.62	0.51
1:A:128:ARG:CB	1:A:131:VAL:HG23	2.34	0.51
1:B:143:VAL:HG22	1:B:297:HIS:CD2	2.45	0.51
1:A:394:ASN:ND2	1:A:414:GLU:H	2.06	0.51
1:B:364:ALA:HA	1:B:676:THR:HG21	1.91	0.51
1:A:446:ASP:HB3	1:A:450:LEU:HD22	1.93	0.51
1:A:236:ASN:HD22	1:A:238:LYS:H	1.59	0.51
1:B:233:THR:HG22	4:B:2378:HOH:O	2.11	0.51
1:A:186:PHE:O	1:A:205:THR:HA	2.11	0.50
1:A:270:THR:OG1	4:A:2337:HOH:O	2.20	0.50
1:B:118:GLY:O	1:B:297:HIS:HE1	1.95	0.50
1:B:264:THR:OG1	1:B:266:ARG:HG2	2.11	0.50
1:A:91:PRO:HG2	1:A:168:LYS:HB2	1.94	0.50
1:A:33:ASN:HD21	1:A:36:MET:H	1.58	0.50
1:A:628:SER:HB3	1:A:674:SER:OG	2.12	0.49
1:B:604:ILE:HG21	1:B:690:ARG:HH11	1.77	0.49
1:B:630:SER:N	1:B:631:PRO:HD2	2.26	0.49
1:B:375:LYS:HG3	4:B:2526:HOH:O	2.12	0.49
1:B:33:ASN:HD22	1:B:33:ASN:C	2.15	0.49
1:A:363:PHE:CG	1:A:629:LEU:HD13	2.47	0.49
1:A:468:VAL:CG2	1:A:477:TYR:HB3	2.42	0.49
1:B:630:SER:O	1:B:634:HIS:HD2	1.95	0.49
1:A:132:ARG:H	1:A:159:SER:HB3	1.77	0.49
1:B:416:HIS:HE1	1:B:418:GLU:OE1	1.95	0.49
1:A:373:ASP:HB3	4:A:2409:HOH:O	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:HG13	1:B:173:ALA:HA	1.95	0.48
1:A:467:ARG:CZ	4:A:2469:HOH:O	2.59	0.48
1:B:171:ILE:HG22	1:B:201:ILE:HD12	1.95	0.48
1:A:101:LEU:HD23	1:A:101:LEU:N	2.27	0.48
1:A:690:ARG:CZ	1:A:690:ARG:HB3	2.43	0.48
1:A:365:PHE:HE2	1:A:439:TYR:HB2	1.78	0.48
1:A:1:MET:HG3	1:A:664:ASN:ND2	2.29	0.48
1:A:419:TRP:HZ2	1:B:420:GLU:CG	2.24	0.47
1:A:419:TRP:CZ2	1:B:420:GLU:HG2	2.39	0.47
1:A:345:LYS:HB2	1:A:353:GLY:HA3	1.94	0.47
1:A:308:SER:CB	1:A:371:ILE:HB	2.43	0.47
1:B:359:ASP:OD2	1:B:629:LEU:HD11	2.15	0.47
1:A:425:GLU:HA	1:A:483:THR:O	2.14	0.47
1:B:319:GLN:HA	1:B:319:GLN:HE21	1.78	0.47
1:B:425:GLU:OE1	1:B:427:HIS:HE1	1.98	0.47
1:A:657:LEU:CD1	1:A:662:TYR:HB2	2.35	0.47
1:A:300:ILE:HA	1:A:303:GLN:HE21	1.80	0.47
1:B:55:TYR:HB3	1:B:81:VAL:HG11	1.97	0.47
1:B:4:ILE:HG13	1:B:5:PHE:CD1	2.48	0.47
1:B:338:ALA:HB1	1:B:379:ASN:ND2	2.30	0.47
1:A:30:SER:CB	1:A:348:THR:HG22	2.45	0.47
1:A:716:ARG:O	1:A:717:ASP:HB2	2.15	0.47
1:B:361:GLU:HB2	1:B:435:ALA:HB2	1.97	0.47
1:A:1:MET:HG3	1:A:664:ASN:HD21	1.80	0.47
1:A:646:LYS:HE3	4:A:2653:HOH:O	2.14	0.47
1:B:361:GLU:H	1:B:361:GLU:CD	2.18	0.46
1:B:311:VAL:O	1:B:709:TYR:HA	2.14	0.46
1:B:699:ALA:N	1:B:700:PRO:HD3	2.30	0.46
1:A:468:VAL:HG22	1:A:469:HIS:N	2.30	0.46
1:A:414:GLU:HG2	1:A:422:THR:HG23	1.98	0.46
1:B:518:GLN:O	1:B:522:LYS:HG3	2.15	0.46
1:A:4:ILE:HG13	1:A:5:PHE:CD1	2.51	0.46
1:B:22:LYS:O	1:B:26:GLU:HG3	2.15	0.46
1:B:119:VAL:CG1	1:B:138:GLN:HG3	2.45	0.46
1:A:166:THR:HG23	1:A:245:THR:HG22	1.96	0.46
1:B:369:LEU:HG	1:B:377:THR:HG21	1.98	0.46
1:A:333:TYR:CZ	1:A:335:GLY:HA2	2.51	0.45
1:B:666:THR:HG22	1:B:666:THR:O	2.16	0.45
1:A:1:MET:HG3	1:A:664:ASN:OD1	2.15	0.45
1:B:312:ILE:O	1:B:319:GLN:HG2	2.16	0.45
1:B:478:MET:CB	1:B:494:ASN:HD21	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLN:HE22	1:B:284:LYS:HZ2	1.64	0.45
1:A:256:LEU:HD23	1:A:256:LEU:C	2.37	0.45
1:A:468:VAL:HG23	1:A:478:MET:O	2.17	0.45
1:A:416:HIS:HE1	1:A:418:GLU:OE1	2.00	0.45
1:A:85:VAL:HG13	1:A:173:ALA:HA	1.99	0.45
1:A:365:PHE:HE1	1:A:380:LEU:HB3	1.81	0.44
1:A:118:GLY:O	1:A:297:HIS:HE1	2.00	0.44
1:B:360:THR:HB	1:B:361:GLU:OE1	2.16	0.44
1:A:110:THR:O	1:A:122:ARG:HA	2.17	0.44
1:B:328:GLN:HB2	1:B:675:MET:CE	2.48	0.44
1:B:679:TRP:CE2	1:B:683:VAL:HG21	2.53	0.44
1:A:181:ASN:O	1:A:183:ASP:N	2.50	0.44
1:A:544:PRO:HB2	1:A:553:VAL:HB	2.00	0.44
1:B:338:ALA:HB1	1:B:379:ASN:HD21	1.81	0.44
1:A:623:THR:HG22	1:A:625:HIS:H	1.83	0.44
1:B:222:ARG:CG	1:B:222:ARG:HH21	2.31	0.44
1:A:280:GLN:NE2	4:A:2345:HOH:O	2.49	0.43
1:A:375:LYS:HG3	4:A:2411:HOH:O	2.18	0.43
1:B:577:ASN:OD1	1:B:578:GLN:HG3	2.18	0.43
1:A:170:SER:HB3	1:A:241:THR:HG22	2.00	0.43
1:B:608:THR:OG1	1:B:611:GLN:HG3	2.18	0.43
1:B:101:LEU:HD13	1:B:106:ILE:HD13	2.01	0.43
1:A:322:ILE:HD11	1:A:678:ALA:HB1	1.95	0.43
1:A:33:ASN:C	1:A:33:ASN:HD22	2.20	0.43
1:A:593:GLN:HB3	1:A:627:SER:HB3	2.00	0.43
1:B:447:SER:O	1:B:451:HIS:HD2	2.01	0.43
1:A:653:ARG:HD3	1:A:662:TYR:CE1	2.53	0.43
1:A:687:ALA:HA	1:A:700:PRO:CB	2.46	0.43
1:A:143:VAL:HG22	1:A:297:HIS:CD2	2.53	0.43
1:A:322:ILE:HD13	1:A:678:ALA:CB	2.48	0.43
1:A:196:ALA:HB1	1:A:229:ASN:ND2	2.31	0.43
1:A:22:LYS:O	1:A:26:GLU:HG3	2.19	0.43
1:A:25:GLN:CD	4:A:2039:HOH:O	2.57	0.43
1:A:689:MET:HA	1:A:697:HIS:O	2.19	0.43
1:A:15:HIS:HA	1:A:109:PHE:O	2.19	0.43
1:A:33:ASN:ND2	1:A:35:TYR:H	2.17	0.42
1:B:355:ALA:HB2	1:B:410:PHE:CE1	2.53	0.42
1:A:401:LYS:HE2	4:A:2466:HOH:O	2.19	0.42
1:A:212:THR:HB	1:A:213:PRO:HD2	2.02	0.42
1:A:449:VAL:HG13	1:A:450:LEU:HD13	2.02	0.42
1:B:461:SER:HB3	1:B:506:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLU:HG3	1:B:432:ILE:HA	2.02	0.42
1:A:130:ALA:O	1:A:159:SER:HB2	2.19	0.42
1:B:256:LEU:C	1:B:256:LEU:HD23	2.39	0.42
1:A:641:LEU:O	1:A:642:HIS:HB2	2.20	0.42
1:B:183:ASP:CG	1:B:183:ASP:O	2.59	0.42
1:A:223:LEU:N	1:A:223:LEU:HD22	2.35	0.41
1:B:228:LYS:HB3	1:B:228:LYS:NZ	2.34	0.41
1:A:200:SER:HA	1:A:219:MET:O	2.20	0.41
1:A:710:THR:HA	1:A:722:VAL:O	2.20	0.41
1:A:733:LEU:CD2	1:A:753:ALA:HB2	2.51	0.41
1:A:80:LYS:NZ	4:A:2129:HOH:O	2.52	0.41
1:B:701:PHE:CD1	1:B:701:PHE:C	2.94	0.41
1:B:186:PHE:O	1:B:205:THR:HA	2.20	0.41
1:A:671:HIS:O	1:A:675:MET:HG3	2.20	0.41
1:B:157:ASN:HD21	1:B:159:SER:CB	2.33	0.41
1:B:375:LYS:HG2	4:B:2211:HOH:O	2.21	0.41
1:A:365:PHE:HZ	1:A:381:LEU:HG	1.86	0.41
1:A:39:ARG:HE	1:A:51:LEU:HB3	1.84	0.41
1:B:204:LYS:HA	1:B:215:PHE:O	2.20	0.41
1:B:110:THR:O	1:B:122:ARG:HA	2.21	0.41
1:B:280:GLN:HG3	4:B:2428:HOH:O	2.19	0.41
1:A:698:TYR:OH	1:A:713:GLN:NE2	2.53	0.41
1:B:689:MET:HA	1:B:697:HIS:O	2.20	0.41
1:B:291:GLU:H	1:B:291:GLU:CD	2.24	0.41
1:A:426:ILE:HD13	1:A:467:ARG:HH11	1.78	0.41
1:A:478:MET:HB3	1:A:494:ASN:OD1	2.20	0.41
1:A:477:TYR:CD2	1:A:537:ILE:HA	2.56	0.41
1:A:182:TYR:HD2	1:A:186:PHE:CZ	2.39	0.41
1:A:160:ASP:O	1:A:161:ALA:CB	2.67	0.41
1:B:212:THR:HB	1:B:213:PRO:HD2	2.02	0.41
1:B:414:GLU:HG2	1:B:422:THR:HG23	2.02	0.41
1:B:361:GLU:HA	1:B:365:PHE:CD1	2.56	0.41
1:A:204:LYS:HA	1:A:215:PHE:O	2.21	0.41
1:B:33:ASN:C	1:B:33:ASN:ND2	2.74	0.40
1:A:22:LYS:HE2	1:A:42:PHE:CE1	2.55	0.40
1:A:682:VAL:O	1:A:686:PHE:HB2	2.22	0.40
1:A:657:LEU:HA	1:A:662:TYR:CD1	2.55	0.40
1:A:375:LYS:HE3	1:A:375:LYS:HB2	1.88	0.40
1:A:388:LEU:HA	1:A:388:LEU:HD12	1.94	0.40
1:A:134:ALA:HB2	1:A:158:LEU:HD11	2.03	0.40
1:A:479:ILE:HB	1:A:499:ASN:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASP:OD2	1:B:206:THR:HG22	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	751/754 (100%)	725 (96%)	24 (3%)	2 (0%)	46	42
1	B	752/754 (100%)	732 (97%)	20 (3%)	0	100	100
All	All	1503/1508 (100%)	1457 (97%)	44 (3%)	2 (0%)	56	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ASP
1	A	182	TYR

### 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	646/647 (100%)	628 (97%)	18 (3%)	51	52
1	B	646/647 (100%)	635 (98%)	11 (2%)	68	74
All	All	1292/1294 (100%)	1263 (98%)	29 (2%)	60	63



All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	51	LEU
1	A	101	LEU
1	A	120	LEU
1	A	157	ASN
1	A	177	ASN
1	A	179	GLU
1	A	198	ARG
1	A	341	ASN
1	A	360	THR
1	A	365	PHE
1	A	380	LEU
1	A	386	LYS
1	A	388	LEU
1	A	420	GLU
1	A	429	ASN
1	A	450	LEU
1	A	629	LEU
1	B	33	ASN
1	B	51	LEU
1	B	157	ASN
1	B	222	ARG
1	B	266	ARG
1	B	319	GLN
1	B	329	LEU
1	B	361	GLU
1	B	420	GLU
1	B	429	ASN
1	B	670	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	11	ASN
1	A	33	ASN
1	A	138	GLN
1	A	145	GLN
1	A	157	ASN
1	A	195	GLN
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	234	GLN
1	A	236	ASN
1	A	271	GLN
1	A	280	GLN
1	A	297	HIS
1	A	303	GLN
1	A	320	GLN
1	A	325	ASN
1	A	341	ASN
1	A	379	ASN
1	A	387	GLN
1	A	394	ASN
1	A	396	GLN
1	A	416	HIS
1	A	429	ASN
1	A	475	ASN
1	A	495	ASN
1	A	499	ASN
1	A	518	GLN
1	A	523	GLN
1	A	554	GLN
1	A	578	GLN
1	A	663	ASN
1	A	671	HIS
1	A	684	GLN
1	A	697	HIS
1	A	713	GLN
1	A	730	HIS
1	B	8	GLN
1	B	11	ASN
1	B	33	ASN
1	B	72	ASN
1	B	138	GLN
1	B	145	GLN
1	B	157	ASN
1	B	195	GLN
1	B	280	GLN
1	B	297	HIS
1	B	303	GLN
1	B	320	GLN
1	B	325	ASN
1	B	328	GLN

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Mol	Chain	Res	Type
1	B	387	GLN
1	B	396	GLN
1	B	416	HIS
1	B	427	HIS
1	B	429	ASN
1	B	451	HIS
1	B	475	ASN
1	B	491	ASN
1	B	494	ASN
1	B	495	ASN
1	B	518	GLN
1	B	523	GLN
1	B	554	GLN
1	B	578	GLN
1	B	611	GLN
1	B	634	HIS
1	B	664	ASN
1	B	695	GLN
1	B	697	HIS
1	B	713	GLN

### 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	B	1755	-	4,4,4	1.20	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	B	1755	-	-	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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.