



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:18 PM UTC

PDB ID : 2OLS / pdb_00002ols
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

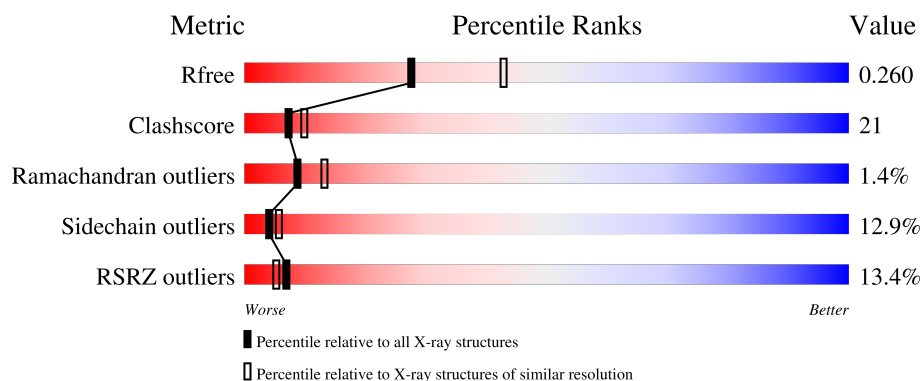
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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
1	A	725	Total	C	N	O	S	0	0	0
			5584	3518	963	1071	32			

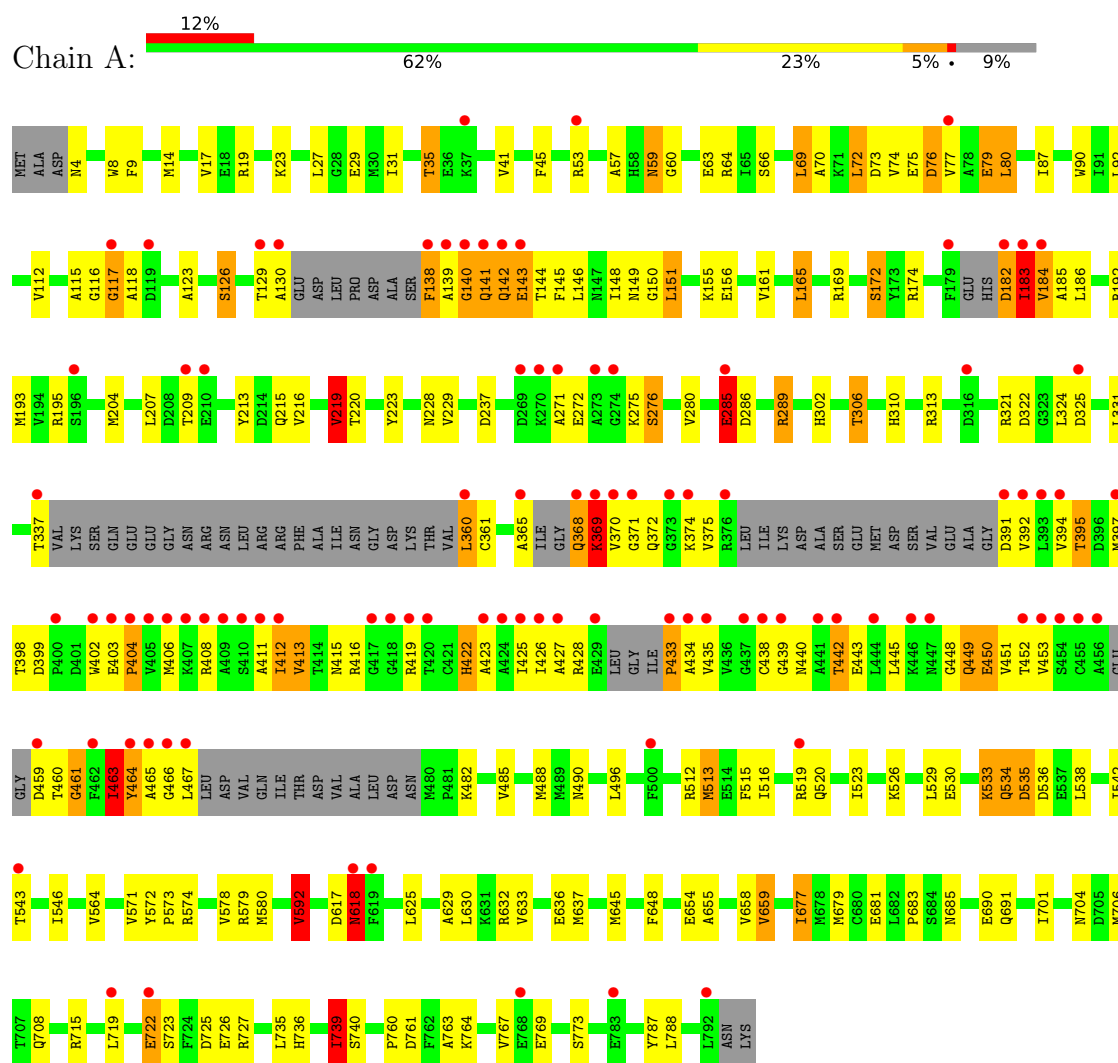
- Molecule 2 is water.

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

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 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 48.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.1 (48.22-2.40) 88.0 (48.22-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.251 0.208 , 0.260	Depositor DCC
R_{free} test set	2313 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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	0.97	6/5678 (0.1%)	0.99	9/7669 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	739	ILE	CA-CB	8.15	1.65	1.54
1	A	618	ASN	CB-CG	6.68	1.68	1.52
1	A	219	VAL	CA-CB	6.07	1.62	1.54
1	A	592	VAL	CA-CB	5.41	1.60	1.54
1	A	677	ILE	CA-CB	5.04	1.60	1.54
1	A	150	GLY	N-CA	5.03	1.49	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASN	N-CA-C	8.42	122.86	112.58
1	A	150	GLY	N-CA-C	6.88	121.19	111.14
1	A	141	GLN	N-CA-C	-5.87	104.47	111.69
1	A	453	VAL	N-CA-C	5.75	115.02	106.85
1	A	228	ASN	N-CA-C	5.58	117.37	111.28
1	A	739	ILE	CA-CB-CG2	5.56	119.95	110.50
1	A	535	ASP	N-CA-C	5.52	117.37	110.91
1	A	313	ARG	N-CA-C	5.34	112.82	108.07
1	A	740	SER	CB-CA-C	-5.01	103.01	110.88

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

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	229	0
2	A	410	0	0	45	0
All	All	5994	0	5511	229	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 21.

All (229) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:183:ILE:CG2	2:A:1142:HOH:O	2.06	1.01
1:A:402:TRP:O	1:A:406:MET:HE3	1.60	1.00
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:445:LEU:HD21	1:A:463:ILE:HD11	1.46	0.94
1:A:450:GLU:O	1:A:450:GLU:HG3	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:O	1:A:722:GLU:HG3	1.67	0.89
1:A:123:ALA:HB2	1:A:193:MET:HE2	1.56	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:HE2	1:A:773:SER:HB2	1.58	0.85
1:A:398:THR:HG21	1:A:406:MET:HE2	1.59	0.84
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:637:MET:SD	2:A:1066:HOH:O	2.39	0.79
1:A:645:MET:HE3	1:A:679:MET:HB2	1.63	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:76:ASP:OD2	1:A:76:ASP:C	2.30	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:488:MET:HE2	1:A:773:SER:CB	2.15	0.73
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:397:MET:HE3	1:A:398:THR:O	1.90	0.71
1:A:123:ALA:HB2	1:A:193:MET:HE3	1.69	0.69
1:A:632:ARG:HG2	1:A:637:MET:HE3	1.74	0.69
1:A:146:LEU:CD2	1:A:193:MET:HE1	2.23	0.69
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:645:MET:HE3	1:A:679:MET:SD	2.33	0.67
1:A:365:ALA:HB2	1:A:461:GLY:N	2.10	0.67
1:A:375:VAL:HG23	1:A:451:VAL:CG2	2.24	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:392:VAL:HG13	1:A:411:ALA:HB3	1.79	0.65
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:460:THR:O	1:A:460:THR:CG2	2.48	0.61
1:A:123:ALA:HB2	1:A:193:MET:HE1	1.76	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:146:LEU:HD22	1:A:193:MET:HE1	1.81	0.60
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:398:THR:CG2	1:A:406:MET:HE2	2.30	0.60
1:A:14:MET:HE1	2:A:972:HOH:O	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:VAL:O	1:A:574:ARG:HB2	2.03	0.59
1:A:645:MET:HE3	1:A:679:MET:CB	2.33	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
1:A:375:VAL:CG2	1:A:451:VAL:CG2	2.82	0.57
1:A:442:THR:HG22	1:A:443:GLU:CD	2.30	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:123:ALA:CA	1:A:193:MET:HE3	2.35	0.56
1:A:392:VAL:HG13	1:A:411:ALA:CB	2.35	0.56
1:A:402:TRP:C	1:A:406:MET:HE3	2.28	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:69:LEU:CD1	1:A:87:ILE:HD11	2.35	0.56
1:A:302:HIS:O	1:A:306:THR:HG23	2.05	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:402:TRP:O	1:A:406:MET:CE	2.47	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:422:HIS:HD1	1:A:422:HIS:C	2.16	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:645:MET:HE1	1:A:679:MET:SD	2.48	0.54
1:A:579:ARG:HD3	1:A:645:MET:HE2	1.90	0.53
1:A:123:ALA:CB	1:A:193:MET:HE3	2.33	0.53
1:A:467:LEU:HD23	1:A:467:LEU:C	2.33	0.53
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:VAL:HG13	1:A:767:VAL:HG22	1.90	0.53
1:A:146:LEU:HD23	1:A:193:MET:HE1	1.90	0.53
1:A:564:VAL:HG13	1:A:578:VAL:HG21	1.92	0.52
1:A:8:TRP:CE2	2:A:1024:HOH:O	2.62	0.52
1:A:360:LEU:HD12	2:A:1170:HOH:O	2.10	0.52
1:A:681:GLU:H	1:A:685:ASN:HD22	1.56	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: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
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:23:LYS:HD3	2:A:849:HOH:O	2.11	0.49
1:A:138:PHE:N	1:A:138:PHE:HD2	2.10	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: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:422:HIS:C	1:A:422:HIS:ND1	2.73	0.47
1:A:466:GLY:O	1:A:467:LEU:HB2	2.14	0.47
1:A:683:PRO:HA	1:A:706:MET:HE1	1.96	0.47
1:A:141:GLN:O	1:A:142:GLN:C	2.58	0.47
1:A:321:ARG:NE	2:A:1182:HOH:O	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:440:ASN:CG	1:A:440:ASN:O	2.58	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
1:A:53:ARG:HG3	2:A:930:HOH:O	2.16	0.45
1:A:427:ALA:HB1	1:A:434:ALA:HB2	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: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: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:9:PHE:HB3	1:A:31:ILE:HD12	2.00	0.42
1:A:74:VAL:HG23	1:A:80:LEU:HD13	2.00	0.42
1:A:428:ARG:NE	2:A:1193:HOH:O	2.52	0.42
1:A:115:ALA:HB1	1:A:192:ARG:HH21	1.84	0.42
1:A:64:ARG:HG2	1:A:90:TRP:CZ3	2.53	0.42
1:A:360:LEU:N	2:A:1199:HOH:O	2.52	0.42
1:A:654:GLU:O	1:A:658:VAL:HG23	2.19	0.42
1:A:683:PRO:CA	1:A:706:MET:HE1	2.49	0.42
1:A:440:ASN:HB2	1:A:443:GLU:CG	2.50	0.42
1:A:579:ARG:HH11	1:A:679:MET:HE1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TYR:CZ	1:A:215:GLN:HB2	2.55	0.41
1:A:580:MET:HE3	1:A:630:LEU:HD12	2.01	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:398:THR:HG21	1:A:406:MET:CE	2.40	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:513:MET:HE3	1:A:516:ILE:HD12	2.03	0.41
1:A:535:ASP:O	1:A:536:ASP:C	2.62	0.41
1:A:139:ALA:HB2	1:A:419:ARG:HH22	1.85	0.41
1:A:763:ALA:HB1	1:A:788:LEU:HD21	2.03	0.41
1:A:72:LEU:CD2	1:A:79:GLU:HB3	2.51	0.41
1:A:438:CYS:O	1:A:439:GLY:C	2.63	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	707/794 (89%)	661 (94%)	36 (5%)	10 (1%)	9 13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY
1	A	183	ILE
1	A	369	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	513 (87%)	76 (13%)	4 6

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	27	LEU
1	A	35	THR
1	A	41	VAL
1	A	63	GLU
1	A	66	SER
1	A	69	LEU
1	A	72	LEU
1	A	75	GLU
1	A	76	ASP
1	A	77	VAL
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	GLU
1	A	144	THR
1	A	149	ASN
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	186	LEU
1	A	207	LEU
1	A	216	VAL
1	A	219	VAL
1	A	229	VAL
1	A	275	LYS
1	A	276	SER
1	A	280	VAL
1	A	285	GLU
1	A	289	ARG
1	A	306	THR
1	A	331	LEU
1	A	337	THR
1	A	360	LEU
1	A	368	GLN
1	A	369	LYS
1	A	374	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	422	HIS
1	A	425	ILE
1	A	442	THR
1	A	450	GLU
1	A	463	ILE
1	A	482	LYS
1	A	496	LEU
1	A	513	MET
1	A	526	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	529	LEU
1	A	533	LYS
1	A	543	THR
1	A	592	VAL
1	A	617	ASP
1	A	618	ASN
1	A	625	LEU
1	A	636	GLU
1	A	648	PHE
1	A	659	VAL
1	A	719	LEU
1	A	722	GLU
1	A	723	SER
1	A	739	ILE
1	A	764	LYS

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	33	GLN
1	A	58	HIS
1	A	142	GLN
1	A	160	HIS
1	A	228	ASN
1	A	279	ASN
1	A	310	HIS
1	A	332	GLN
1	A	372	GLN
1	A	447	ASN
1	A	590	ASN
1	A	595	ASN
1	A	618	ASN
1	A	665	ASN
1	A	672	ASN
1	A	685	ASN
1	A	708	GLN
1	A	736	HIS
1	A	759	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 oligosaccharides 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%)	0.68	97 (13%) 7 5	27, 52, 99, 109	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	PRO	6.4
1	A	427	ALA	6.0
1	A	405	VAL	6.0
1	A	138	PHE	5.8
1	A	392	VAL	5.8
1	A	456	ALA	5.7
1	A	142	GLN	5.4
1	A	139	ALA	5.1
1	A	411	ALA	4.8
1	A	365	ALA	4.8
1	A	442	THR	4.8
1	A	183	ILE	4.6
1	A	184	VAL	4.5
1	A	467	LEU	4.5
1	A	454	SER	4.5
1	A	360	LEU	4.4
1	A	368	GLN	4.4
1	A	370	VAL	4.2
1	A	412	ILE	4.1
1	A	409	ALA	4.0
1	A	434	ALA	3.9
1	A	273	ALA	3.8
1	A	404	PRO	3.7
1	A	406	MET	3.7
1	A	407	LYS	3.7
1	A	394	VAL	3.6
1	A	129	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	425	ILE	3.5
1	A	459	ASP	3.5
1	A	140	GLY	3.5
1	A	426	ILE	3.4
1	A	543	THR	3.4
1	A	337	THR	3.4
1	A	402	TRP	3.3
1	A	453	VAL	3.3
1	A	419	ARG	3.2
1	A	400	PRO	3.2
1	A	369	LYS	3.1
1	A	792	LEU	3.0
1	A	182	ASP	3.0
1	A	179	PHE	3.0
1	A	376	ARG	3.0
1	A	77	VAL	3.0
1	A	374	LYS	3.0
1	A	397	MET	2.9
1	A	418	GLY	2.9
1	A	210	GLU	2.9
1	A	429	GLU	2.9
1	A	391	ASP	2.9
1	A	446	LYS	2.8
1	A	441	ALA	2.8
1	A	141	GLN	2.8
1	A	408	ARG	2.8
1	A	53	ARG	2.7
1	A	373	GLY	2.7
1	A	371	GLY	2.6
1	A	143	GLU	2.6
1	A	783	GLU	2.6
1	A	435	VAL	2.6
1	A	466	GLY	2.6
1	A	618	ASN	2.6
1	A	423	ALA	2.5
1	A	274	GLY	2.5
1	A	768	GLU	2.5
1	A	452	THR	2.5
1	A	719	LEU	2.5
1	A	465	ALA	2.5
1	A	410	SER	2.4
1	A	444	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	519	ARG	2.4
1	A	462	PHE	2.4
1	A	417	GLY	2.4
1	A	619	PHE	2.4
1	A	447	ASN	2.4
1	A	271	ALA	2.4
1	A	403	GLU	2.3
1	A	424	ALA	2.3
1	A	464	TYR	2.3
1	A	117	GLY	2.2
1	A	316	ASP	2.2
1	A	325	ASP	2.2
1	A	285	GLU	2.2
1	A	437	GLY	2.2
1	A	722	GLU	2.2
1	A	500	PHE	2.2
1	A	393	LEU	2.2
1	A	119	ASP	2.2
1	A	420	THR	2.1
1	A	439	GLY	2.1
1	A	196	SER	2.1
1	A	37	LYS	2.1
1	A	209	THR	2.1
1	A	130	ALA	2.1
1	A	270	LYS	2.1
1	A	438	CYS	2.0
1	A	455	CYS	2.0
1	A	269	ASP	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 oligosaccharides 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.