



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 AM GMT

PDB ID : 2GMV
Title : PEPCK complex with a GTP-competitive inhibitor
Authors : Dunten, P.
Deposited on : 2006-04-07
Resolution : 2.30 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

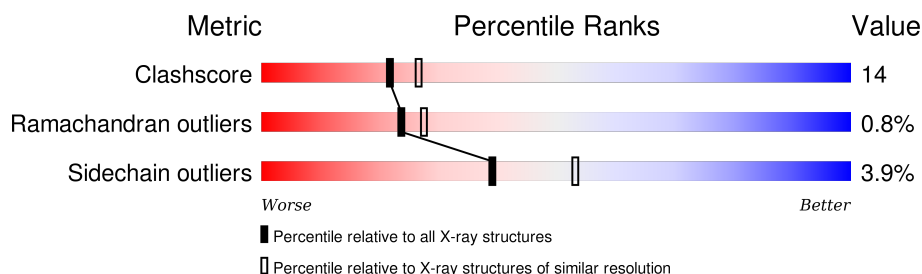
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	625	 76% 19% . .
1	B	625	 61% 33% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9624 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 carboxykinase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4715	3009	806	865	35			
1	B	602	Total	C	N	O	S	0	0	0
			4715	3009	806	865	35			

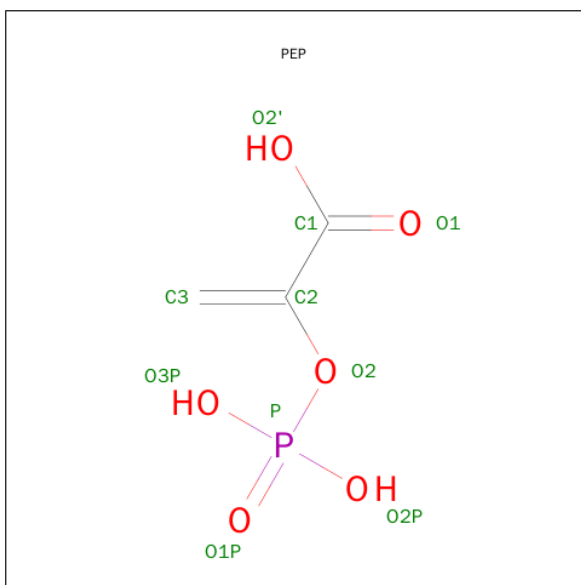
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P35558
A	-1	GLU	-	CLONING ARTIFACT	UNP P35558
A	0	LEU	-	CLONING ARTIFACT	UNP P35558
A	184	LEU	VAL	VARIANT	UNP P35558
A	267	VAL	ILE	VARIANT	UNP P35558
A	586	ASP	GLU	VARIANT	UNP P35558
A	597	VAL	GLU	VARIANT	UNP P35558
B	-2	GLY	-	CLONING ARTIFACT	UNP P35558
B	-1	GLU	-	CLONING ARTIFACT	UNP P35558
B	0	LEU	-	CLONING ARTIFACT	UNP P35558
B	184	LEU	VAL	VARIANT	UNP P35558
B	267	VAL	ILE	VARIANT	UNP P35558
B	586	ASP	GLU	VARIANT	UNP P35558
B	597	VAL	GLU	VARIANT	UNP P35558

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

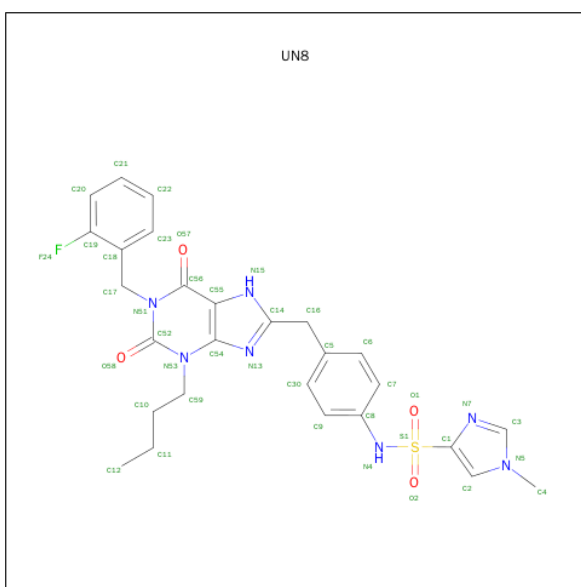
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C₃H₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 4 is N-(4-{[3-BUTYL-1-(2-FLUOROBENZYL)-2,6-DIOXO-2,3,6,7-TETRAHYDRO-1H-PURIN-8-YL]METHYL}PHENYL)-1-METHYL-1H-IMIDAZOLE-4-SULFONAMIDE (three-letter code: UN8) (formula: C₂₇H₂₈FN₇O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			40	27	1	7	4	1		

- Molecule 5 is water.

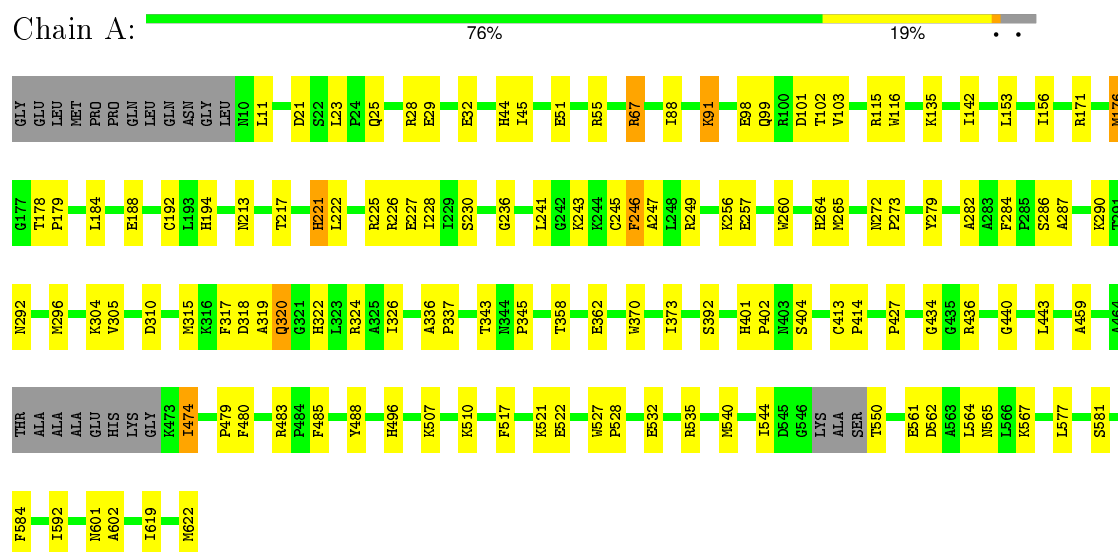
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total 107	O 107	0	0
5	B	25	Total 25	O 25	0	0

3 Residue-property plots

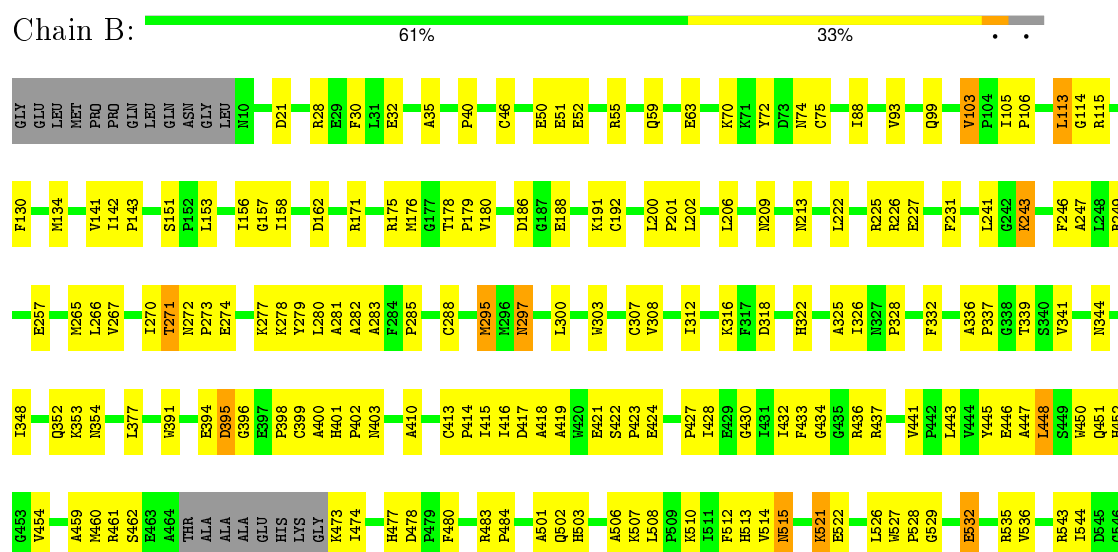
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 carboxykinase, cytosolic



- Molecule 1: Phosphoenolpyruvate carboxykinase, cytosolic





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.01Å 66.13Å 137.36Å 90.00° 145.09° 90.00°	Depositor
Resolution (Å)	39.31 – 2.30	Depositor
% Data completeness (in resolution range)	75.7 (39.31-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9624	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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: UN8, MN, PEP

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	0.33	0/4836	0.52	0/6549
1	B	0.31	0/4836	0.52	0/6549
All	All	0.32	0/9672	0.52	0/13098

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	4715	0	4658	78	0
1	B	4715	0	4658	190	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
4	A	40	0	28	2	0
5	A	107	0	0	1	0
5	B	25	0	0	0	0
All	All	9624	0	9348	263	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 14.

All (263) 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:B:448:LEU:HD21	1:B:618:ARG:NH1	1.68	1.09
1:B:448:LEU:HD21	1:B:618:ARG:HH12	1.20	0.98
1:B:272:ASN:HB2	1:B:273:PRO:HD2	1.46	0.95
1:B:295:MET:HA	1:B:415:ILE:HD11	1.53	0.90
1:B:527:TRP:CD1	1:B:529:GLY:HA2	2.09	0.87
1:B:437:ARG:HB2	1:B:515:ASN:HD21	1.38	0.86
1:B:613:LEU:HA	1:B:616:LYS:HB3	1.55	0.86
1:A:319:ALA:HB1	1:B:423:PRO:HB2	1.56	0.85
1:B:543:ARG:HA	1:B:543:ARG:HH11	1.41	0.85
1:B:434:GLY:HA2	1:B:513:HIS:NE2	1.93	0.83
1:B:437:ARG:HB2	1:B:515:ASN:ND2	1.94	0.81
1:B:604:LEU:HD12	1:B:605:PRO:HD2	1.63	0.80
1:B:272:ASN:CB	1:B:273:PRO:HD2	2.12	0.78
1:B:583:GLU:O	1:B:587:LYS:HG2	1.82	0.78
1:B:265:MET:HG2	1:B:283:ALA:HB2	1.69	0.75
1:A:257:GLU:HB3	1:B:188:GLU:HG3	1.70	0.73
1:B:527:TRP:HD1	1:B:529:GLY:HA2	1.53	0.73
1:B:460:MET:HG3	1:B:480:PHE:H	1.53	0.73
1:B:551:LYS:HD3	1:B:558:ILE:HD11	1.70	0.72
1:B:554:PRO:HB3	1:B:618:ARG:O	1.90	0.72
1:B:501:ALA:HA	1:B:508:LEU:HD11	1.71	0.72
1:B:443:LEU:HD13	1:B:577:LEU:HD21	1.73	0.71
1:B:271:THR:HG22	1:B:272:ASN:H	1.55	0.70
1:B:206:LEU:HD23	1:B:209:ASN:HA	1.73	0.70
1:B:153:LEU:HD12	1:B:326:ILE:HG23	1.73	0.70
1:B:175:ARG:HH21	1:B:421:GLU:HG3	1.54	0.70
1:A:21:ASP:HA	1:A:28:ARG:HH12	1.56	0.69
1:B:142:ILE:HG23	1:B:176:MET:HG3	1.74	0.69
1:B:551:LYS:HB3	1:B:558:ILE:HG13	1.74	0.69
1:B:153:LEU:HD21	1:B:316:LYS:HB3	1.74	0.68
1:A:102:THR:HG22	1:A:103:VAL:HG13	1.76	0.68
1:B:307:CYS:O	1:B:416:ILE:HD12	1.94	0.67
1:B:527:TRP:CD1	1:B:529:GLY:CA	2.78	0.67
1:B:510:LYS:HE3	1:B:544:ILE:HA	1.76	0.67
1:B:559:PRO:HB2	1:B:564:LEU:HD11	1.76	0.66
1:B:564:LEU:HD12	1:B:574:MET:HE1	1.75	0.66
1:B:613:LEU:HA	1:B:616:LYS:CB	2.25	0.66
1:A:345:PRO:HD2	5:A:771:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:HG3	1:A:55:ARG:NH1	2.11	0.65
1:B:451:GLN:O	1:B:611:GLU:HG3	1.97	0.65
1:A:243:LYS:O	1:A:247:ALA:HB3	1.97	0.65
1:B:609:GLU:O	1:B:612:ILE:HB	1.97	0.64
1:B:271:THR:HA	1:B:277:LYS:HA	1.80	0.64
1:B:332:PHE:CE1	1:B:410:ALA:HA	2.33	0.64
1:B:30:PHE:CE1	1:B:191:LYS:HB3	2.34	0.63
1:B:134:MET:HG2	1:B:162:ASP:HB3	1.80	0.63
1:A:21:ASP:HA	1:A:28:ARG:NH1	2.14	0.63
1:A:153:LEU:HB2	1:A:326:ILE:HD13	1.81	0.62
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.82	0.61
1:A:459:ALA:HB1	1:A:592:ILE:HD13	1.82	0.61
1:B:543:ARG:NH1	1:B:543:ARG:HA	2.12	0.60
1:B:555:ILE:HG22	1:B:615:LEU:HD11	1.82	0.60
1:B:280:LEU:HD22	1:B:432:ILE:HD11	1.83	0.60
1:B:437:ARG:HG3	1:B:441:VAL:HG21	1.84	0.60
1:B:175:ARG:NH2	1:B:421:GLU:HG3	2.17	0.60
1:A:318:ASP:OD2	1:A:324:ARG:HD2	2.02	0.60
1:A:188:GLU:HG2	1:B:257:GLU:HB3	1.83	0.59
1:B:448:LEU:CD2	1:B:618:ARG:HH12	2.04	0.59
1:B:295:MET:HG3	1:B:344:ASN:HD21	1.66	0.59
1:B:454:VAL:HG12	1:B:608:ILE:HD11	1.85	0.59
1:B:273:PRO:HD3	1:B:303:TRP:NE1	2.18	0.59
1:B:344:ASN:O	1:B:348:ILE:HG12	2.03	0.59
1:B:434:GLY:HA2	1:B:513:HIS:CE1	2.38	0.59
1:A:619:ILE:O	1:A:622:MET:HG2	2.03	0.59
1:B:434:GLY:HA2	1:B:513:HIS:CD2	2.37	0.58
1:B:99:GLN:HG2	1:B:105:ILE:HD11	1.84	0.58
1:A:436:ARG:HG3	1:A:517:PHE:CG	2.38	0.58
1:B:595:TYR:CE1	1:B:599:GLN:HG3	2.38	0.58
1:B:510:LYS:CE	1:B:544:ILE:HA	2.33	0.58
1:A:292:ASN:HB3	4:A:703:UN8:C23	2.34	0.57
1:B:459:ALA:HB1	1:B:592:ILE:HD13	1.85	0.57
1:B:527:TRP:CD1	1:B:529:GLY:N	2.72	0.57
1:B:151:SER:HB2	1:B:423:PRO:HA	1.86	0.57
1:B:582:LYS:HE3	1:B:619:ILE:O	2.05	0.56
1:A:370:TRP:CD1	1:A:373:ILE:HB	2.40	0.56
1:B:564:LEU:CD1	1:B:574:MET:HE1	2.36	0.56
1:B:513:HIS:CE1	1:B:514:VAL:O	2.59	0.56
1:A:153:LEU:HD12	1:A:326:ILE:HG23	1.88	0.56
1:B:503:HIS:O	1:B:506:ALA:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:HIS:HB2	1:B:186:ASP:OD2	2.07	0.55
1:B:295:MET:HA	1:B:415:ILE:CD1	2.31	0.55
1:B:446:GLU:HB3	1:B:557:TYR:HD1	1.70	0.55
1:B:441:VAL:HG23	1:B:584:PHE:CZ	2.42	0.54
1:B:247:ALA:HB1	1:B:312:ILE:HG21	1.90	0.54
1:B:613:LEU:HD23	1:B:616:LYS:HE3	1.90	0.54
1:A:565:ASN:OD1	1:A:567:LYS:HG3	2.07	0.54
1:B:282:ALA:HB2	1:B:432:ILE:HB	1.88	0.53
1:B:448:LEU:HD21	1:B:618:ARG:CZ	2.35	0.53
1:A:178:THR:N	1:A:179:PRO:CD	2.71	0.53
1:B:575:MET:O	1:B:579:SER:HB3	2.08	0.53
1:B:430:GLY:HA2	1:B:510:LYS:O	2.09	0.53
1:A:142:ILE:CG2	1:A:176:MET:HG3	2.38	0.53
1:B:581:SER:OG	1:B:584:PHE:HB3	2.09	0.53
1:B:441:VAL:HG23	1:B:584:PHE:HZ	1.74	0.52
1:B:267:VAL:HG12	1:B:308:VAL:HB	1.91	0.52
1:B:243:LYS:O	1:B:247:ALA:HB3	2.09	0.52
1:B:105:ILE:HG23	1:B:106:PRO:HD2	1.91	0.52
1:A:188:GLU:CG	1:B:257:GLU:HB3	2.39	0.51
1:A:222:LEU:N	1:A:222:LEU:HD12	2.24	0.51
1:B:265:MET:CG	1:B:283:ALA:HB2	2.40	0.51
1:B:93:VAL:HG12	1:B:115:ARG:NH1	2.25	0.51
1:B:272:ASN:CB	1:B:273:PRO:CD	2.86	0.51
1:B:51:GLU:HB3	1:B:55:ARG:HH12	1.76	0.51
1:A:246:PHE:C	1:A:246:PHE:HD1	2.14	0.51
1:B:551:LYS:NZ	1:B:561:GLU:HB2	2.26	0.51
1:A:246:PHE:C	1:A:246:PHE:CD1	2.85	0.51
1:A:535:ARG:HD3	1:A:565:ASN:O	2.11	0.51
1:B:74:ASN:O	1:B:354:ASN:HA	2.11	0.50
1:B:46:CYS:HA	1:B:52:GLU:OE2	2.12	0.50
1:B:202:LEU:HD11	1:B:206:LEU:HD13	1.94	0.50
1:A:25:GLN:O	1:A:29:GLU:HG3	2.12	0.50
1:B:460:MET:HB2	1:B:478:ASP:O	2.12	0.50
1:A:156:ILE:HD12	1:A:184:LEU:HB2	1.94	0.50
1:B:419:ALA:HB1	1:B:422:SER:HB2	1.94	0.49
1:A:23:LEU:HD11	1:A:45:ILE:HD11	1.93	0.49
1:B:312:ILE:HG22	1:B:328:PRO:HG3	1.95	0.49
1:B:341:VAL:HA	1:B:348:ILE:HG13	1.95	0.49
1:B:249:ARG:HG3	1:B:249:ARG:HH11	1.78	0.48
1:A:99:GLN:HA	1:A:116:TRP:CD1	2.48	0.48
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD23	1:A:32:GLU:HG2	1.95	0.48
1:A:440:GLY:HA3	1:A:584:PHE:CZ	2.48	0.48
1:B:555:ILE:HA	1:B:615:LEU:CD1	2.44	0.47
1:B:613:LEU:CA	1:B:616:LYS:HB3	2.36	0.47
1:A:401:HIS:CD2	1:A:402:PRO:HD2	2.49	0.47
1:B:527:TRP:HH2	1:B:535:ARG:HD2	1.79	0.47
1:A:474:ILE:HA	1:A:474:ILE:HD13	1.72	0.47
1:A:228:ILE:HG21	1:A:245:CYS:HB3	1.96	0.47
1:A:249:ARG:HG2	1:A:485:PHE:O	2.15	0.47
1:B:527:TRP:CH2	1:B:535:ARG:HD2	2.49	0.46
1:B:588:GLU:C	1:B:590:GLU:H	2.18	0.46
1:A:343:THR:HG22	4:A:703:UN8:H43	1.97	0.46
1:A:284:PHE:CE2	1:A:434:GLY:HA3	2.51	0.46
1:B:587:LYS:O	1:B:590:GLU:HB2	2.15	0.46
1:A:221:HIS:NE2	1:A:249:ARG:HD2	2.30	0.46
1:B:532:GLU:OE1	1:B:532:GLU:HA	2.11	0.46
1:A:142:ILE:HG23	1:A:176:MET:HG3	1.97	0.46
1:B:88:ILE:O	1:B:88:ILE:HG23	2.15	0.46
1:A:320:GLN:HA	1:A:320:GLN:OE1	2.16	0.46
1:A:135:LYS:HD2	1:A:135:LYS:HA	1.83	0.46
1:B:614:ALA:HB1	1:B:618:ARG:NH1	2.31	0.46
1:B:433:PHE:O	1:B:514:VAL:HG22	2.16	0.46
1:B:605:PRO:O	1:B:608:ILE:HB	2.14	0.46
1:B:206:LEU:CD2	1:B:209:ASN:HA	2.42	0.46
1:B:192:CYS:HB3	1:B:241:LEU:HD12	1.97	0.46
1:A:44:HIS:CD2	1:A:44:HIS:C	2.89	0.46
1:B:141:VAL:O	1:B:143:PRO:HD3	2.16	0.46
1:B:50:GLU:HG3	1:B:171:ARG:NH2	2.31	0.46
1:B:559:PRO:HB3	1:B:564:LEU:HD21	1.98	0.46
1:A:527:TRP:HA	1:A:528:PRO:HD2	1.75	0.46
1:B:300:LEU:HD21	1:B:535:ARG:NH1	2.31	0.46
1:B:249:ARG:HG3	1:B:249:ARG:NH1	2.31	0.46
1:A:443:LEU:HB2	1:A:577:LEU:HD11	1.97	0.46
1:A:532:GLU:OE1	1:A:532:GLU:HA	2.16	0.45
1:B:247:ALA:HB3	1:B:312:ILE:HD13	1.98	0.45
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.80	0.45
1:B:200:LEU:HA	1:B:201:PRO:C	2.36	0.45
1:A:67:ARG:HD3	1:A:362:GLU:OE1	2.17	0.45
1:B:157:GLY:O	1:B:158:ILE:HD13	2.16	0.45
1:B:51:GLU:CB	1:B:55:ARG:HH12	2.28	0.45
1:A:91:LYS:HG2	1:A:217:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:TRP:HA	1:B:528:PRO:HD2	1.78	0.45
1:B:450:TRP:C	1:B:452:HIS:N	2.69	0.45
1:A:260:TRP:HB2	1:A:315:MET:O	2.17	0.45
1:B:461:ARG:NH1	1:B:588:GLU:OE1	2.50	0.44
1:B:559:PRO:CB	1:B:564:LEU:HD21	2.46	0.44
1:A:320:GLN:O	1:A:507:LYS:HE2	2.17	0.44
1:B:526:LEU:HD11	1:B:576:GLU:OE2	2.16	0.44
1:B:564:LEU:O	1:B:566:LEU:HG	2.17	0.44
1:B:273:PRO:HG2	1:B:274:GLU:OE1	2.17	0.44
1:B:543:ARG:NH1	1:B:543:ARG:CA	2.79	0.44
1:A:88:ILE:HD13	1:A:91:LYS:HD3	2.00	0.44
1:A:264:HIS:CD2	1:A:290:LYS:NZ	2.86	0.44
1:A:115:ARG:HB3	1:A:115:ARG:NH1	2.33	0.44
1:B:21:ASP:HA	1:B:28:ARG:NH1	2.32	0.44
1:B:59:GLN:O	1:B:63:GLU:HG2	2.17	0.44
1:B:297:ASN:C	1:B:297:ASN:HD22	2.19	0.44
1:B:103:VAL:CG1	1:B:114:GLY:HA3	2.47	0.44
1:B:443:LEU:HD21	1:B:536:VAL:HG21	2.00	0.44
1:B:50:GLU:HG3	1:B:171:ARG:HH22	1.82	0.44
1:B:278:LYS:HD3	1:B:544:ILE:CD1	2.48	0.44
1:B:619:ILE:O	1:B:622:MET:HG2	2.17	0.44
1:B:446:GLU:CG	1:B:447:ALA:N	2.81	0.44
1:B:417:ASP:OD1	1:B:418:ALA:N	2.51	0.44
1:B:535:ARG:HD3	1:B:565:ASN:O	2.17	0.43
1:B:615:LEU:O	1:B:619:ILE:HG13	2.18	0.43
1:B:178:THR:N	1:B:179:PRO:CD	2.80	0.43
1:B:617:GLN:C	1:B:619:ILE:H	2.21	0.43
1:A:317:PHE:HA	1:A:322:HIS:O	2.18	0.43
1:B:574:MET:HE3	1:B:574:MET:HB3	1.93	0.43
1:B:222:LEU:N	1:B:222:LEU:HD12	2.34	0.43
1:B:436:ARG:O	1:B:437:ARG:HD2	2.18	0.43
1:B:416:ILE:HA	1:B:416:ILE:HD12	1.89	0.43
1:B:615:LEU:HG	1:B:619:ILE:HD11	2.01	0.43
1:A:601:ASN:HB3	1:A:602:ALA:H	1.60	0.43
1:B:510:LYS:HD2	1:B:512:PHE:HZ	1.84	0.43
1:B:483:ARG:N	1:B:484:PRO:CD	2.82	0.43
1:B:266:LEU:O	1:B:281:ALA:HA	2.18	0.43
1:A:225:ARG:HB3	1:A:227:GLU:OE2	2.18	0.43
1:A:358:THR:O	1:A:404:SER:HB2	2.18	0.43
1:B:553:THR:HB	1:B:554:PRO:CD	2.49	0.43
1:B:130:PHE:CZ	1:B:231:PHE:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:PRO:HG3	1:B:462:SER:HB2	2.01	0.43
1:B:401:HIS:CE1	1:B:403:ASN:HB3	2.54	0.43
1:B:391:TRP:CD2	1:B:399:CYS:HB3	2.53	0.43
1:A:23:LEU:HD11	1:A:45:ILE:CD1	2.49	0.43
1:B:394:GLU:C	1:B:396:GLY:H	2.22	0.43
1:A:192:CYS:HB3	1:A:241:LEU:HD12	2.01	0.43
1:B:339:THR:HG22	1:B:348:ILE:CD1	2.49	0.43
1:B:398:PRO:HB2	1:B:400:ALA:O	2.18	0.43
1:B:443:LEU:HB2	1:B:577:LEU:HD11	2.01	0.42
1:B:267:VAL:CG1	1:B:308:VAL:HB	2.49	0.42
1:B:521:LYS:HG3	1:B:522:GLU:N	2.34	0.42
1:B:272:ASN:HB2	1:B:303:TRP:CZ2	2.53	0.42
1:B:35:ALA:O	1:B:40:PRO:HD2	2.19	0.42
1:B:225:ARG:O	1:B:227:GLU:HG3	2.18	0.42
1:B:113:LEU:HD11	1:B:599:GLN:HB3	2.01	0.42
1:B:461:ARG:HG2	1:B:477:HIS:ND1	2.34	0.42
1:B:401:HIS:CG	1:B:402:PRO:HD2	2.54	0.42
1:A:296:MET:HE3	1:A:305:VAL:HG21	2.02	0.42
1:B:156:ILE:HD13	1:B:180:VAL:HG13	2.01	0.42
1:A:540:MET:O	1:A:544:ILE:HG13	2.19	0.42
1:B:551:LYS:HZ2	1:B:561:GLU:HB2	1.85	0.42
1:A:11:LEU:HD12	1:A:11:LEU:HA	1.77	0.42
1:A:256:LYS:HD2	1:A:488:TYR:CE1	2.54	0.42
1:B:510:LYS:HD2	1:B:512:PHE:CZ	2.55	0.42
1:A:483:ARG:HH11	1:A:483:ARG:HG2	1.84	0.42
1:B:582:LYS:HD2	1:B:622:MET:C	2.40	0.41
1:B:592:ILE:O	1:B:596:LEU:HG	2.20	0.41
1:B:270:ILE:HG23	1:B:270:ILE:O	2.20	0.41
1:A:194:HIS:HA	1:A:230:SER:O	2.20	0.41
1:B:437:ARG:CB	1:B:515:ASN:HD21	2.22	0.41
1:A:221:HIS:ND1	1:A:221:HIS:N	2.68	0.41
1:B:72:TYR:HB2	1:B:75:CYS:HB2	2.02	0.41
1:B:325:ALA:HB2	1:B:428:ILE:HG13	2.03	0.41
1:A:265:MET:HA	1:A:282:ALA:O	2.20	0.41
1:B:588:GLU:HA	1:B:588:GLU:OE1	2.19	0.41
1:B:460:MET:HG3	1:B:480:PHE:N	2.29	0.41
1:A:279:TYR:HB2	1:A:427:PRO:O	2.21	0.41
1:B:446:GLU:HG3	1:B:447:ALA:H	1.85	0.41
1:A:171:ARG:HA	1:A:176:MET:HE2	2.02	0.41
1:A:479:PRO:O	1:A:480:PHE:HB2	2.21	0.41
1:A:413:CYS:HA	1:A:414:PRO:HD2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:PRO:HG2	1:B:608:ILE:CG1	2.51	0.41
1:B:348:ILE:O	1:B:352:GLN:HG2	2.21	0.41
1:B:445:TYR:CE2	1:B:513:HIS:HB3	2.56	0.41
1:B:461:ARG:HG2	1:B:477:HIS:CE1	2.56	0.41
1:B:588:GLU:C	1:B:590:GLU:N	2.73	0.41
1:A:98:GLU:HB2	1:A:101:ASP:OD2	2.21	0.41
1:B:295:MET:CA	1:B:415:ILE:HD11	2.36	0.40
1:B:477:HIS:CD2	1:B:595:TYR:CG	3.09	0.40
1:B:279:TYR:HB2	1:B:427:PRO:O	2.20	0.40
1:A:272:ASN:HB2	1:A:273:PRO:CD	2.50	0.40
1:B:339:THR:HG22	1:B:348:ILE:HD11	2.03	0.40
1:B:318:ASP:OD1	1:B:322:HIS:N	2.54	0.40
1:A:286:SER:O	1:A:287:ALA:HB3	2.21	0.40
1:B:437:ARG:HA	1:B:437:ARG:HD2	1.76	0.40
1:B:501:ALA:HB3	1:B:502:GLN:NE2	2.36	0.40
1:A:336:ALA:O	1:A:337:PRO:C	2.59	0.40
1:B:535:ARG:NH1	1:B:565:ASN:O	2.53	0.40
1:B:543:ARG:CZ	1:B:543:ARG:HB3	2.52	0.40
1:A:561:GLU:O	1:A:562:ASP:HB2	2.22	0.40
1:B:413:CYS:HA	1:B:414:PRO:HD3	1.91	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	596/625 (95%)	571 (96%)	24 (4%)	1 (0%)	52	64
1	B	596/625 (95%)	539 (90%)	49 (8%)	8 (1%)	15	15
All	All	1192/1250 (95%)	1110 (93%)	73 (6%)	9 (1%)	24	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	565	ASN
1	A	236	GLY
1	B	448	LEU
1	B	618	ARG
1	B	243	LYS
1	B	271	THR
1	B	515	ASN
1	B	395	ASP
1	B	570	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	507/523 (97%)	490 (97%)	17 (3%)	44	59
1	B	507/523 (97%)	484 (96%)	23 (4%)	34	46
All	All	1014/1046 (97%)	974 (96%)	40 (4%)	39	53

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	91	LYS
1	A	176	MET
1	A	213	ASN
1	A	221	HIS
1	A	226	ARG
1	A	246	PHE
1	A	304	LYS
1	A	310	ASP
1	A	320	GLN
1	A	392	SER
1	A	474	ILE
1	A	510	LYS
1	A	521	LYS
1	A	522	GLU

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Mol	Chain	Res	Type
1	A	550	THR
1	A	581	SER
1	B	32	GLU
1	B	70	LYS
1	B	103	VAL
1	B	113	LEU
1	B	213	ASN
1	B	226	ARG
1	B	246	PHE
1	B	288	CYS
1	B	295	MET
1	B	297	ASN
1	B	353	LYS
1	B	377	LEU
1	B	395	ASP
1	B	424	GLU
1	B	473	LYS
1	B	474	ILE
1	B	507	LYS
1	B	521	LYS
1	B	532	GLU
1	B	557	TYR
1	B	567	LYS
1	B	588	GLU
1	B	616	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	297	ASN
1	B	10	ASN
1	B	213	ASN
1	B	297	ASN
1	B	502	GLN
1	B	571	HIS

5.3.3 RNA ⓘ

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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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$
3	PEP	A	702	-	5,9,9	1.26	0	8,13,13	1.19	1 (12%)
4	UN8	A	703	-	34,44,44	1.96	6 (17%)	40,64,64	2.65	11 (27%)
3	PEP	B	702	-	5,9,9	1.13	0	8,13,13	2.18	1 (12%)

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
3	PEP	A	702	-	-	0/5/9/9	0/0/0/0
4	UN8	A	703	-	-	0/17/23/23	0/5/5/5
3	PEP	B	702	-	-	0/5/9/9	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	UN8	O1-S1	-3.14	1.40	1.43
4	A	703	UN8	O2-S1	-2.45	1.40	1.43
4	A	703	UN8	C9-C8	2.18	1.42	1.39
4	A	703	UN8	C56-C55	2.93	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	UN8	S1-N4	4.03	1.70	1.63
4	A	703	UN8	C54-N13	7.99	1.40	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	UN8	C55-C56-N51	-9.95	114.66	120.52
3	B	702	PEP	O2-C2-C3	-5.37	113.87	124.73
4	A	703	UN8	C17-N51-C52	-5.20	111.89	118.05
4	A	703	UN8	C7-C8-C9	-3.65	113.99	119.06
4	A	703	UN8	C54-C55-N15	-3.59	106.40	109.55
4	A	703	UN8	O1-S1-N4	-3.01	99.05	106.69
4	A	703	UN8	O1-S1-C1	-2.45	104.25	107.67
4	A	703	UN8	C30-C9-C8	2.21	122.77	120.28
4	A	703	UN8	C6-C7-C8	2.43	123.02	120.28
3	A	702	PEP	P-O2-C2	2.57	128.67	122.96
4	A	703	UN8	C59-N53-C54	3.81	122.89	119.15
4	A	703	UN8	C56-C55-C54	5.48	123.85	119.93
4	A	703	UN8	O1-S1-O2	5.60	126.97	119.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	UN8	2	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.