Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:25 PM GMT

PDB ID	:	1FIY
Title	:	THREE-DIMENSIONAL STRUCTURE OF PHOSPHOENOLPYRUVATE CARBOXYLASE FROM ESCHERICHIA COLI AT 2.8 A RESOLUTION
Authors	:	Kai, Y.; Matsumura, H.; Inoue, T.; Terada, K.; Nagara, Y.; Yoshinaga, T.; Kihara, A.; Izui, K.
Deposited on	:	1998-05-02
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

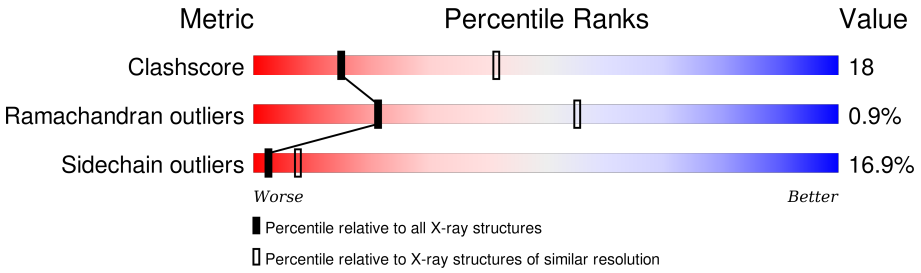
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	883	56% 35% 7%

2 Entry composition

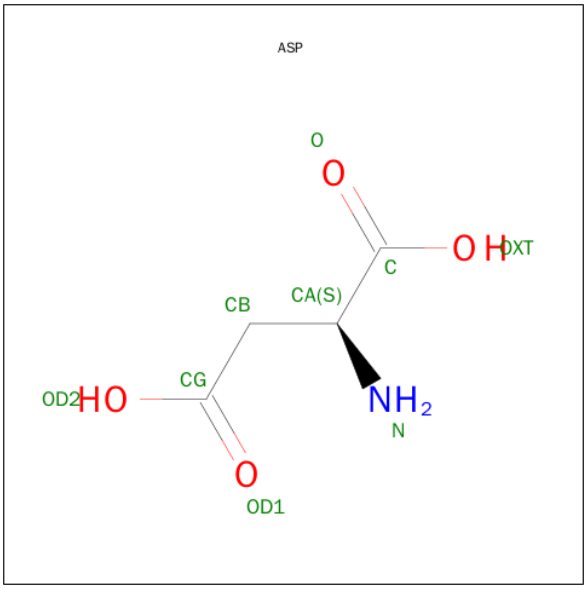
There are 3 unique types of molecules in this entry. The entry contains 6936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	873	Total	C	N	O	S	0	0	0
			6888	4358	1203	1296	31			

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		

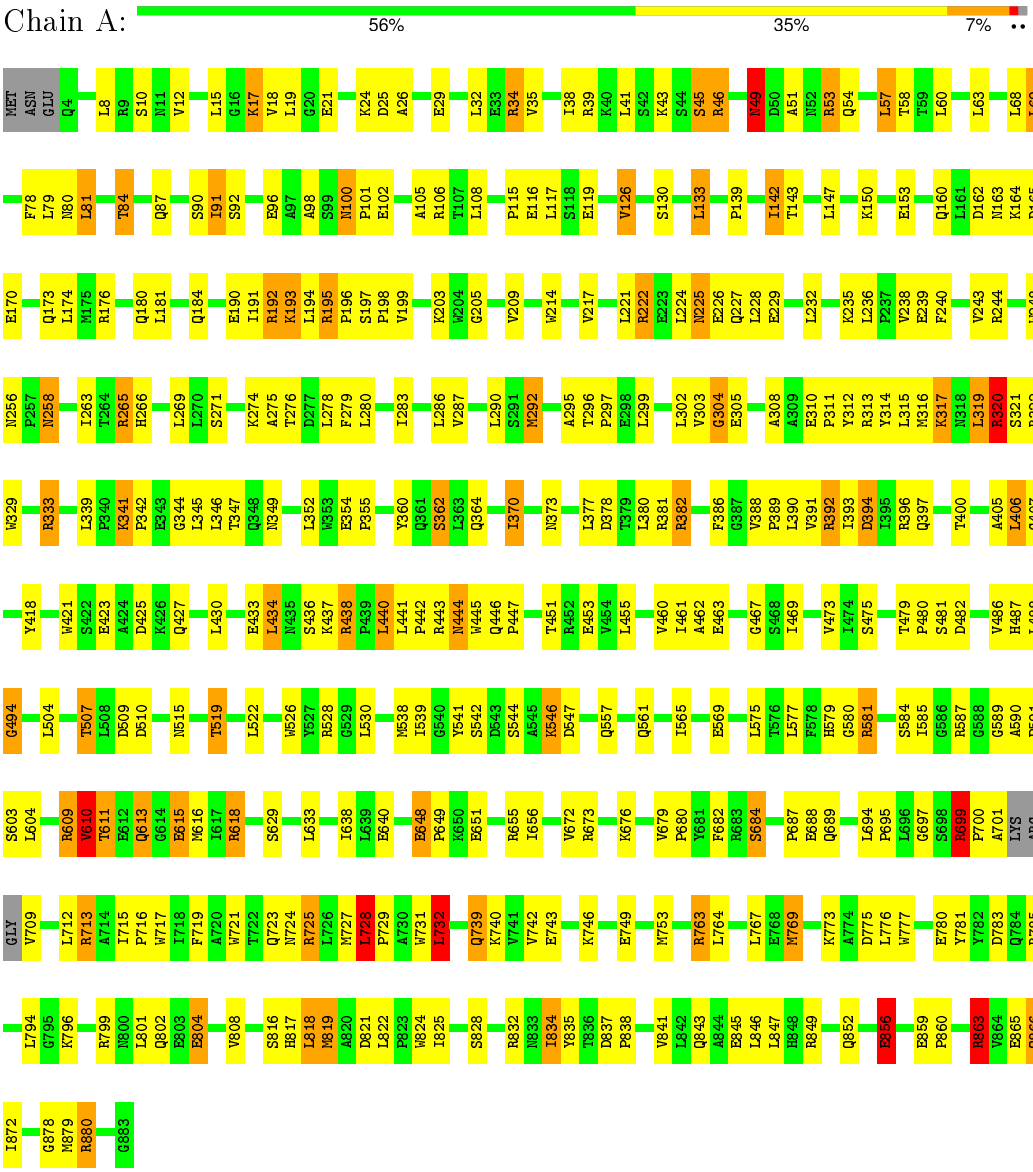
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: PHOSPHOENOLPYRUVATE CARBOXYLASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	117.60Å 248.40Å 82.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6936	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

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	0.56	0/7022	1.20	32/9522 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	618	ARG	CD-NE-CZ	13.33	142.26	123.60
1	A	699	ARG	CD-NE-CZ	11.00	139.00	123.60
1	A	320	ARG	CD-NE-CZ	9.95	137.53	123.60
1	A	320	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	618	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	46	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	382	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	863	ARG	CD-NE-CZ	8.55	135.57	123.60
1	A	382	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	725	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	880	ARG	NE-CZ-NH1	-7.73	116.43	120.30
1	A	863	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	394	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	392	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	713	ARG	NE-CZ-NH1	-6.59	117.01	120.30
1	A	580	GLY	C-N-CA	6.39	137.68	121.70
1	A	394	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	438	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	438	ARG	CD-NE-CZ	6.17	132.24	123.60
1	A	166	ILE	N-CA-CB	5.89	124.35	110.80
1	A	609	ARG	CD-NE-CZ	5.88	131.83	123.60
1	A	819	MET	CA-CB-CG	5.76	123.10	113.30
1	A	222	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	609	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	763	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	438	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	411	ARG	NE-CZ-NH1	-5.41	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	610	VAL	CB-CA-C	-5.30	101.33	111.40
1	A	265	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	A	856	GLU	CA-CB-CG	5.20	124.84	113.40
1	A	482	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	728	LEU	CA-CB-CG	5.07	126.96	115.30

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	6888	0	6933	243	0
2	A	9	0	3	3	0
3	A	39	0	0	1	0
All	All	6936	0	6936	243	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 18.

All (243) 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:142:ILE:HD11	1:A:869:MET:HB3	1.41	1.00
1:A:507:THR:HG22	1:A:510:ASP:H	1.31	0.94
1:A:776:LEU:HD22	1:A:799:ARG:HG2	1.49	0.92
1:A:84:THR:HG22	1:A:618:ARG:HH22	1.34	0.89
1:A:817:HIS:O	1:A:818:LEU:HB2	1.75	0.85
1:A:326:THR:HG21	1:A:346:LEU:H	1.43	0.83
1:A:60:LEU:HB3	1:A:845:GLU:HG3	1.58	0.83
1:A:863:ARG:HG3	1:A:863:ARG:HH11	1.49	0.75
1:A:195:ARG:NH2	1:A:701:ALA:HB2	2.03	0.73
1:A:319:LEU:HD22	1:A:323:LEU:HD22	1.70	0.73
1:A:287:VAL:O	1:A:313:ARG:HD3	1.89	0.72
1:A:526:TRP:CH2	1:A:530:LEU:HD22	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ILE:O	1:A:569:GLU:HG3	1.90	0.72
1:A:87:GLN:HE22	1:A:618:ARG:HE	1.38	0.72
1:A:326:THR:HB	1:A:345:LEU:HD12	1.72	0.72
1:A:139:PRO:HD2	1:A:615:GLU:HG3	1.72	0.71
1:A:49:ASN:HD22	1:A:51:ALA:H	1.36	0.71
1:A:349:ASN:ND2	1:A:388:VAL:H	1.88	0.71
1:A:837:ASP:HB3	1:A:838:PRO:HD3	1.73	0.70
1:A:487:HIS:CD2	1:A:530:LEU:HD21	2.26	0.70
1:A:286:LEU:HD13	1:A:316:MET:HE1	1.75	0.69
1:A:329:TRP:CZ2	1:A:333:ARG:HD3	2.28	0.68
1:A:776:LEU:HD21	1:A:802:GLN:NE2	2.09	0.67
1:A:377:LEU:O	1:A:381:ARG:HG3	1.94	0.66
1:A:68:LEU:HD11	1:A:849:ARG:HH11	1.61	0.66
1:A:283:ILE:HD12	1:A:316:MET:HE3	1.77	0.65
1:A:728:LEU:HD13	1:A:732:LEU:HG	1.78	0.65
1:A:87:GLN:NE2	1:A:618:ARG:HE	1.94	0.64
1:A:15:LEU:HB3	1:A:81:LEU:HG	1.78	0.64
1:A:780:GLU:HG3	1:A:799:ARG:NH1	2.13	0.64
1:A:378:ASP:O	1:A:382:ARG:HG3	1.97	0.64
1:A:822:LEU:HD22	1:A:825:ILE:HD12	1.79	0.63
1:A:142:ILE:CD1	1:A:869:MET:HB3	2.24	0.63
1:A:326:THR:CG2	1:A:346:LEU:H	2.11	0.62
1:A:418:TYR:OH	1:A:430:LEU:HD11	1.99	0.62
1:A:253:ARG:HG3	1:A:397:GLN:NE2	2.14	0.62
1:A:694:LEU:HD11	1:A:868:LEU:HD13	1.80	0.61
1:A:441:LEU:HD21	1:A:455:LEU:HD22	1.82	0.61
1:A:142:ILE:HD11	1:A:869:MET:SD	2.40	0.61
1:A:80:ASN:O	1:A:84:THR:HG23	2.01	0.60
1:A:236:LEU:HD13	1:A:240:PHE:CE2	2.36	0.60
1:A:236:LEU:HD13	1:A:240:PHE:CD2	2.36	0.59
1:A:769:MET:HG3	2:A:884:ASP:O	2.02	0.59
1:A:515:ASN:O	1:A:519:THR:HG23	2.02	0.59
1:A:423:GLU:OE2	1:A:427:GLN:NE2	2.22	0.59
1:A:214:TRP:CE2	1:A:382:ARG:HD3	2.37	0.59
1:A:651:GLU:OE2	1:A:655:ARG:NH2	2.36	0.59
1:A:49:ASN:ND2	1:A:51:ALA:H	1.99	0.58
1:A:258:ASN:ND2	1:A:700:PRO:HD3	2.18	0.58
1:A:724:ASN:O	1:A:725:ARG:HB2	2.04	0.58
1:A:126:VAL:CG1	1:A:236:LEU:HD21	2.33	0.58
1:A:304:GLY:O	1:A:305:GLU:HB2	2.03	0.58
1:A:442:PRO:HB2	1:A:445:TRP:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ILE:HD13	1:A:596:LEU:HD23	1.86	0.58
1:A:406:LEU:HD21	1:A:488:LEU:HD23	1.85	0.58
1:A:648:GLU:HG3	1:A:649:PRO:HD2	1.86	0.58
1:A:49:ASN:HD21	1:A:51:ALA:HB3	1.68	0.58
1:A:164:LYS:O	1:A:165:ASP:HB2	2.04	0.58
1:A:880:ARG:HD2	2:A:884:ASP:OD2	2.02	0.57
1:A:225:ASN:ND2	1:A:235:LYS:HB3	2.19	0.57
1:A:364:GLN:HE22	1:A:373:ASN:HD21	1.52	0.57
1:A:68:LEU:HD22	1:A:846:LEU:HD21	1.86	0.57
1:A:53:ARG:HH21	1:A:781:TYR:HD1	1.53	0.57
1:A:60:LEU:HB3	1:A:845:GLU:CG	2.32	0.56
1:A:126:VAL:HG13	1:A:236:LEU:HD21	1.88	0.56
1:A:615:GLU:HG2	1:A:719:PHE:HZ	1.71	0.56
1:A:238:VAL:HG21	1:A:360:TYR:CZ	2.41	0.56
1:A:46:ARG:HH22	1:A:775:ASP:CG	2.08	0.56
1:A:475:SER:HA	1:A:504:LEU:HB3	1.87	0.56
1:A:715:ILE:HB	1:A:716:PRO:HD3	1.89	0.55
1:A:105:ALA:HB2	1:A:227:GLN:OE1	2.07	0.55
1:A:522:LEU:O	1:A:528:ARG:HD3	2.07	0.55
1:A:310:GLU:HG3	1:A:313:ARG:HB3	1.89	0.54
1:A:728:LEU:CD1	1:A:732:LEU:HG	2.37	0.54
1:A:409:LEU:HD21	1:A:440:LEU:HD23	1.89	0.54
1:A:322:ARG:HG3	1:A:344:GLY:O	2.08	0.54
1:A:585:ILE:HD13	1:A:596:LEU:CD2	2.38	0.54
1:A:205:GLY:O	1:A:209:VAL:HG23	2.08	0.54
1:A:557:GLN:HG3	1:A:561:GLN:HE21	1.72	0.54
1:A:303:VAL:HG13	1:A:314:TYR:CD2	2.42	0.54
1:A:581:ARG:HG3	1:A:611:THR:HG21	1.89	0.53
1:A:860:PRO:HB2	1:A:865:GLU:OE2	2.08	0.53
1:A:198:PRO:HB2	1:A:263:ILE:HG21	1.89	0.53
1:A:167:ALA:HB1	1:A:169:TYR:CE1	2.43	0.53
1:A:163:ASN:ND2	1:A:164:LYS:O	2.42	0.53
1:A:34:ARG:O	1:A:38:ILE:HG12	2.07	0.53
1:A:804:GLU:O	1:A:808:VAL:HG23	2.09	0.53
1:A:547:ASP:OD1	1:A:673:ARG:NH2	2.41	0.53
1:A:868:LEU:HD22	1:A:872:ILE:CD1	2.39	0.53
1:A:96:GLU:HG3	1:A:824:TRP:CD1	2.44	0.53
1:A:863:ARG:HG3	1:A:863:ARG:NH1	2.19	0.52
1:A:393:ILE:HG22	1:A:394:ASP:N	2.25	0.52
1:A:199:VAL:HG12	1:A:203:LYS:HD2	1.92	0.52
1:A:326:THR:HG21	1:A:346:LEU:N	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD12	1:A:442:PRO:HD2	1.91	0.52
1:A:386:PHE:HB3	1:A:390:LEU:O	2.09	0.51
1:A:584:SER:HA	1:A:587:ARG:HG3	1.92	0.51
1:A:769:MET:CE	1:A:773:LYS:HD2	2.41	0.51
1:A:274:LYS:HE3	1:A:278:LEU:HD21	1.92	0.51
1:A:504:LEU:HD13	1:A:538:MET:SD	2.50	0.51
1:A:8:LEU:O	1:A:12:VAL:HG13	2.10	0.51
1:A:49:ASN:C	1:A:49:ASN:HD22	2.12	0.51
1:A:312:TYR:HE1	1:A:362:SER:HG	1.57	0.51
1:A:715:ILE:HB	1:A:716:PRO:CD	2.40	0.51
1:A:60:LEU:HD11	1:A:841:VAL:HG12	1.91	0.51
1:A:773:LYS:HB3	1:A:879:MET:HE3	1.92	0.51
1:A:349:ASN:HD21	1:A:388:VAL:H	1.58	0.51
1:A:45:SER:OG	1:A:53:ARG:HA	2.11	0.51
1:A:84:THR:HG22	1:A:618:ARG:NH2	2.14	0.50
1:A:229:GLU:HB2	1:A:235:LYS:HG2	1.94	0.50
1:A:303:VAL:HG13	1:A:314:TYR:HD2	1.76	0.50
1:A:323:LEU:HD13	1:A:346:LEU:CD1	2.42	0.50
1:A:133:LEU:N	1:A:133:LEU:HD22	2.26	0.50
1:A:319:LEU:HD21	1:A:352:LEU:HD23	1.94	0.50
1:A:445:TRP:CE3	1:A:447:PRO:HG3	2.47	0.50
1:A:597:LEU:HD21	1:A:640:GLU:HB3	1.94	0.49
1:A:539:ILE:HG21	1:A:557:GLN:HG3	1.95	0.49
1:A:817:HIS:O	1:A:818:LEU:CB	2.55	0.49
1:A:87:GLN:O	1:A:91:ILE:HD13	2.13	0.49
1:A:195:ARG:HD3	1:A:699:ARG:O	2.13	0.49
1:A:393:ILE:HG22	1:A:394:ASP:H	1.76	0.49
1:A:279:PHE:O	1:A:283:ILE:HG12	2.13	0.49
1:A:546:LYS:HG3	1:A:717:TRP:CD1	2.47	0.49
1:A:167:ALA:HB3	1:A:170:GLU:HG3	1.95	0.48
1:A:832:ARG:HH22	2:A:884:ASP:CG	2.16	0.48
1:A:783:ASP:HA	1:A:787:VAL:HG23	1.94	0.48
1:A:54:GLN:O	1:A:58:THR:HG23	2.13	0.48
1:A:305:GLU:H	1:A:308:ALA:HB2	1.78	0.48
1:A:364:GLN:NE2	1:A:373:ASN:HD21	2.12	0.48
1:A:193:LYS:CE	1:A:193:LYS:H	2.27	0.48
1:A:100:ASN:HD22	1:A:101:PRO:N	2.11	0.48
1:A:731:TRP:CE3	1:A:732:LEU:HA	2.49	0.48
1:A:868:LEU:HD22	1:A:872:ILE:HD11	1.95	0.47
1:A:100:ASN:C	1:A:100:ASN:HD22	2.17	0.47
1:A:589:GLY:HA2	1:A:633:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:HG12	1:A:221:LEU:HD12	1.96	0.47
1:A:341:LYS:HB2	1:A:345:LEU:HD22	1.95	0.47
1:A:191:ILE:HG21	1:A:866:GLN:HG2	1.95	0.47
1:A:68:LEU:HD21	1:A:849:ARG:NH1	2.30	0.47
1:A:394:ASP:OD2	1:A:609:ARG:NH2	2.48	0.47
1:A:682:PHE:CZ	1:A:688:GLU:HG3	2.49	0.47
1:A:143:THR:HG22	1:A:190:GLU:O	2.14	0.47
1:A:579:HIS:HB2	1:A:610:VAL:HG13	1.96	0.47
1:A:723:GLN:HB3	1:A:843:GLN:HE22	1.80	0.46
1:A:275:ALA:HB2	1:A:390:LEU:HB2	1.98	0.46
1:A:98:ALA:HB1	1:A:629:SER:OG	2.15	0.46
1:A:590:ALA:HB3	1:A:591:PRO:HD3	1.96	0.46
1:A:868:LEU:O	1:A:872:ILE:HD12	2.16	0.46
1:A:310:GLU:N	1:A:311:PRO:HD3	2.30	0.46
1:A:672:VAL:HG13	1:A:709:VAL:HG21	1.98	0.46
1:A:589:GLY:HA2	1:A:633:LEU:HD13	1.96	0.46
1:A:396:ARG:HB2	1:A:473:VAL:HB	1.98	0.46
1:A:763:ARG:HH21	1:A:767:LEU:HD22	1.81	0.46
1:A:192:ARG:CZ	1:A:196:PRO:HB3	2.46	0.46
1:A:615:GLU:CG	1:A:719:PHE:HZ	2.28	0.46
1:A:725:ARG:NE	1:A:879:MET:HE1	2.30	0.46
1:A:405:ALA:HA	1:A:451:THR:HG23	1.97	0.46
1:A:290:LEU:HA	1:A:292:MET:SD	2.55	0.46
1:A:581:ARG:N	1:A:581:ARG:HD2	2.31	0.46
1:A:633:LEU:HA	1:A:633:LEU:HD23	1.81	0.46
1:A:283:ILE:O	1:A:287:VAL:HG23	2.16	0.45
1:A:445:TRP:CD2	1:A:447:PRO:HG3	2.50	0.45
1:A:515:ASN:O	1:A:519:THR:CG2	2.64	0.45
1:A:35:VAL:HG13	1:A:75:PHE:CE1	2.51	0.45
1:A:541:TYR:HB2	1:A:557:GLN:NE2	2.31	0.45
1:A:728:LEU:HD12	1:A:728:LEU:C	2.37	0.45
1:A:615:GLU:HG2	1:A:719:PHE:CZ	2.50	0.45
1:A:725:ARG:CZ	1:A:879:MET:HE1	2.47	0.45
1:A:21:GLU:O	1:A:24:LYS:HB3	2.15	0.45
1:A:832:ARG:HD2	1:A:878:GLY:O	2.17	0.45
1:A:613:GLN:HG2	1:A:616:MET:HB2	1.98	0.45
1:A:266:HIS:O	1:A:269:LEU:HB2	2.17	0.45
1:A:142:ILE:HD11	1:A:869:MET:CB	2.28	0.45
1:A:195:ARG:HG3	1:A:697:GLY:O	2.17	0.45
1:A:310:GLU:N	1:A:311:PRO:CD	2.80	0.45
1:A:434:LEU:HG	1:A:526:TRP:CH2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:MET:HE2	1:A:773:LYS:HD2	1.99	0.44
1:A:69:LEU:HD22	1:A:73:ARG:HG3	1.98	0.44
1:A:370:ILE:HG12	1:A:370:ILE:H	1.46	0.44
1:A:299:LEU:HD11	1:A:315:LEU:HD11	1.99	0.44
1:A:271:SER:HB3	1:A:389:PRO:O	2.16	0.44
1:A:460:VAL:O	1:A:461:ILE:C	2.55	0.44
1:A:575:LEU:HD21	1:A:577:LEU:HD21	2.00	0.44
1:A:436:SER:O	1:A:491:LYS:NZ	2.44	0.44
1:A:341:LYS:HA	1:A:342:PRO:HD3	1.89	0.44
1:A:504:LEU:HD13	1:A:538:MET:CG	2.48	0.44
1:A:739:GLN:O	1:A:743:GLU:HG3	2.17	0.44
1:A:173:GLN:HG2	1:A:176:ARG:HH22	1.83	0.44
1:A:712:LEU:HD22	1:A:716:PRO:HB2	1.99	0.43
1:A:687:PRO:HB3	1:A:847:LEU:HD11	1.99	0.43
1:A:541:TYR:HB2	1:A:557:GLN:HE22	1.84	0.43
1:A:79:LEU:O	1:A:79:LEU:HD12	2.19	0.43
1:A:388:VAL:HB	1:A:389:PRO:HD3	2.01	0.43
1:A:248:TRP:CD1	1:A:394:ASP:HB2	2.53	0.43
1:A:292:MET:SD	1:A:292:MET:N	2.90	0.43
1:A:856:GLU:HG2	1:A:856:GLU:O	2.18	0.43
1:A:837:ASP:HB3	1:A:838:PRO:CD	2.46	0.43
1:A:433:GLU:HA	1:A:433:GLU:OE1	2.19	0.43
1:A:354:GLU:CB	1:A:355:PRO:HD3	2.48	0.43
1:A:443:ARG:HD3	1:A:444:ASN:N	2.33	0.43
1:A:684:SER:HB3	1:A:787:VAL:HG22	2.00	0.42
1:A:487:HIS:NE2	1:A:530:LEU:HD21	2.33	0.42
1:A:727:MET:CE	1:A:879:MET:HE3	2.49	0.42
1:A:715:ILE:HG12	1:A:715:ILE:H	1.64	0.42
1:A:115:PRO:O	1:A:116:GLU:HB2	2.19	0.42
1:A:24:LYS:HD2	1:A:29:GLU:HG2	2.01	0.42
1:A:299:LEU:HD22	1:A:362:SER:OG	2.18	0.42
1:A:834:ILE:HD11	1:A:835:TYR:CE2	2.54	0.42
1:A:392:ARG:HG2	1:A:467:GLY:O	2.20	0.42
1:A:108:LEU:HD22	1:A:232:LEU:HG	2.00	0.42
1:A:406:LEU:HA	1:A:406:LEU:HD12	1.81	0.42
1:A:317:LYS:HG2	1:A:320:ARG:NH1	2.35	0.42
1:A:160:GLN:HB3	1:A:174:LEU:HD11	2.02	0.42
1:A:312:TYR:O	1:A:316:MET:HG2	2.20	0.42
1:A:214:TRP:CZ2	1:A:382:ARG:HD3	2.54	0.42
1:A:265:ARG:HD2	1:A:265:ARG:HH11	1.55	0.42
1:A:441:LEU:HA	1:A:442:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:MET:HE3	1:A:773:LYS:HD2	2.02	0.42
1:A:613:GLN:HE21	1:A:613:GLN:H	1.68	0.42
1:A:407:GLY:O	1:A:411:ARG:HD2	2.20	0.42
1:A:421:TRP:HB3	1:A:425:ASP:HB2	2.01	0.42
1:A:296:THR:O	1:A:297:PRO:C	2.58	0.42
1:A:604:LEU:HD22	1:A:638:ILE:HD12	2.02	0.41
1:A:818:LEU:O	1:A:819:MET:C	2.58	0.41
1:A:615:GLU:CD	1:A:615:GLU:H	2.22	0.41
1:A:96:GLU:HG3	1:A:824:TRP:CG	2.55	0.41
1:A:299:LEU:HD22	1:A:362:SER:HG	1.85	0.41
1:A:721:TRP:CD1	1:A:729:PRO:HD3	2.55	0.41
1:A:224:LEU:O	1:A:228:LEU:HG	2.20	0.41
1:A:17:LYS:HD2	1:A:17:LYS:HA	1.70	0.41
1:A:411:ARG:HD3	1:A:411:ARG:HH11	1.50	0.41
1:A:191:ILE:HB	3:A:895:HOH:O	2.20	0.41
1:A:694:LEU:HB3	1:A:695:PRO:HD2	2.02	0.40
1:A:423:GLU:OE2	1:A:481:SER:HB3	2.21	0.40
1:A:462:ALA:HB1	1:A:494:GLY:O	2.21	0.40
1:A:713:ARG:HD2	1:A:713:ARG:N	2.36	0.40
1:A:19:LEU:HD23	1:A:78:PHE:CD1	2.56	0.40
1:A:295:ALA:HB1	1:A:299:LEU:HD23	2.03	0.40
1:A:63:LEU:O	1:A:849:ARG:NH2	2.47	0.40
1:A:24:LYS:HZ2	1:A:29:GLU:HB3	1.87	0.40
1:A:679:VAL:HB	1:A:680:PRO:HD3	2.03	0.40
1:A:57:LEU:HD21	1:A:785:ARG:HD3	2.03	0.40
1:A:479:THR:HB	1:A:480:PRO:CD	2.52	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	869/883 (98%)	794 (91%)	67 (8%)	8 (1%)	21 55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ALA
1	A	603	SER
1	A	732	LEU
1	A	818	LEU
1	A	304	GLY
1	A	49	ASN
1	A	258	ASN
1	A	494	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	739/747 (99%)	614 (83%)	125 (17%)	2 7

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	17	LYS
1	A	18	VAL
1	A	25	ASP
1	A	32	LEU
1	A	34	ARG
1	A	39	ARG
1	A	41	LEU
1	A	43	LYS
1	A	45	SER
1	A	49	ASN
1	A	53	ARG
1	A	57	LEU

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Mol	Chain	Res	Type
1	A	69	LEU
1	A	81	LEU
1	A	84	THR
1	A	90	SER
1	A	91	ILE
1	A	92	SER
1	A	100	ASN
1	A	102	GLU
1	A	106	ARG
1	A	117	LEU
1	A	119	GLU
1	A	126	VAL
1	A	130	SER
1	A	133	LEU
1	A	142	ILE
1	A	147	LEU
1	A	150	LYS
1	A	153	GLU
1	A	162	ASP
1	A	180	GLN
1	A	181	LEU
1	A	184	GLN
1	A	192	ARG
1	A	193	LYS
1	A	194	LEU
1	A	195	ARG
1	A	197	SER
1	A	222	ARG
1	A	225	ASN
1	A	226	GLU
1	A	239	GLU
1	A	243	VAL
1	A	244	ARG
1	A	249	MET
1	A	253	ARG
1	A	256	ASN
1	A	276	THR
1	A	280	LEU
1	A	292	MET
1	A	302	LEU
1	A	317	LYS
1	A	319	LEU

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Mol	Chain	Res	Type
1	A	320	ARG
1	A	321	SER
1	A	323	LEU
1	A	326	THR
1	A	333	ARG
1	A	339	LEU
1	A	341	LYS
1	A	347	THR
1	A	362	SER
1	A	370	ILE
1	A	380	LEU
1	A	391	VAL
1	A	400	THR
1	A	406	LEU
1	A	408	GLU
1	A	411	ARG
1	A	434	LEU
1	A	437	LYS
1	A	438	ARG
1	A	440	LEU
1	A	444	ASN
1	A	446	GLN
1	A	453	GLU
1	A	463	GLU
1	A	469	ILE
1	A	486	VAL
1	A	492	GLU
1	A	507	THR
1	A	509	ASP
1	A	519	THR
1	A	542	SER
1	A	544	SER
1	A	546	LYS
1	A	581	ARG
1	A	610	VAL
1	A	611	THR
1	A	613	GLN
1	A	615	GLU
1	A	648	GLU
1	A	656	ILE
1	A	676	LYS
1	A	684	SER

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Mol	Chain	Res	Type
1	A	689	GLN
1	A	699	ARG
1	A	728	LEU
1	A	732	LEU
1	A	739	GLN
1	A	740	LYS
1	A	742	VAL
1	A	746	LYS
1	A	749	GLU
1	A	753	MET
1	A	764	LEU
1	A	769	MET
1	A	777	TRP
1	A	789	LYS
1	A	794	LEU
1	A	796	LYS
1	A	801	LEU
1	A	804	GLU
1	A	816	SER
1	A	821	ASP
1	A	828	SER
1	A	834	ILE
1	A	852	GLN
1	A	856	GLU
1	A	859	GLU
1	A	863	ARG
1	A	866	GLN
1	A	868	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	54	GLN
1	A	77	GLN
1	A	87	GLN
1	A	100	ASN
1	A	163	ASN
1	A	225	ASN
1	A	231	ASN
1	A	256	ASN
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	266	HIS
1	A	349	ASN
1	A	364	GLN
1	A	535	GLN
1	A	557	GLN
1	A	561	GLN
1	A	599	GLN
1	A	613	GLN
1	A	724	ASN
1	A	802	GLN
1	A	843	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

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	ASP	A	884	-	2,8,8	0.36	0	0,10,10	0.00	-

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
2	ASP	A	884	-	-	0/2/8/8	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	884	ASP	3	0

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 will therefore be empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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