



# Full wwPDB X-ray Structure Validation Report i

Apr 27, 2024 – 11:24 am BST

PDB ID : 2WQD  
Title : Crystal structure of enzyme I of the phosphoenolpyruvate:sugar phosphotransferase system in the dephosphorylated state  
Authors : Oberholzer, A.E.; Schneider, P.; Siebold, C.; Baumann, U.; Erni, B.  
Deposited on : 2009-08-19  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

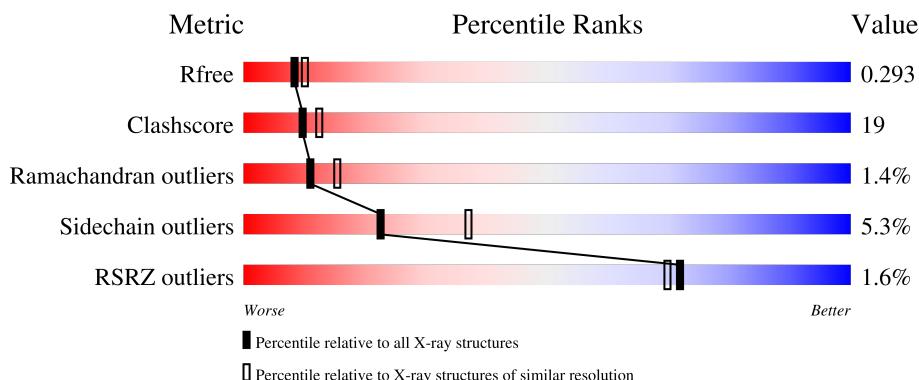
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	572	2%	63% 32% .

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4480 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 PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	570	4324	2711	732	865	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	ALA	HIS	engineered mutation	UNP P51183
A	365	SER	CYS	engineered mutation	UNP P51183

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

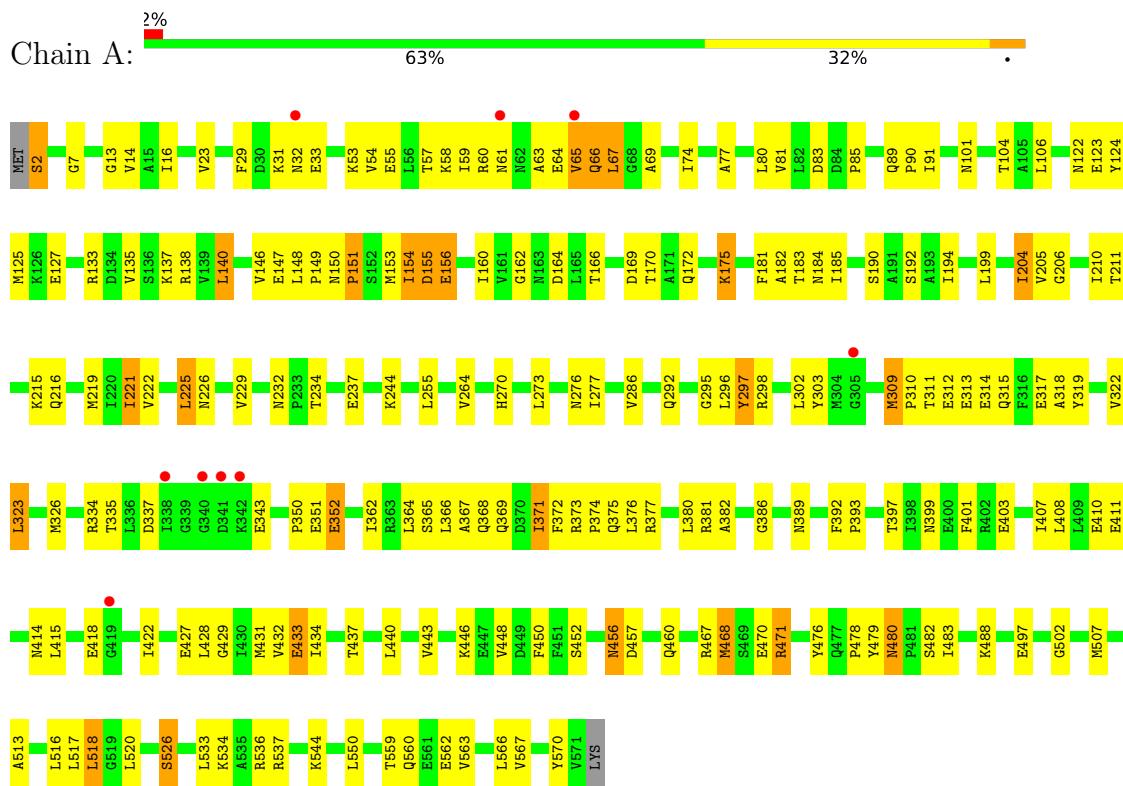
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	155	Total O 155 155	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.34Å    98.34Å    105.11Å 90.00°    90.00°    120.00°	Depositor
Resolution (Å)	35.91 – 2.40 35.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.91-2.40) 100.0 (35.91-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.52 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
$R$ , $R_{free}$	0.228 , 0.295 0.227 , 0.293	Depositor DCC
$R_{free}$ test set	1747 reflections (7.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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	0.24	0/4377	0.43	2/5931 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	151	PRO	N-CA-CB	6.15	110.68	103.30
1	A	350	PRO	N-CA-CB	5.80	110.26	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	4324	0	4264	166	0
2	A	1	0	0	0	0
3	A	155	0	0	3	0
All	All	4480	0	4264	166	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 19.

All (166) 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:175:LYS:HE2	1:A:175:LYS:H	1.13	1.10
1:A:470:GLU:HB2	1:A:471:ARG:HH21	1.29	0.95
1:A:184:ASN:HD21	1:A:211:THR:H	1.16	0.94
1:A:2:SER:OG	1:A:232:ASN:O	1.87	0.92
1:A:297:TYR:HE2	1:A:322:VAL:HG21	1.37	0.88
1:A:170:THR:HG21	1:A:192:SER:HB2	1.60	0.83
1:A:460:GLN:HE21	1:A:467:ARG:H	1.27	0.81
1:A:362:ILE:HA	1:A:365:SER:HB3	1.64	0.79
1:A:456:ASN:HD22	1:A:457:ASP:H	1.30	0.79
1:A:153:MET:HA	1:A:154:ILE:CB	2.14	0.77
1:A:175:LYS:H	1:A:175:LYS:CE	1.97	0.74
1:A:175:LYS:HE2	1:A:175:LYS:N	1.98	0.73
1:A:480:ASN:HD22	1:A:482:SER:H	1.37	0.72
1:A:480:ASN:ND2	1:A:482:SER:H	1.89	0.70
1:A:434:ILE:O	1:A:437:THR:HG22	1.93	0.68
1:A:559:THR:HG23	1:A:562:GLU:H	1.58	0.68
1:A:91:ILE:HD12	1:A:106:LEU:HA	1.75	0.67
1:A:313:GLU:O	1:A:317:GLU:HG2	1.96	0.65
1:A:234:THR:HG21	3:A:2065:HOH:O	1.95	0.65
1:A:429:GLY:HA2	1:A:448:VAL:HG13	1.76	0.65
1:A:55:GLU:O	1:A:59:ILE:HG12	1.97	0.65
1:A:122:ASN:HD22	1:A:125:MET:HG2	1.62	0.64
1:A:335:THR:HB	1:A:393:PRO:HD3	1.79	0.64
1:A:369:GLN:O	1:A:373:ARG:HB2	1.98	0.63
1:A:460:GLN:NE2	1:A:467:ARG:H	1.95	0.63
1:A:393:PRO:HA	1:A:431:MET:HB3	1.79	0.63
1:A:31:LYS:H	1:A:31:LYS:HD2	1.64	0.63
1:A:13:GLY:H	1:A:225:LEU:HD13	1.64	0.62
1:A:302:LEU:HD21	1:A:315:GLN:HG2	1.80	0.62
1:A:276:ASN:OD1	1:A:526:SER:HB3	2.00	0.62
1:A:81:VAL:HG11	1:A:135:VAL:HG21	1.83	0.61
1:A:366:LEU:O	1:A:367:ALA:HB3	2.01	0.60
1:A:295:GLY:HA3	1:A:526:SER:OG	2.01	0.60
1:A:318:ALA:O	1:A:322:VAL:HG23	2.02	0.59
1:A:59:ILE:HD12	1:A:172:GLN:HE21	1.67	0.59
1:A:53:LYS:O	1:A:57:THR:HG23	2.03	0.58
1:A:64:GLU:C	1:A:66:GLN:H	2.06	0.58
1:A:160:ILE:HB	1:A:181:PHE:HB3	1.85	0.58
1:A:210:ILE:HD11	1:A:229:VAL:HG21	1.86	0.58
1:A:446:LYS:HE3	1:A:497:GLU:OE2	2.04	0.58
1:A:106:LEU:HD23	1:A:140:LEU:HG	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:O	1:A:377:ARG:HG2	2.04	0.57
1:A:264:VAL:HG22	1:A:270:HIS:CD2	2.38	0.57
1:A:64:GLU:CB	1:A:69:ALA:HA	2.35	0.56
1:A:433:GLU:HB2	1:A:457:ASP:HB2	1.88	0.56
1:A:337:ASP:HB2	1:A:393:PRO:HG2	1.87	0.56
1:A:362:ILE:HD12	1:A:392:PHE:HB3	1.89	0.55
1:A:480:ASN:HD22	1:A:482:SER:N	2.02	0.55
1:A:204:ILE:CD1	1:A:229:VAL:HG23	2.36	0.55
1:A:364:LEU:HD12	1:A:368:GLN:HG3	1.89	0.54
1:A:312:GLU:OE1	1:A:377:ARG:HD3	2.08	0.54
1:A:315:GLN:HB3	1:A:319:TYR:CE2	2.43	0.54
1:A:518:LEU:HD22	1:A:544:LYS:HG3	1.89	0.53
1:A:184:ASN:HD21	1:A:211:THR:N	1.96	0.53
1:A:456:ASN:HD22	1:A:457:ASP:N	2.01	0.53
1:A:23:VAL:O	1:A:149:PRO:HG3	2.09	0.52
1:A:476:TYR:O	1:A:478:PRO:HD3	2.10	0.52
1:A:371:ILE:O	1:A:371:ILE:HD13	2.09	0.52
1:A:432:VAL:HG13	1:A:437:THR:CG2	2.40	0.52
1:A:32:ASN:H	1:A:104:THR:HG21	1.75	0.52
1:A:234:THR:HG23	1:A:237:GLU:H	1.75	0.51
1:A:399:ASN:O	1:A:403:GLU:HG3	2.10	0.51
1:A:64:GLU:HB2	1:A:69:ALA:HA	1.91	0.51
1:A:204:ILE:HG23	1:A:222:VAL:HG13	1.92	0.51
1:A:479:TYR:HB2	1:A:560:GLN:HG3	1.92	0.51
1:A:16:ILE:HG23	1:A:219:MET:HE1	1.91	0.51
1:A:29:PHE:HE1	1:A:104:THR:HG23	1.76	0.51
1:A:298:ARG:HG2	1:A:334:ARG:NH2	2.26	0.51
1:A:297:TYR:CE2	1:A:322:VAL:HG21	2.29	0.50
1:A:381:ARG:HG2	1:A:415:LEU:HD13	1.94	0.50
1:A:488:LYS:HB2	1:A:520:LEU:HD22	1.93	0.50
1:A:407:ILE:O	1:A:410:GLU:HB2	2.12	0.50
1:A:89:GLN:HB2	1:A:90:PRO:HD3	1.94	0.50
1:A:440:LEU:HG	1:A:443:VAL:HB	1.93	0.49
1:A:67:LEU:HD22	1:A:199:LEU:HD21	1.94	0.49
1:A:550:LEU:HD13	1:A:570:TYR:CD1	2.48	0.49
1:A:60:ARG:HH21	1:A:61:ASN:HB2	1.78	0.49
1:A:215:LYS:HD3	1:A:216:GLN:O	2.13	0.49
1:A:470:GLU:HB2	1:A:471:ARG:NH2	2.13	0.48
1:A:452:SER:HA	1:A:502:GLY:O	2.13	0.48
1:A:155:ASP:HA	1:A:156:GLU:HA	1.55	0.48
1:A:460:GLN:HE21	1:A:467:ARG:N	2.05	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLU:CD	1:A:123:GLU:H	2.17	0.48
1:A:392:PHE:CE2	1:A:428:LEU:HD11	2.48	0.48
1:A:377:ARG:O	1:A:381:ARG:HG3	2.13	0.48
1:A:7:GLY:HA3	1:A:204:ILE:HD12	1.96	0.48
1:A:33:GLU:HB3	1:A:101:ASN:HD22	1.79	0.47
1:A:456:ASN:ND2	1:A:456:ASN:N	2.62	0.47
1:A:471:ARG:N	1:A:471:ARG:HE	2.12	0.47
1:A:303:TYR:CD2	1:A:310:PRO:HD2	2.49	0.47
1:A:302:LEU:CD2	1:A:315:GLN:HG2	2.43	0.47
1:A:311:THR:HG23	1:A:314:GLU:H	1.79	0.47
1:A:255:LEU:HD21	1:A:534:LYS:HD3	1.94	0.47
1:A:372:PHE:CE2	1:A:376:LEU:HD11	2.50	0.47
1:A:162:GLY:O	1:A:183:THR:HA	2.15	0.47
1:A:534:LYS:H	1:A:534:LYS:HE2	1.78	0.47
1:A:204:ILE:HD13	1:A:229:VAL:HG23	1.97	0.47
1:A:392:PHE:CZ	1:A:428:LEU:HD21	2.50	0.47
1:A:471:ARG:HE	1:A:471:ARG:H	1.62	0.47
1:A:537:ARG:HB3	1:A:537:ARG:NH1	2.30	0.47
1:A:376:LEU:O	1:A:380:LEU:HD13	2.15	0.46
1:A:122:ASN:ND2	1:A:125:MET:HG2	2.28	0.46
1:A:411:GLU:HA	1:A:414:ASN:HB2	1.97	0.46
1:A:563:VAL:O	1:A:567:VAL:HG23	2.16	0.46
1:A:414:ASN:O	1:A:418:GLU:HG3	2.15	0.45
1:A:166:THR:HG22	1:A:169:ASP:CG	2.37	0.45
1:A:351:GLU:O	1:A:352:GLU:HG2	2.17	0.45
1:A:401:PHE:CE1	1:A:448:VAL:HG22	2.51	0.45
1:A:478:PRO:O	1:A:507:MET:HE1	2.17	0.45
1:A:146:VAL:HG22	1:A:147:GLU:H	1.82	0.45
1:A:392:PHE:HE2	1:A:428:LEU:HD11	1.82	0.45
1:A:13:GLY:H	1:A:225:LEU:CD1	2.27	0.45
1:A:133:ARG:O	1:A:137:LYS:HG3	2.17	0.45
1:A:59:ILE:O	1:A:63:ALA:HB2	2.16	0.45
1:A:286:VAL:HG11	1:A:326:MET:HE3	1.99	0.44
1:A:164:ASP:HB2	1:A:185:ILE:HG12	1.99	0.44
1:A:182:ALA:HB1	1:A:210:ILE:CD1	2.47	0.44
1:A:315:GLN:NE2	1:A:375:GLN:HA	2.32	0.44
1:A:399:ASN:N	3:A:2105:HOH:O	2.50	0.44
1:A:29:PHE:HE1	1:A:104:THR:CG2	2.30	0.44
1:A:153:MET:CA	1:A:154:ILE:CB	2.93	0.44
1:A:190:SER:O	1:A:194:ILE:HG13	2.17	0.44
1:A:74:ILE:O	1:A:77:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:THR:HG23	1:A:169:ASP:H	1.83	0.44
1:A:123:GLU:HG2	1:A:124:TYR:H	1.83	0.43
1:A:513:ALA:O	1:A:517:LEU:HG	2.18	0.43
1:A:448:VAL:HG12	1:A:450:PHE:H	1.82	0.43
1:A:480:ASN:HB3	1:A:483:ILE:HG12	2.00	0.43
1:A:170:THR:CG2	1:A:192:SER:HB2	2.40	0.43
1:A:286:VAL:HG11	1:A:326:MET:CE	2.48	0.43
1:A:297:TYR:C	1:A:297:TYR:CD1	2.90	0.43
1:A:433:GLU:CB	1:A:457:ASP:HB2	2.48	0.43
1:A:64:GLU:C	1:A:66:GLN:N	2.71	0.43
1:A:534:LYS:H	1:A:534:LYS:CE	2.32	0.43
1:A:123:GLU:O	1:A:127:GLU:HG2	2.18	0.43
1:A:234:THR:CG2	1:A:237:GLU:H	2.31	0.43
1:A:14:VAL:HG21	1:A:244:LYS:HG2	2.01	0.42
1:A:64:GLU:O	1:A:65:VAL:HB	2.18	0.42
1:A:323:LEU:HB3	1:A:386:GLY:H	1.84	0.42
1:A:380:LEU:HD11	1:A:408:LEU:HD11	2.00	0.42
1:A:518:LEU:CD2	1:A:544:LYS:HG3	2.48	0.42
1:A:323:LEU:HD23	1:A:382:ALA:O	2.19	0.42
1:A:64:GLU:HB3	1:A:69:ALA:HA	2.00	0.42
1:A:146:VAL:HG22	1:A:147:GLU:N	2.34	0.42
1:A:205:VAL:HG22	1:A:206:GLY:H	1.84	0.42
1:A:468:MET:HA	1:A:468:MET:CE	2.50	0.42
1:A:292:GLN:HE21	1:A:536:ARG:HH21	1.66	0.42
1:A:297:TYR:C	1:A:297:TYR:HD1	2.23	0.42
1:A:559:THR:HG22	1:A:562:GLU:HG3	2.02	0.42
1:A:54:VAL:O	1:A:58:LYS:HG2	2.20	0.41
1:A:309:MET:HA	1:A:310:PRO:HD3	1.92	0.41
1:A:160:ILE:HB	1:A:181:PHE:CB	2.49	0.41
1:A:534:LYS:HA	1:A:537:ARG:NH1	2.36	0.41
1:A:138:ARG:HA	1:A:148:LEU:HD11	2.01	0.41
1:A:392:PHE:HA	1:A:393:PRO:HD3	1.83	0.41
1:A:397:THR:CB	3:A:2105:HOH:O	2.68	0.41
1:A:389:ASN:ND2	1:A:427:GLU:HB2	2.36	0.41
1:A:373:ARG:N	1:A:374:PRO:CD	2.84	0.41
1:A:83:ASP:O	1:A:85:PRO:HD3	2.21	0.41
1:A:221:ILE:O	1:A:221:ILE:HG13	2.20	0.41
1:A:273:LEU:H	1:A:292:GLN:NE2	2.19	0.41
1:A:234:THR:HG22	1:A:237:GLU:CG	2.50	0.40
1:A:277:ILE:O	1:A:277:ILE:HG13	2.21	0.40
1:A:380:LEU:O	1:A:422:ILE:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LYS:HE2	1:A:534:LYS:HB2	1.96	0.40
1:A:516:LEU:HD23	1:A:516:LEU:HA	1.88	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	568/572 (99%)	539 (95%)	21 (4%)	8 (1%)	11 15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	151	PRO
1	A	343	GLU
1	A	352	GLU
1	A	150	ASN
1	A	154	ILE
1	A	155	ASP
1	A	67	LEU

### 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	454/481 (94%)	430 (95%)	24 (5%)	22   37

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	66	GLN
1	A	80	LEU
1	A	140	LEU
1	A	156	GLU
1	A	175	LYS
1	A	204	ILE
1	A	221	ILE
1	A	225	LEU
1	A	226	ASN
1	A	296	LEU
1	A	297	TYR
1	A	309	MET
1	A	323	LEU
1	A	371	ILE
1	A	433	GLU
1	A	456	ASN
1	A	468	MET
1	A	471	ARG
1	A	480	ASN
1	A	518	LEU
1	A	526	SER
1	A	533	LEU
1	A	566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	46	ASN
1	A	66	GLN
1	A	78	HIS
1	A	89	GLN
1	A	99	ASN
1	A	112	GLN
1	A	122	ASN
1	A	172	GLN

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	226	ASN
1	A	270	HIS
1	A	292	GLN
1	A	315	GLN
1	A	456	ASN
1	A	460	GLN
1	A	477	GLN
1	A	480	ASN
1	A	568	ASN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	570/572 (99%)	-0.28	9 (1%) 72 70	28, 55, 110, 159	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	GLY	4.0
1	A	305	GLY	3.9
1	A	340	GLY	3.9
1	A	65	VAL	3.5
1	A	61	ASN	2.8
1	A	32	ASN	2.6
1	A	338	ILE	2.6
1	A	342	LYS	2.5
1	A	341	ASP	2.5

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

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

### 6.3 Carbohydrates i

There are no monosaccharides in this entry.

### 6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	1572	1/1	0.94	0.26	78,78,78,78	0

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

There are no such residues in this entry.