



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 03:47 PM EST

PDB ID : 1SP9
Title : 4-Hydroxyphenylpyruvate Dioxygenase
Authors : Fritze, I.M.; Linden, L.; Freigang, J.; Auerbach, G.; Huber, R.; Steinbacher, S.
Deposited on : 2004-03-16
Resolution : 3.00 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 : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

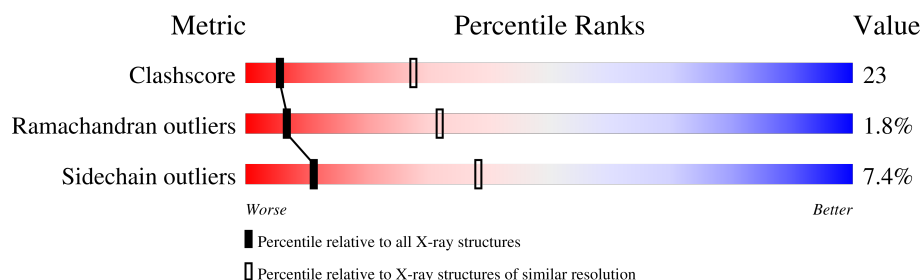
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	
1	B	445	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5745 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 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	164	0	0
			2819	1793	487	526	13			
1	B	374	Total	C	N	O	S	179	0	0
			2924	1860	501	550	13			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

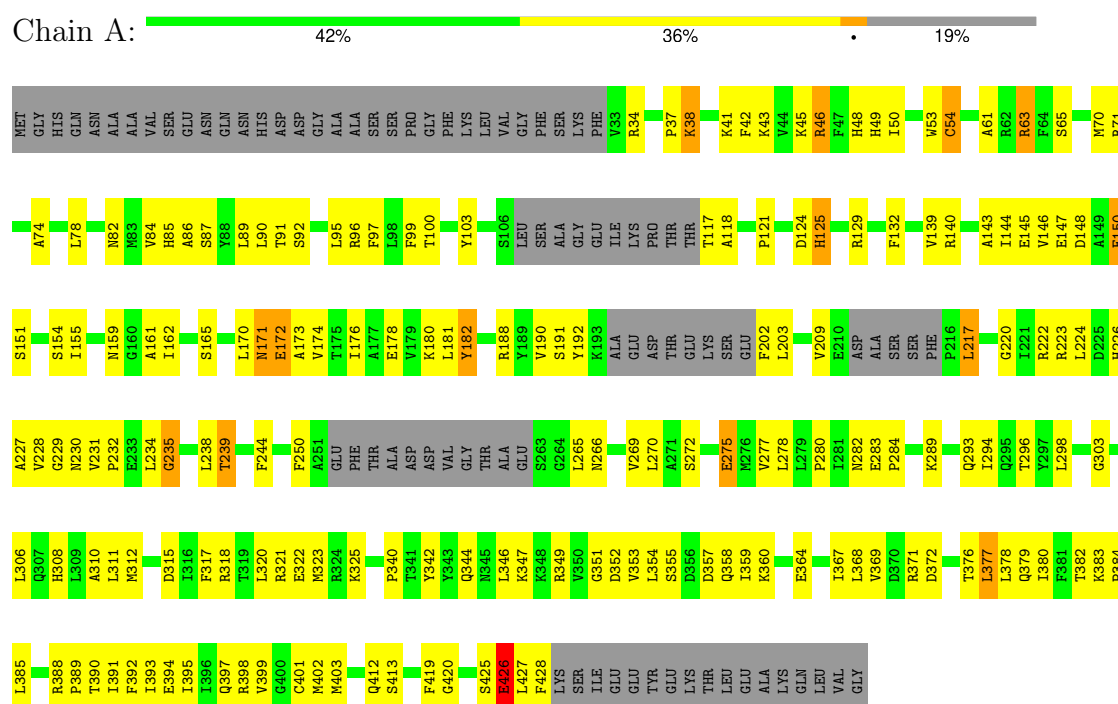
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

3 Residue-property plots

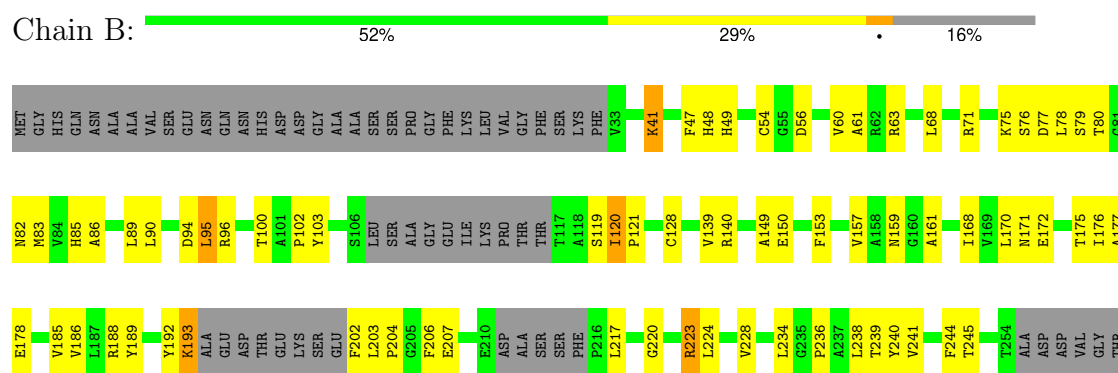
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

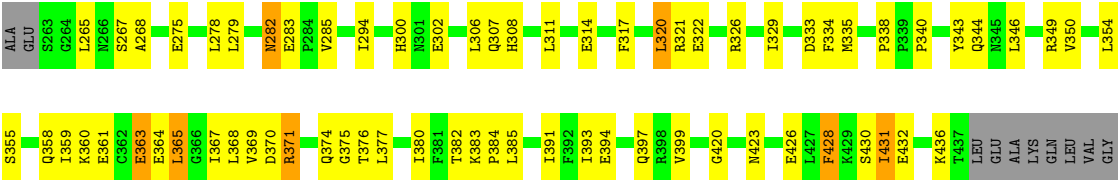
Note EDS was not executed.

• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.20Å 95.20Å 185.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.83 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (16.83-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5745	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: FE2

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	0.43	0/2882	0.69	0/3886
1	B	0.44	0/2989	0.67	0/4029
All	All	0.43	0/5871	0.68	0/7915

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	2819	0	2768	135	2
1	B	2924	0	2866	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	5745	0	5634	244	2

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 23.

All (244) 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:284:PRO:HG3	1:A:294:ILE:HG22	1.35	1.02
1:A:234:LEU:HB2	1:A:283:GLU:HB2	1.44	0.99
1:B:346:LEU:HD23	1:B:359:ILE:HG23	1.46	0.96
1:B:223:ARG:HH21	1:B:223:ARG:HB2	1.43	0.82
1:A:48:HIS:HD2	1:A:49:HIS:HD1	1.27	0.81
1:B:265:LEU:HA	1:B:285:VAL:HG23	1.66	0.78
1:B:121:PRO:HG3	1:B:170:LEU:HD11	1.64	0.78
1:B:63:ARG:HG2	1:B:63:ARG:HH21	1.48	0.77
1:B:320:LEU:HG	1:B:367:ILE:HD11	1.68	0.76
1:A:234:LEU:HB2	1:A:283:GLU:CB	2.17	0.75
1:B:294:ILE:HD12	1:B:294:ILE:H	1.51	0.75
1:B:192:TYR:HB3	1:B:193:LYS:HD3	1.69	0.75
1:A:376:THR:HB	1:A:399:VAL:HG13	1.69	0.74
1:A:45:LYS:HB3	1:A:46:ARG:HD2	1.70	0.73
1:A:48:HIS:CD2	1:A:49:HIS:HD1	2.06	0.72
1:A:265:LEU:HB3	1:A:294:ILE:HD12	1.73	0.71
1:A:323:MET:HE2	1:A:395:ILE:HG12	1.72	0.71
1:A:228:VAL:HG22	1:A:280:PRO:HB2	1.74	0.70
1:A:41:LYS:HB3	1:A:155:ILE:HG21	1.74	0.70
1:A:282:ASN:HB3	1:A:294:ILE:HD13	1.74	0.70
1:A:176:ILE:CD1	1:A:190:VAL:HG22	2.23	0.69
1:B:320:LEU:HD21	1:B:380:ILE:HG21	1.74	0.69
1:B:376:THR:HB	1:B:399:VAL:CG1	2.23	0.68
1:A:89:LEU:HD11	1:A:96:ARG:HB3	1.76	0.67
1:B:49:HIS:HE2	1:B:188:ARG:HH11	1.43	0.67
1:A:293:GLN:O	1:A:296:THR:HB	1.95	0.66
1:A:426:GLU:HA	1:A:428:PHE:CZ	2.31	0.66
1:A:377:LEU:HD12	1:A:398:ARG:NH1	2.12	0.64
1:A:78:LEU:HG	1:A:103:TYR:CE1	2.32	0.64
1:B:423:ASN:HA	1:B:426:GLU:HB3	1.79	0.64
1:A:226:HIS:HB3	1:A:278:LEU:HB2	1.79	0.63
1:A:377:LEU:HD12	1:A:398:ARG:HH12	1.64	0.63
1:B:61:ALA:O	1:B:90:LEU:HD11	1.99	0.63
1:A:346:LEU:HD11	1:A:369:VAL:HB	1.79	0.63
1:B:48:HIS:HD2	1:B:49:HIS:ND1	1.98	0.62
1:B:294:ILE:HD12	1:B:294:ILE:N	2.15	0.61
1:A:360:LYS:O	1:A:364:GLU:HG3	2.01	0.61
1:A:402:MET:SD	1:A:412:GLN:HB2	2.40	0.61
1:B:95:LEU:HD23	1:B:224:LEU:HB2	1.83	0.61
1:B:139:VAL:HG11	1:B:306:LEU:HD13	1.81	0.61
1:B:364:GLU:O	1:B:365:LEU:HG	2.01	0.61
1:A:384:PRO:HG2	1:A:389:PRO:HA	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ARG:HG2	1:B:375:GLY:O	2.01	0.60
1:A:143:ALA:HB2	1:A:188:ARG:HB3	1.84	0.60
1:B:346:LEU:HD11	1:B:369:VAL:HB	1.83	0.60
1:B:170:LEU:HB3	1:B:204:PRO:HG2	1.83	0.60
1:A:176:ILE:HD11	1:A:190:VAL:HG22	1.83	0.59
1:A:385:LEU:HG	1:A:391:ILE:O	2.02	0.59
1:B:244:PHE:CD1	1:B:245:THR:HG23	2.38	0.59
1:B:161:ALA:HB2	1:B:244:PHE:CB	2.33	0.58
1:B:244:PHE:CE1	1:B:245:THR:HG23	2.38	0.58
1:B:56:ASP:O	1:B:60:VAL:HG23	2.03	0.58
1:B:294:ILE:H	1:B:294:ILE:CD1	2.16	0.58
1:A:91:THR:HG22	1:A:96:ARG:HG2	1.86	0.58
1:A:223:ARG:HG3	1:A:312:MET:HB3	1.86	0.58
1:B:317:PHE:O	1:B:321:ARG:HG3	2.04	0.58
1:A:162:ILE:HB	1:A:180:LYS:HG3	1.85	0.58
1:B:307:GLN:O	1:B:391:ILE:HA	2.04	0.57
1:B:153:PHE:CD1	1:B:177:ALA:HB1	2.40	0.57
1:B:239:THR:HG23	1:B:240:TYR:N	2.20	0.57
1:B:228:VAL:HG21	1:B:308:HIS:CE1	2.39	0.57
1:A:74:ALA:HA	1:A:209:VAL:HG23	1.87	0.56
1:B:139:VAL:HG23	1:B:391:ILE:HD12	1.88	0.56
1:A:278:LEU:HD13	1:A:419:PHE:CZ	2.41	0.56
1:B:161:ALA:HB2	1:B:244:PHE:CG	2.41	0.56
1:A:321:ARG:O	1:A:325:LYS:HG3	2.06	0.56
1:A:202:PHE:O	1:A:203:LEU:HD12	2.06	0.56
1:A:278:LEU:HD13	1:A:419:PHE:HZ	1.70	0.56
1:A:265:LEU:CB	1:A:294:ILE:HD12	2.36	0.56
1:A:231:VAL:HB	1:A:232:PRO:HD2	1.87	0.55
1:A:235:GLY:O	1:A:239:THR:HG23	2.06	0.55
1:B:376:THR:O	1:B:399:VAL:HG12	2.05	0.55
1:B:431:ILE:HG13	1:B:431:ILE:O	2.07	0.55
1:A:342:TYR:CZ	1:A:368:LEU:HD23	2.42	0.55
1:B:86:ALA:O	1:B:100:THR:HA	2.06	0.55
1:B:360:LYS:HG3	1:B:364:GLU:OE2	2.06	0.55
1:A:43:LYS:HG2	1:A:147:GLU:HG2	1.88	0.55
1:A:228:VAL:HG21	1:A:308:HIS:CE1	2.43	0.54
1:A:383:LYS:HB3	1:A:384:PRO:CD	2.37	0.54
1:A:148:ASP:HB3	1:A:151:SER:HB3	1.90	0.54
1:A:176:ILE:HD11	1:A:188:ARG:HD3	1.89	0.54
1:A:340:PRO:O	1:A:344:GLN:HG3	2.07	0.54
1:B:89:LEU:HD22	1:B:202:PHE:CD1	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:CYS:HB3	1:A:413:SER:OG	2.07	0.54
1:B:430:SER:C	1:B:432:GLU:H	2.11	0.54
1:A:369:VAL:HG13	1:A:378:LEU:HD23	1.90	0.54
1:A:320:LEU:HD11	1:A:380:ILE:HD13	1.89	0.53
1:A:394:GLU:C	1:A:395:ILE:HD12	2.29	0.53
1:A:383:LYS:HB3	1:A:384:PRO:HD2	1.91	0.53
1:A:284:PRO:HG3	1:A:294:ILE:CG2	2.24	0.53
1:B:220:GLY:O	1:B:314:GLU:HG2	2.09	0.53
1:B:77:ASP:HB2	1:B:103:TYR:OH	2.09	0.53
1:A:376:THR:HB	1:A:399:VAL:CG1	2.39	0.53
1:B:265:LEU:HA	1:B:285:VAL:CG2	2.36	0.53
1:A:87:SER:HA	1:A:99:PHE:O	2.08	0.52
1:B:338:PRO:HG2	1:B:368:LEU:CD2	2.38	0.52
1:B:355:SER:OG	1:B:358:GLN:HG3	2.09	0.52
1:A:146:VAL:HG23	1:A:191:SER:HB3	1.91	0.52
1:B:192:TYR:O	1:B:193:LYS:C	2.46	0.52
1:B:77:ASP:HA	1:B:82:ASN:HB3	1.91	0.52
1:A:95:LEU:HD23	1:A:224:LEU:N	2.25	0.52
1:A:354:LEU:O	1:A:359:ILE:HD11	2.10	0.52
1:B:82:ASN:HD21	1:B:85:HIS:CE1	2.28	0.52
1:B:275:GLU:O	1:B:278:LEU:HD21	2.10	0.52
1:A:48:HIS:HD2	1:A:49:HIS:ND1	2.02	0.51
1:A:346:LEU:HD12	1:A:349:ARG:HH12	1.76	0.51
1:A:382:THR:HG22	1:A:383:LYS:O	2.10	0.51
1:B:223:ARG:HH21	1:B:223:ARG:CB	2.17	0.51
1:B:78:LEU:O	1:B:80:THR:N	2.44	0.51
1:B:150:GLU:CD	1:B:175:THR:HG21	2.31	0.51
1:A:298:LEU:O	1:A:303:GLY:N	2.43	0.51
1:B:193:LYS:HD3	1:B:193:LYS:N	2.26	0.51
1:A:121:PRO:HG3	1:A:170:LEU:HD21	1.94	0.50
1:A:230:ASN:OD1	1:A:282:ASN:HB2	2.12	0.50
1:A:78:LEU:HA	1:A:82:ASN:O	2.11	0.50
1:B:47:PHE:CD2	1:B:224:LEU:HD12	2.47	0.50
1:A:86:ALA:O	1:A:100:THR:HA	2.11	0.50
1:B:140:ARG:O	1:B:186:VAL:HG22	2.12	0.50
1:A:278:LEU:C	1:A:280:PRO:HD3	2.32	0.50
1:A:226:HIS:CB	1:A:278:LEU:HB2	2.42	0.49
1:A:234:LEU:H	1:A:283:GLU:HG3	1.77	0.49
1:B:322:GLU:O	1:B:326:ARG:NH2	2.43	0.49
1:A:37:PRO:O	1:A:38:LYS:C	2.50	0.49
1:A:84:VAL:HG13	1:A:125:HIS:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PHE:HB3	1:A:99:PHE:CE1	2.47	0.49
1:A:269:VAL:HG22	1:A:280:PRO:HG3	1.94	0.49
1:B:343:TYR:CZ	1:B:363:GLU:HA	2.48	0.49
1:A:384:PRO:CG	1:A:389:PRO:HA	2.42	0.49
1:B:193:LYS:NZ	1:B:193:LYS:HB2	2.27	0.49
1:A:275:GLU:O	1:A:278:LEU:HD21	2.13	0.48
1:B:76:SER:OG	1:B:119:SER:HB2	2.13	0.48
1:B:78:LEU:HG	1:B:103:TYR:CZ	2.48	0.48
1:A:231:VAL:O	1:A:284:PRO:HD3	2.13	0.48
1:B:202:PHE:O	1:B:203:LEU:HD12	2.13	0.48
1:B:393:ILE:CG2	1:B:394:GLU:N	2.75	0.48
1:A:346:LEU:HD12	1:A:349:ARG:NH1	2.29	0.48
1:B:78:LEU:C	1:B:80:THR:H	2.17	0.48
1:A:174:VAL:HG12	1:A:192:TYR:CD2	2.49	0.48
1:A:227:ALA:O	1:A:280:PRO:HD2	2.13	0.48
1:A:85:HIS:HD2	1:A:87:SER:OG	1.96	0.48
1:B:265:LEU:HD12	1:B:282:ASN:HB3	1.95	0.47
1:A:250:PHE:HD2	1:A:275:GLU:HG2	1.79	0.47
1:B:391:ILE:HG23	1:B:391:ILE:O	2.14	0.47
1:A:139:VAL:HB	1:A:306:LEU:HD13	1.97	0.47
1:B:41:LYS:HG2	1:B:159:ASN:ND2	2.29	0.47
1:B:239:THR:CG2	1:B:240:TYR:N	2.78	0.47
1:A:65:SER:O	1:A:217:LEU:HD23	2.15	0.47
1:A:182:TYR:CZ	1:A:229:GLY:HA3	2.49	0.47
1:A:220:GLY:O	1:A:222:ARG:HG2	2.15	0.47
1:A:388:ARG:C	1:A:390:THR:H	2.17	0.47
1:A:161:ALA:HB2	1:A:244:PHE:CG	2.49	0.47
1:B:176:ILE:HD11	1:B:188:ARG:NE	2.29	0.47
1:A:139:VAL:CB	1:A:306:LEU:HD13	2.45	0.46
1:A:150:GLU:HG3	1:A:151:SER:N	2.30	0.46
1:A:371:ARG:HG2	1:A:372:ASP:N	2.29	0.46
1:B:207:GLU:HA	1:B:207:GLU:OE1	2.16	0.46
1:A:393:ILE:CG2	1:A:394:GLU:N	2.78	0.46
1:B:329:ILE:O	1:B:329:ILE:HG13	2.15	0.46
1:A:250:PHE:CD2	1:A:275:GLU:HG2	2.51	0.46
1:A:379:GLN:OE1	1:A:420:GLY:HA3	2.15	0.46
1:A:265:LEU:N	1:A:265:LEU:HD23	2.31	0.46
1:B:334:PHE:CE1	1:B:382:THR:HG22	2.51	0.46
1:B:360:LYS:O	1:B:364:GLU:HG3	2.16	0.46
1:A:85:HIS:CD2	1:A:87:SER:OG	2.69	0.46
1:B:149:ALA:HB3	1:B:175:THR:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG23	1:A:139:VAL:HG13	1.98	0.46
1:B:343:TYR:CG	1:B:363:GLU:HB2	2.51	0.46
1:A:70:MET:HG2	1:A:92:SER:HB2	1.99	0.45
1:A:84:VAL:HB	1:A:118:ALA:HB2	1.98	0.45
1:B:121:PRO:HB2	1:B:168:ILE:CD1	2.46	0.45
1:B:75:LYS:O	1:B:206:PHE:HA	2.17	0.45
1:A:53:TRP:CE2	1:A:140:ARG:HG2	2.50	0.45
1:A:323:MET:CE	1:A:395:ILE:HG12	2.43	0.45
1:B:360:LYS:HZ2	1:B:364:GLU:CD	2.20	0.45
1:A:63:ARG:C	1:A:63:ARG:HD3	2.36	0.45
1:B:63:ARG:HH21	1:B:63:ARG:CG	2.23	0.45
1:B:178:GLU:HG2	1:B:188:ARG:HB2	1.99	0.45
1:A:155:ILE:O	1:A:159:ASN:ND2	2.50	0.44
1:A:353:VAL:HG11	1:A:376:THR:HB	1.99	0.44
1:B:176:ILE:HA	1:B:189:TYR:O	2.16	0.44
1:B:333:ASP:HB2	1:B:383:LYS:HE3	1.99	0.44
1:B:385:LEU:HD21	1:B:393:ILE:HG13	1.99	0.44
1:B:153:PHE:O	1:B:157:VAL:HG23	2.17	0.44
1:B:95:LEU:HB2	1:B:223:ARG:HA	2.00	0.44
1:B:338:PRO:CG	1:B:368:LEU:HD21	2.47	0.44
1:A:165:SER:HB3	1:A:178:GLU:HB2	1.99	0.44
1:B:358:GLN:HA	1:B:361:GLU:OE1	2.18	0.44
1:B:338:PRO:HG2	1:B:368:LEU:HD21	1.98	0.44
1:A:151:SER:O	1:A:154:SER:HB3	2.18	0.44
1:A:355:SER:OG	1:A:358:GLN:HG3	2.18	0.44
1:A:382:THR:O	1:A:392:PHE:HB2	2.18	0.44
1:A:272:SER:OG	1:A:277:VAL:HB	2.18	0.43
1:A:395:ILE:HD12	1:A:395:ILE:N	2.33	0.43
1:A:238:LEU:HD11	1:A:270:LEU:HD21	2.01	0.43
1:A:171:ASN:O	1:A:173:ALA:N	2.52	0.43
1:B:168:ILE:O	1:B:175:THR:HA	2.18	0.43
1:B:370:ASP:OD2	1:B:420:GLY:HA2	2.19	0.43
1:A:315:ASP:HB3	1:A:318:ARG:HB3	2.00	0.43
1:A:425:SER:O	1:A:428:PHE:CD1	2.72	0.43
1:A:54:CYS:HA	1:A:132:PHE:CE1	2.54	0.43
1:A:317:PHE:HE2	1:A:367:ILE:HD12	1.83	0.43
1:B:89:LEU:HD13	1:B:202:PHE:CE1	2.53	0.43
1:B:176:ILE:HD11	1:B:188:ARG:CD	2.49	0.43
1:B:326:ARG:HA	1:B:329:ILE:HG12	2.00	0.43
1:A:377:LEU:HD21	1:A:379:GLN:CD	2.39	0.43
1:A:427:LEU:N	1:A:427:LEU:HD22	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:CA	1:B:82:ASN:HB3	2.49	0.42
1:A:388:ARG:O	1:A:390:THR:N	2.49	0.42
1:A:89:LEU:HD12	1:A:97:PHE:O	2.19	0.42
1:A:181:LEU:HG	1:A:182:TYR:CD2	2.54	0.42
1:A:346:LEU:HD11	1:A:369:VAL:CB	2.49	0.42
1:A:306:LEU:HD23	1:A:306:LEU:C	2.39	0.42
1:B:236:PRO:O	1:B:239:THR:HG22	2.19	0.42
1:B:63:ARG:CG	1:B:63:ARG:NH2	2.83	0.42
1:B:185:VAL:HG12	1:B:186:VAL:H	1.85	0.42
1:A:61:ALA:O	1:A:90:LEU:HD11	2.20	0.41
1:A:385:LEU:HD21	1:A:393:ILE:N	2.35	0.41
1:A:143:ALA:HA	1:A:188:ARG:O	2.20	0.41
1:B:71:ARG:O	1:B:90:LEU:HA	2.19	0.41
1:B:120:ILE:HA	1:B:121:PRO:HD2	1.77	0.41
1:B:300:HIS:C	1:B:302:GLU:H	2.21	0.41
1:B:333:ASP:CB	1:B:383:LYS:HE3	2.50	0.41
1:A:266:ASN:HD22	1:A:266:ASN:HA	1.63	0.41
1:B:121:PRO:HD3	1:B:170:LEU:HD21	2.02	0.41
1:B:340:PRO:O	1:B:344:GLN:HG3	2.20	0.41
1:B:241:VAL:HA	1:B:244:PHE:CE2	2.56	0.41
1:A:226:HIS:NE2	1:A:310:ALA:HB2	2.36	0.41
1:A:228:VAL:HA	1:A:280:PRO:O	2.20	0.41
1:A:311:LEU:HD12	1:A:311:LEU:N	2.35	0.41
1:B:78:LEU:C	1:B:80:THR:N	2.73	0.41
1:A:238:LEU:HD12	1:A:270:LEU:HD11	2.03	0.41
1:A:390:THR:OG1	1:A:391:ILE:N	2.51	0.41
1:B:102:PRO:HD3	1:B:128:CYS:SG	2.61	0.41
1:A:171:ASN:O	1:A:172:GLU:C	2.59	0.41
1:A:181:LEU:HG	1:A:182:TYR:CE2	2.56	0.41
1:A:278:LEU:O	1:A:280:PRO:HD3	2.20	0.41
1:B:428:PHE:H	1:B:428:PHE:HD1	1.69	0.41
1:A:71:ARG:O	1:A:90:LEU:HA	2.21	0.41
1:B:94:ASP:O	1:B:96:ARG:HG3	2.21	0.41
1:A:283:GLU:HA	1:A:284:PRO:HD3	1.92	0.40
1:B:238:LEU:HD21	1:B:268:ALA:HB3	2.03	0.40
1:B:234:LEU:H	1:B:283:GLU:HB3	1.86	0.40
1:B:267:SER:HB3	1:B:282:ASN:HB3	2.03	0.40
1:A:401:CYS:O	1:A:403:MET:HG3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:OE2	1:A:322:GLU:OE2[7_555]	1.99	0.21
1:A:315:ASP:OD1	1:A:315:ASP:OD1[7_555]	2.03	0.17

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	352/445 (79%)	303 (86%)	41 (12%)	8 (2%)	5	26
1	B	364/445 (82%)	320 (88%)	39 (11%)	5 (1%)	9	37
All	All	716/890 (80%)	623 (87%)	80 (11%)	13 (2%)	7	32

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	GLU
1	A	125	HIS
1	A	351	GLY
1	A	352	ASP
1	B	79	SER
1	B	365	LEU
1	B	436	LYS
1	A	289	LYS
1	B	431	ILE
1	A	38	LYS
1	A	426	GLU
1	A	235	GLY
1	B	350	VAL

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	305/371 (82%)	284 (93%)	21 (7%)	13	42
1	B	317/371 (85%)	292 (92%)	25 (8%)	10	35
All	All	622/742 (84%)	576 (93%)	46 (7%)	11	38

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	42	PHE
1	A	46	ARG
1	A	54	CYS
1	A	63	ARG
1	A	117	THR
1	A	124	ASP
1	A	129	ARG
1	A	144	ILE
1	A	145	GLU
1	A	150	GLU
1	A	171	ASN
1	A	182	TYR
1	A	217	LEU
1	A	239	THR
1	A	275	GLU
1	A	347	LYS
1	A	357	ASP
1	A	377	LEU
1	A	397	GLN
1	A	426	GLU
1	B	41	LYS
1	B	54	CYS
1	B	68	LEU
1	B	83	MET
1	B	95	LEU
1	B	120	ILE
1	B	171	ASN
1	B	172	GLU
1	B	193	LYS
1	B	217	LEU
1	B	223	ARG
1	B	279	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	282	ASN
1	B	311	LEU
1	B	320	LEU
1	B	335	MET
1	B	349	ARG
1	B	354	LEU
1	B	363	GLU
1	B	371	ARG
1	B	374	GLN
1	B	377	LEU
1	B	384	PRO
1	B	397	GLN
1	B	428	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	85	HIS
1	A	159	ASN
1	A	266	ASN
1	A	379	GLN
1	A	423	ASN
1	B	48	HIS
1	B	85	HIS
1	B	159	ASN
1	B	249	GLN
1	B	266	ASN
1	B	295	GLN
1	B	423	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.