



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:35 am BST

PDB ID : 2OLS
Title : The crystal structure of the phosphoenolpyruvate synthase from *Neisseria meningitidis*
Authors : Zhang, R.; Duggan, E.; Bargassa, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-01-19
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

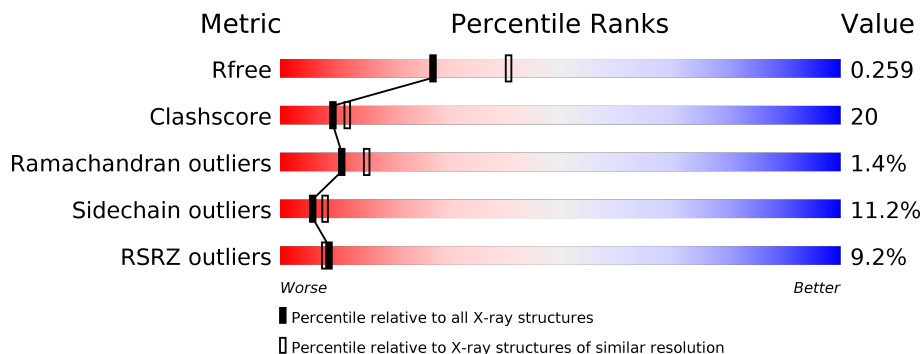
1 Overall quality at a glance

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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	794	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5994 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 synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	5584	3518	963	1071	32	0	0	0

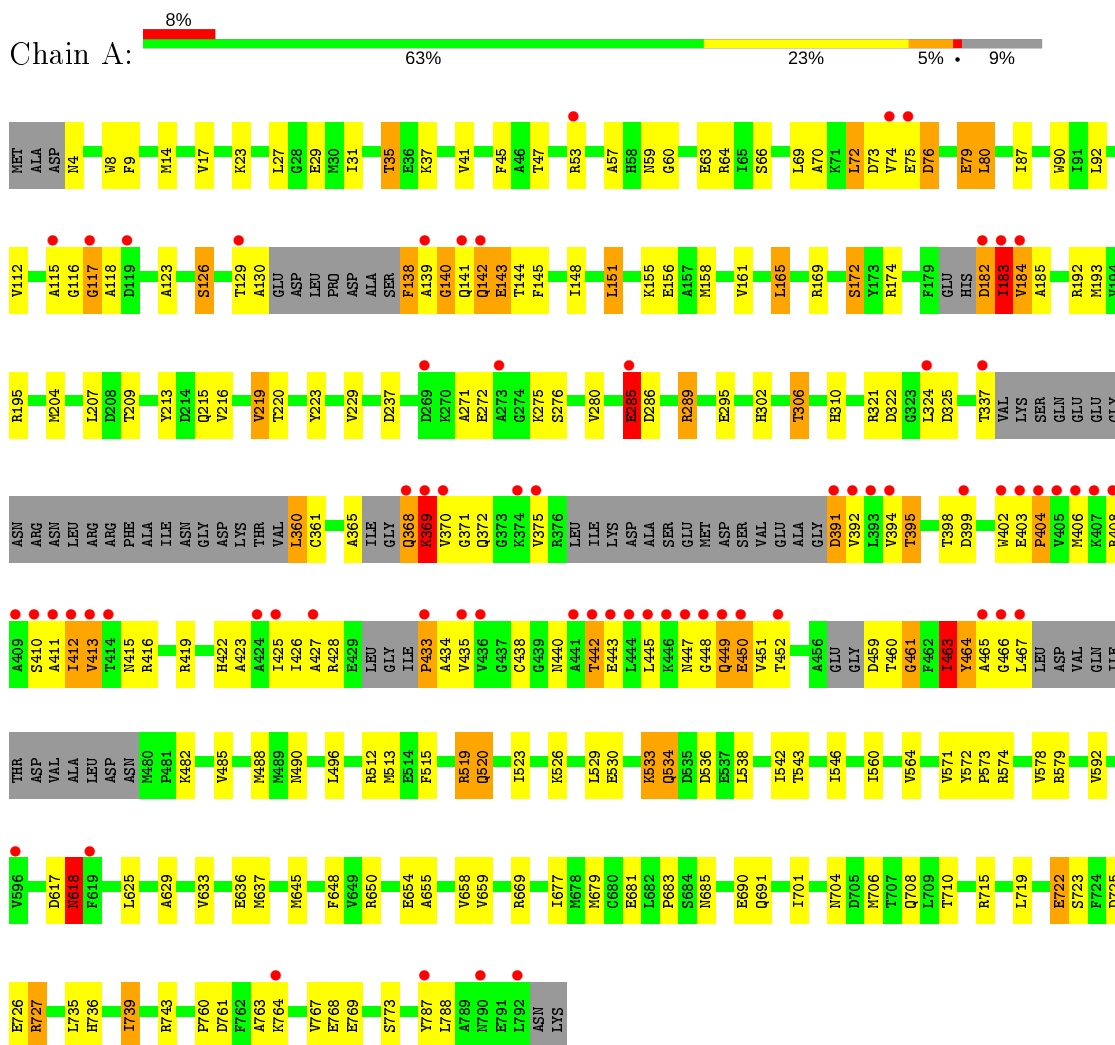
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	410	Total	O	0	0
			410	410		

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 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 synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	183.05Å 183.05Å 72.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.40 48.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	88.1 (48.22-2.40) 82.8 (48.20-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.251 0.208 , 0.259	Depositor DCC
R_{free} test set	2313 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtrriage
Anisotropy	0.727	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5994	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.79	5/5678 (0.1%)	0.81	7/7669 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	618	ASN	CB-CG	7.70	1.68	1.51
1	A	768	GLU	CG-CD	6.98	1.62	1.51
1	A	295	GLU	CG-CD	5.88	1.60	1.51
1	A	520	GLN	CG-CD	5.15	1.62	1.51
1	A	37	LYS	CD-CE	5.09	1.64	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	519	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	650	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	669	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	669	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	743	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	519	ARG	NE-CZ-NH2	-5.68	117.46	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	183	ILE	CA
1	A	535	ASP	CA
1	A	543	THR	CB

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	GLY	Peptide
1	A	182	ASP	Peptide
1	A	433	PRO	Peptide
1	A	449	GLN	Peptide
1	A	464	TYR	Peptide
1	A	534	GLN	Peptide
1	A	59	ASN	Peptide

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	5584	0	5511	219	0
2	A	410	0	0	45	0
All	All	5994	0	5511	219	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 20.

All (219) 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:123:ALA:HB2	1:A:193:MET:CE	1.72	1.17
1:A:182:ASP:CB	1:A:183:ILE:HA	1.71	1.17
1:A:534:GLN:CG	1:A:538:LEU:HD23	1.76	1.15
1:A:534:GLN:HG2	1:A:538:LEU:HD23	1.23	1.13
1:A:182:ASP:HB2	1:A:183:ILE:HA	1.10	1.09
1:A:368:GLN:O	1:A:369:LYS:HB2	1.42	1.08
1:A:45:PHE:HB3	2:A:1024:HOH:O	1.56	1.05
1:A:306:THR:HG21	2:A:912:HOH:O	1.55	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:CG2	2:A:1142:HOH:O	2.06	1.01
1:A:271:ALA:HB2	2:A:1158:HOH:O	1.59	1.00
1:A:182:ASP:HB2	1:A:183:ILE:CA	1.94	0.95
1:A:488:MET:HE2	1:A:773:SER:HB2	1.45	0.94
1:A:445:LEU:HD21	1:A:463:ILE:HD11	1.46	0.94
1:A:450:GLU:HG3	1:A:450:GLU:O	1.66	0.94
1:A:449:GLN:HB2	1:A:450:GLU:CB	2.00	0.91
1:A:183:ILE:HG23	1:A:184:VAL:H	1.37	0.90
1:A:722:GLU:HG3	1:A:722:GLU:O	1.67	0.89
1:A:123:ALA:HB2	1:A:193:MET:HE2	1.55	0.88
1:A:463:ILE:HD13	1:A:463:ILE:O	1.76	0.86
1:A:445:LEU:HD21	1:A:463:ILE:CD1	2.04	0.85
1:A:488:MET:CE	1:A:773:SER:HB2	2.09	0.83
1:A:488:MET:CE	1:A:773:SER:CB	2.56	0.82
1:A:534:GLN:HG3	1:A:538:LEU:HD23	1.62	0.81
1:A:406:MET:SD	1:A:426:ILE:HD12	2.22	0.80
1:A:645:MET:HE3	1:A:679:MET:SD	2.21	0.79
1:A:637:MET:SD	2:A:1066:HOH:O	2.39	0.79
1:A:31:ILE:O	1:A:35:THR:HG23	1.82	0.78
1:A:618:ASN:H	1:A:618:ASN:HD22	1.31	0.78
1:A:618:ASN:H	1:A:618:ASN:ND2	1.81	0.77
1:A:183:ILE:CG2	1:A:184:VAL:N	2.46	0.77
1:A:645:MET:CE	1:A:679:MET:SD	2.72	0.77
1:A:375:VAL:HG23	1:A:451:VAL:HG22	1.68	0.76
1:A:488:MET:SD	2:A:1120:HOH:O	2.41	0.76
1:A:183:ILE:HG23	1:A:184:VAL:N	2.01	0.76
1:A:534:GLN:HG2	1:A:538:LEU:CD2	2.09	0.76
1:A:195:ARG:HG3	1:A:324:LEU:HD22	1.69	0.75
1:A:79:GLU:OE2	1:A:79:GLU:HA	1.87	0.75
1:A:449:GLN:HB2	1:A:450:GLU:HB2	1.68	0.75
1:A:130:ALA:HB1	2:A:1109:HOH:O	1.86	0.74
1:A:449:GLN:HB2	1:A:450:GLU:CA	2.17	0.74
1:A:706:MET:SD	2:A:1087:HOH:O	2.45	0.74
1:A:394:VAL:HG22	1:A:413:VAL:CG1	2.18	0.73
1:A:118:ALA:HB2	2:A:1128:HOH:O	1.88	0.73
1:A:31:ILE:O	1:A:35:THR:CG2	2.37	0.73
1:A:460:THR:O	1:A:460:THR:HG22	1.88	0.72
1:A:402:TRP:O	1:A:406:MET:HB2	1.88	0.72
1:A:530:GLU:O	1:A:534:GLN:NE2	2.22	0.71
1:A:123:ALA:HB2	1:A:193:MET:HE1	1.71	0.71
1:A:76:ASP:C	1:A:76:ASP:OD2	2.30	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:O	2:A:1011:HOH:O	2.10	0.68
1:A:394:VAL:HG22	1:A:413:VAL:HG12	1.75	0.68
1:A:118:ALA:HB1	2:A:1068:HOH:O	1.93	0.67
1:A:365:ALA:HB2	1:A:461:GLY:CA	2.23	0.67
1:A:375:VAL:HG23	1:A:451:VAL:CG2	2.24	0.67
1:A:365:ALA:HB2	1:A:461:GLY:N	2.10	0.67
1:A:123:ALA:CB	1:A:193:MET:CE	2.62	0.67
1:A:368:GLN:O	1:A:369:LYS:CB	2.30	0.67
1:A:415:ASN:HA	1:A:438:CYS:O	1.95	0.67
1:A:701:ILE:HG21	1:A:735:LEU:HD22	1.77	0.66
1:A:449:GLN:CB	1:A:450:GLU:CA	2.73	0.66
1:A:223:TYR:CZ	1:A:286:ASP:HB3	2.31	0.65
1:A:391:ASP:N	1:A:410:SER:HG	1.94	0.65
1:A:392:VAL:HG13	1:A:411:ALA:HB3	1.79	0.65
1:A:123:ALA:HB2	1:A:193:MET:HE3	1.75	0.64
1:A:464:TYR:HA	1:A:465:ALA:HB3	1.79	0.64
1:A:536:ASP:HB2	2:A:1033:HOH:O	1.97	0.64
1:A:375:VAL:CG2	1:A:451:VAL:HG21	2.29	0.63
1:A:618:ASN:HB3	2:A:940:HOH:O	1.99	0.63
1:A:618:ASN:HD22	1:A:618:ASN:N	1.96	0.63
1:A:14:MET:HE1	2:A:972:HOH:O	1.99	0.62
1:A:402:TRP:O	1:A:406:MET:CE	2.47	0.62
1:A:460:THR:O	1:A:460:THR:CG2	2.48	0.61
1:A:209:THR:HB	2:A:1149:HOH:O	2.01	0.61
1:A:445:LEU:CD2	1:A:463:ILE:HD11	2.25	0.61
1:A:115:ALA:O	1:A:117:GLY:N	2.33	0.61
1:A:450:GLU:OE2	1:A:467:LEU:HD13	2.01	0.60
1:A:395:THR:HG21	1:A:402:TRP:CZ3	2.36	0.60
1:A:735:LEU:O	1:A:739:ILE:HG23	2.01	0.59
1:A:530:GLU:HB3	1:A:533:LYS:HG3	1.84	0.59
1:A:690:GLU:HG3	2:A:805:HOH:O	2.01	0.59
1:A:130:ALA:HB3	2:A:1092:HOH:O	2.02	0.59
1:A:571:VAL:O	1:A:574:ARG:HB2	2.03	0.59
1:A:488:MET:HE2	1:A:773:SER:CB	2.20	0.59
1:A:123:ALA:CB	1:A:193:MET:HE2	2.31	0.59
1:A:4:ASN:ND2	2:A:934:HOH:O	2.36	0.58
1:A:14:MET:O	1:A:17:VAL:HG23	2.04	0.58
1:A:183:ILE:HG21	2:A:1142:HOH:O	1.86	0.58
1:A:182:ASP:HB3	1:A:183:ILE:HA	1.76	0.58
1:A:365:ALA:HB2	1:A:461:GLY:H	1.68	0.57
1:A:130:ALA:HB2	2:A:1084:HOH:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:CG2	1:A:451:VAL:CG2	2.82	0.57
1:A:271:ALA:HB1	1:A:276:SER:HB3	1.85	0.57
1:A:572:TYR:CG	1:A:573:PRO:HA	2.39	0.57
1:A:392:VAL:HG13	1:A:411:ALA:CB	2.35	0.56
1:A:464:TYR:CA	1:A:465:ALA:HB3	2.35	0.56
1:A:182:ASP:CB	1:A:183:ILE:CA	2.57	0.56
1:A:302:HIS:O	1:A:306:THR:HG23	2.05	0.56
1:A:69:LEU:CD1	1:A:87:ILE:HD11	2.35	0.56
1:A:74:VAL:HG21	1:A:172:SER:HA	1.87	0.56
1:A:271:ALA:CB	2:A:1158:HOH:O	2.35	0.55
1:A:440:ASN:HB2	1:A:443:GLU:HG2	1.88	0.55
1:A:139:ALA:HB3	1:A:140:GLY:HA2	1.87	0.55
1:A:151:LEU:HD22	1:A:155:LYS:HE2	1.89	0.55
1:A:117:GLY:HA3	2:A:1128:HOH:O	2.05	0.55
1:A:69:LEU:HD13	1:A:87:ILE:HD11	1.88	0.55
1:A:53:ARG:NH1	1:A:185:ALA:HB2	2.23	0.54
1:A:515:PHE:CE1	1:A:519:ARG:HD3	2.42	0.54
1:A:655:ALA:O	1:A:659:VAL:HG13	2.07	0.54
1:A:736:HIS:HD2	1:A:769:GLU:OE1	1.90	0.54
1:A:413:VAL:HG23	1:A:435:VAL:HB	1.88	0.54
1:A:701:ILE:HG21	1:A:735:LEU:CD2	2.38	0.54
1:A:449:GLN:CB	1:A:450:GLU:HB2	2.35	0.54
1:A:370:VAL:HG12	1:A:371:GLY:H	1.74	0.53
1:A:372:GLN:HA	1:A:452:THR:HG22	1.90	0.53
1:A:485:VAL:HG13	1:A:767:VAL:HG22	1.90	0.53
1:A:402:TRP:O	1:A:406:MET:HE3	2.08	0.53
1:A:442:THR:HG22	1:A:443:GLU:CD	2.30	0.52
1:A:564:VAL:HG13	1:A:578:VAL:HG21	1.92	0.52
1:A:360:LEU:HD12	2:A:1170:HOH:O	2.10	0.52
1:A:398:THR:HG21	1:A:406:MET:CE	2.40	0.52
1:A:681:GLU:H	1:A:685:ASN:HD22	1.56	0.52
1:A:8:TRP:CE2	2:A:1024:HOH:O	2.62	0.52
1:A:285:GLU:HG2	1:A:289:ARG:NH2	2.25	0.51
1:A:57:ALA:O	1:A:60:GLY:HA2	2.10	0.51
1:A:165:LEU:O	1:A:174:ARG:NH2	2.43	0.51
1:A:402:TRP:O	1:A:406:MET:HE2	2.11	0.51
1:A:23:LYS:CE	1:A:142:GLN:HE21	2.24	0.51
1:A:691:GLN:HG2	2:A:851:HOH:O	2.11	0.51
1:A:523:ILE:HG12	1:A:592:VAL:HG22	1.92	0.50
1:A:139:ALA:H	1:A:140:GLY:HA2	1.76	0.50
1:A:464:TYR:HA	1:A:465:ALA:CB	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TYR:HB3	1:A:465:ALA:HB3	1.94	0.50
1:A:138:PHE:N	1:A:138:PHE:CD2	2.79	0.50
1:A:449:GLN:CB	1:A:450:GLU:HA	2.41	0.50
1:A:138:PHE:N	1:A:138:PHE:HD2	2.10	0.49
1:A:23:LYS:HD3	2:A:849:HOH:O	2.11	0.49
1:A:708:GLN:HE21	1:A:715:ARG:H	1.59	0.49
1:A:488:MET:CE	1:A:773:SER:OG	2.60	0.49
1:A:442:THR:HG22	1:A:443:GLU:OE1	2.12	0.49
1:A:72:LEU:HD22	1:A:73:ASP:N	2.27	0.48
1:A:467:LEU:HD23	1:A:467:LEU:C	2.33	0.48
1:A:618:ASN:CB	2:A:940:HOH:O	2.58	0.48
1:A:534:GLN:CG	1:A:538:LEU:CD2	2.70	0.48
1:A:139:ALA:HB3	1:A:140:GLY:CA	2.44	0.48
1:A:490:ASN:OD1	1:A:512:ARG:NH1	2.46	0.48
1:A:452:THR:HG21	1:A:467:LEU:HA	1.96	0.47
1:A:322:ASP:HB3	1:A:325:ASP:HB2	1.95	0.47
1:A:392:VAL:HA	1:A:411:ALA:HB3	1.96	0.47
1:A:427:ALA:HB1	1:A:433:PRO:HA	1.96	0.47
1:A:520:GLN:HG2	2:A:1124:HOH:O	2.14	0.47
1:A:726:GLU:HG3	2:A:1006:HOH:O	2.13	0.47
1:A:466:GLY:O	1:A:467:LEU:HB2	2.14	0.47
1:A:321:ARG:NE	2:A:1182:HOH:O	2.47	0.47
1:A:706:MET:HE2	1:A:710:THR:OG1	2.15	0.47
1:A:272:GLU:HB2	2:A:1035:HOH:O	2.14	0.47
1:A:403:GLU:N	1:A:404:PRO:CD	2.78	0.47
1:A:223:TYR:CE2	1:A:286:ASP:HB3	2.50	0.47
1:A:183:ILE:HG23	2:A:1142:HOH:O	1.93	0.46
1:A:760:PRO:HB3	1:A:787:TYR:CZ	2.50	0.46
1:A:182:ASP:HB3	2:A:990:HOH:O	2.15	0.46
1:A:725:ASP:OD1	1:A:727:ARG:HG2	2.16	0.46
1:A:394:VAL:HG22	1:A:413:VAL:HG11	1.92	0.46
1:A:398:THR:HG21	1:A:406:MET:HE1	1.98	0.46
1:A:302:HIS:HD2	2:A:1070:HOH:O	1.98	0.46
1:A:450:GLU:OE2	1:A:467:LEU:CD1	2.63	0.46
1:A:459:ASP:HA	2:A:1196:HOH:O	2.15	0.46
1:A:645:MET:HA	1:A:677:ILE:O	2.15	0.46
1:A:488:MET:HE1	1:A:773:SER:CB	2.42	0.46
1:A:485:VAL:CG1	1:A:767:VAL:HG22	2.46	0.46
1:A:204:MET:HG2	1:A:219:VAL:HB	1.99	0.45
1:A:406:MET:HG3	1:A:412:ILE:HD11	1.98	0.45
1:A:412:ILE:HG21	1:A:423:ALA:HB1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:HB1	1:A:434:ALA:HB2	1.98	0.45
1:A:53:ARG:HG3	2:A:930:HOH:O	2.16	0.45
1:A:513:MET:HE1	1:A:560:ILE:HG23	1.98	0.45
1:A:370:VAL:HG12	1:A:371:GLY:N	2.31	0.45
1:A:704:ASN:HB2	2:A:1151:HOH:O	2.17	0.45
1:A:285:GLU:CG	1:A:289:ARG:NH2	2.80	0.44
1:A:645:MET:HE2	1:A:679:MET:HB2	1.99	0.44
1:A:306:THR:HG22	2:A:1059:HOH:O	2.17	0.44
1:A:361:CYS:HB3	1:A:463:ILE:HD12	1.99	0.44
1:A:139:ALA:N	1:A:140:GLY:HA2	2.31	0.44
1:A:375:VAL:HG22	1:A:451:VAL:HG21	2.00	0.44
1:A:427:ALA:CB	1:A:434:ALA:HB2	2.47	0.44
1:A:47:THR:HG21	1:A:158:MET:HE1	2.00	0.44
1:A:683:PRO:HA	1:A:706:MET:HE1	2.00	0.44
1:A:118:ALA:CB	2:A:1128:HOH:O	2.57	0.43
1:A:183:ILE:HG22	1:A:184:VAL:N	2.32	0.43
1:A:408:ARG:NH1	2:A:1197:HOH:O	2.51	0.43
1:A:29:GLU:OE2	1:A:310:HIS:HE1	2.01	0.43
1:A:413:VAL:HA	1:A:435:VAL:O	2.18	0.43
1:A:761:ASP:HB2	2:A:1041:HOH:O	2.18	0.43
1:A:140:GLY:HA3	1:A:142:GLN:HB2	2.01	0.42
1:A:422:HIS:ND1	1:A:422:HIS:C	2.73	0.42
1:A:9:PHE:HB3	1:A:31:ILE:HD12	2.00	0.42
1:A:428:ARG:NE	2:A:1193:HOH:O	2.52	0.42
1:A:74:VAL:HG23	1:A:80:LEU:HD13	2.00	0.42
1:A:115:ALA:HB1	1:A:192:ARG:HH21	1.84	0.42
1:A:360:LEU:N	2:A:1199:HOH:O	2.52	0.42
1:A:64:ARG:HG2	1:A:90:TRP:CZ3	2.53	0.42
1:A:141:GLN:O	1:A:142:GLN:C	2.58	0.42
1:A:654:GLU:O	1:A:658:VAL:HG23	2.19	0.42
1:A:440:ASN:HB2	1:A:443:GLU:CG	2.50	0.42
1:A:213:TYR:CZ	1:A:215:GLN:HB2	2.55	0.41
1:A:440:ASN:O	1:A:440:ASN:CG	2.58	0.41
1:A:715:ARG:NH1	2:A:1151:HOH:O	2.53	0.41
1:A:145:PHE:HB3	1:A:148:ILE:HD11	2.02	0.41
1:A:466:GLY:O	1:A:467:LEU:CB	2.68	0.41
1:A:143:GLU:HG3	2:A:1188:HOH:O	2.20	0.41
1:A:139:ALA:HB2	1:A:419:ARG:HH22	1.85	0.41
1:A:645:MET:CE	1:A:679:MET:HB2	2.51	0.41
1:A:763:ALA:HB1	1:A:788:LEU:HD21	2.03	0.41
1:A:579:ARG:HH11	1:A:679:MET:HE1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:CD2	1:A:79:GLU:HB3	2.51	0.41
1:A:220:THR:HA	1:A:237:ASP:O	2.20	0.40
1:A:464:TYR:CA	1:A:465:ALA:CB	3.00	0.40
1:A:629:ALA:O	1:A:633:VAL:HG23	2.21	0.40
1:A:126:SER:HB2	1:A:161:VAL:HG13	2.02	0.40
1:A:542:ILE:O	1:A:546:ILE:HG23	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	707/794 (89%)	661 (94%)	36 (5%)	10 (1%)	11 15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY
1	A	183	ILE
1	A	369	LYS
1	A	448	GLY
1	A	285	GLU
1	A	404	PRO
1	A	461	GLY
1	A	70	ALA
1	A	463	ILE
1	A	117	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	589/649 (91%)	523 (89%)	66 (11%)	6 8

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	35	THR
1	A	41	VAL
1	A	63	GLU
1	A	66	SER
1	A	72	LEU
1	A	75	GLU
1	A	76	ASP
1	A	79	GLU
1	A	80	LEU
1	A	92	LEU
1	A	112	VAL
1	A	126	SER
1	A	129	THR
1	A	138	PHE
1	A	142	GLN
1	A	143	GLU
1	A	144	THR
1	A	151	LEU
1	A	156	GLU
1	A	165	LEU
1	A	169	ARG
1	A	172	SER
1	A	183	ILE
1	A	184	VAL
1	A	207	LEU
1	A	216	VAL
1	A	219	VAL
1	A	229	VAL
1	A	275	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	280	VAL
1	A	285	GLU
1	A	289	ARG
1	A	306	THR
1	A	337	THR
1	A	360	LEU
1	A	368	GLN
1	A	369	LYS
1	A	391	ASP
1	A	395	THR
1	A	399	ASP
1	A	412	ILE
1	A	413	VAL
1	A	416	ARG
1	A	425	ILE
1	A	442	THR
1	A	447	ASN
1	A	450	GLU
1	A	463	ILE
1	A	482	LYS
1	A	496	LEU
1	A	526	LYS
1	A	529	LEU
1	A	533	LYS
1	A	543	THR
1	A	617	ASP
1	A	618	ASN
1	A	625	LEU
1	A	636	GLU
1	A	648	PHE
1	A	719	LEU
1	A	722	GLU
1	A	723	SER
1	A	727	ARG
1	A	739	ILE
1	A	764	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	58	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	142	GLN
1	A	228	ASN
1	A	279	ASN
1	A	310	HIS
1	A	332	GLN
1	A	447	ASN
1	A	595	ASN
1	A	618	ASN
1	A	672	ASN
1	A	685	ASN
1	A	708	GLN
1	A	736	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	725/794 (91%)	0.50	67 (9%) 9 8	27, 52, 99, 109	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	ALA	7.9
1	A	409	ALA	6.9
1	A	392	VAL	6.1
1	A	407	LYS	5.7
1	A	466	GLY	5.2
1	A	405	VAL	5.0
1	A	411	ALA	4.6
1	A	446	LYS	4.6
1	A	370	VAL	4.5
1	A	183	ILE	4.4
1	A	369	LYS	4.2
1	A	433	PRO	4.1
1	A	406	MET	4.1
1	A	444	LEU	4.1
1	A	402	TRP	4.1
1	A	139	ALA	3.9
1	A	412	ILE	3.8
1	A	129	THR	3.7
1	A	404	PRO	3.7
1	A	445	LEU	3.7
1	A	368	GLN	3.6
1	A	394	VAL	3.5
1	A	449	GLN	3.4
1	A	53	ARG	3.3
1	A	448	GLY	3.3
1	A	142	GLN	3.3
1	A	117	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	374	LYS	3.2
1	A	441	ALA	3.2
1	A	425	ILE	3.1
1	A	375	VAL	3.0
1	A	596	VAL	3.0
1	A	324	LEU	2.8
1	A	391	ASP	2.8
1	A	787	TYR	2.8
1	A	408	ARG	2.8
1	A	403	GLU	2.7
1	A	184	VAL	2.7
1	A	792	LEU	2.7
1	A	393	LEU	2.7
1	A	75	GLU	2.7
1	A	452	THR	2.7
1	A	790	ASN	2.7
1	A	465	ALA	2.6
1	A	399	ASP	2.6
1	A	414	THR	2.5
1	A	436	VAL	2.5
1	A	337	THR	2.5
1	A	619	PHE	2.5
1	A	119	ASP	2.5
1	A	410	SER	2.4
1	A	764	LYS	2.4
1	A	447	ASN	2.4
1	A	450	GLU	2.3
1	A	74	VAL	2.3
1	A	443	GLU	2.3
1	A	269	ASP	2.2
1	A	413	VAL	2.2
1	A	141	GLN	2.2
1	A	182	ASP	2.2
1	A	442	THR	2.2
1	A	115	ALA	2.2
1	A	467	LEU	2.1
1	A	424	ALA	2.1
1	A	273	ALA	2.1
1	A	435	VAL	2.0
1	A	285	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.