



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:37 AM GMT

PDB ID : 2P9C
Title : Crystal structure of serine bound G336V mutant of E.coli phosphoglycerate dehydrogenase
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2007-03-24
Resolution : 2.46 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

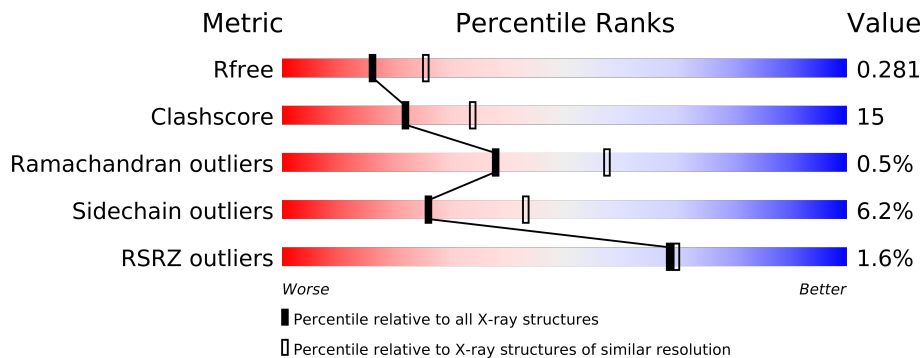
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.46 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}	66092	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	410	
1	B	410	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SER	A	451	-	X
3	SER	A	551	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6296 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

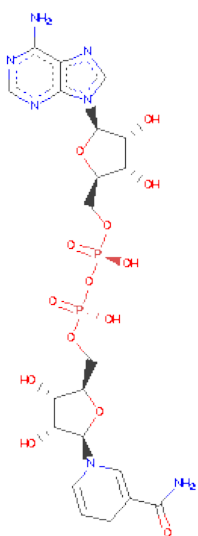
- Molecule 1 is a protein called D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3070	1947	533	582	8			
1	B	405	Total	C	N	O	S	0	0	0
			3070	1947	533	582	8			

There are 10 discrepancies between the modelled and reference sequences:

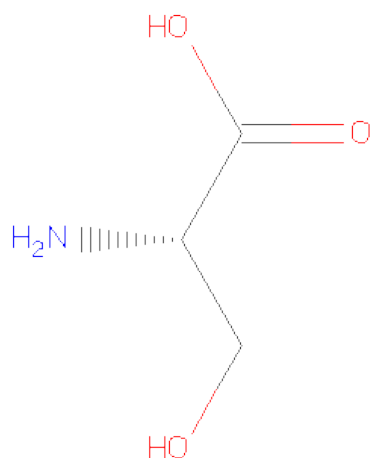
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ALA	CYS	ENGINEERED	UNP P0A9T0
A	83	ALA	CYS	ENGINEERED	UNP P0A9T0
A	250	ALA	CYS	ENGINEERED	UNP P0A9T0
A	282	ALA	CYS	ENGINEERED	UNP P0A9T0
A	336	VAL	GLY	ENGINEERED	UNP P0A9T0
B	81	ALA	CYS	ENGINEERED	UNP P0A9T0
B	83	ALA	CYS	ENGINEERED	UNP P0A9T0
B	250	ALA	CYS	ENGINEERED	UNP P0A9T0
B	282	ALA	CYS	ENGINEERED	UNP P0A9T0
B	336	VAL	GLY	ENGINEERED	UNP P0A9T0

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDEADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SERINE (three-letter code: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			14	6	2	6		

- Molecule 4 is water.

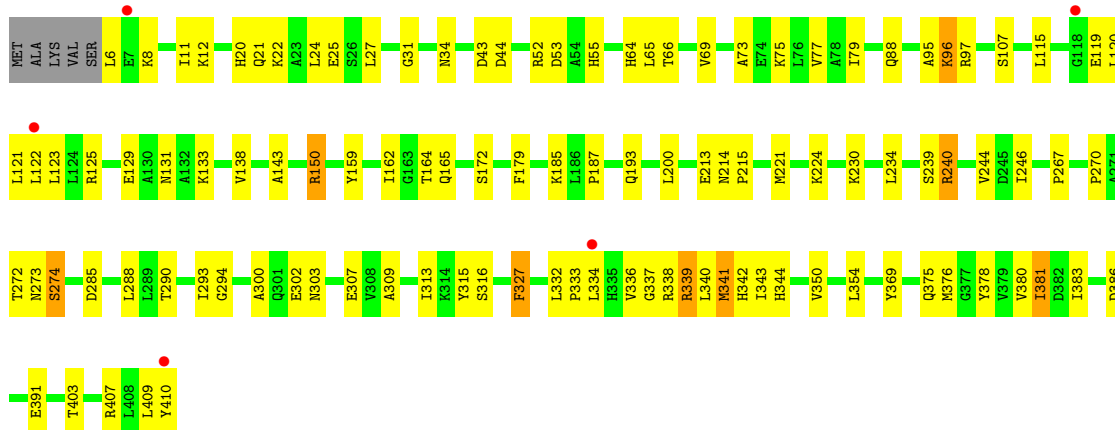
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	B	21	Total 21	O 21	0	0

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.

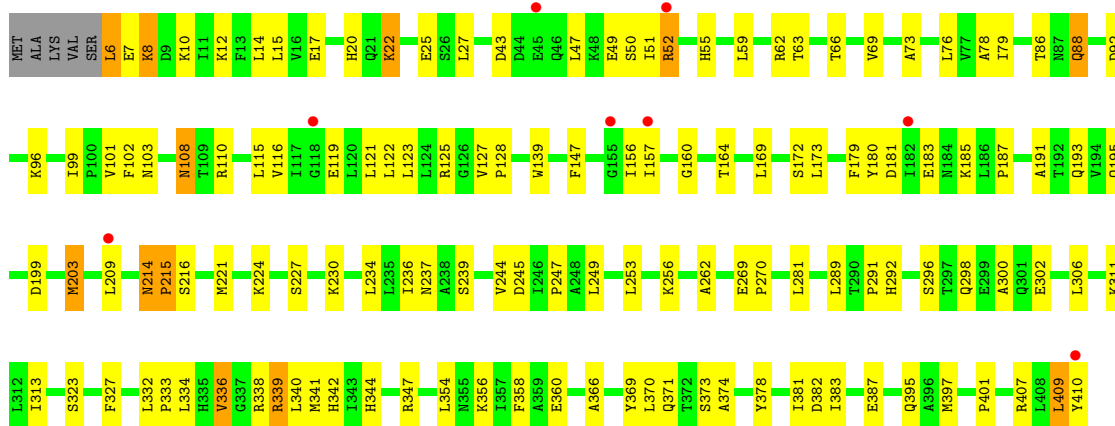
- Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain A: 



- Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.14Å 130.78Å 50.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.46 34.73 – 2.46	Depositor EDS
% Data completeness (in resolution range)	88.6 (35.00-2.46) 88.6 (34.73-2.46)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.219 , 0.281 0.218 , 0.281	Depositor DCC
R_{free} test set	1552 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 30948 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6296	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI

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	0.55	0/3123	0.67	1/4233 (0.0%)
1	B	0.53	0/3123	0.66	0/4233
All	All	0.54	0/6246	0.67	1/8466 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ILE	CB-CA-C	-5.10	101.39	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3070	0	3117	97	0
1	B	3070	0	3117	99	0
2	A	44	0	27	1	0
2	B	44	0	27	1	0
3	A	14	0	8	0	0
4	A	33	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	0	0	0
All	All	6296	0	6296	189	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (189) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:133:LYS:HB3	1:A:138:VAL:HG13	1.29	1.10
1:B:12:LYS:H	1:B:55:HIS:CD2	1.76	1.03
1:A:133:LYS:HB3	1:A:138:VAL:CG1	1.90	1.01
1:B:12:LYS:H	1:B:55:HIS:HD2	1.04	1.01
1:B:341:MET:HG2	1:B:409:LEU:HD21	1.49	0.92
1:B:88:GLN:N	1:B:88:GLN:HE21	1.66	0.91
1:B:160:GLY:O	1:B:164:THR:HG23	1.71	0.91
1:B:88:GLN:H	1:B:88:GLN:NE2	1.69	0.89
1:A:339:ARG:HD3	1:A:380:VAL:CG1	2.02	0.88
1:A:22:LYS:HD2	1:A:302:GLU:HG3	1.56	0.87
1:B:27:LEU:HD23	1:B:313:ILE:HD11	1.59	0.84
1:A:354:LEU:HD21	1:A:381:ILE:HD11	1.64	0.79
1:A:77:VAL:HG12	1:A:315:TYR:HE2	1.45	0.79
1:A:133:LYS:CB	1:A:138:VAL:CG1	2.61	0.77
1:A:133:LYS:HG2	1:A:138:VAL:HG11	1.67	0.77
1:A:354:LEU:HD21	1:A:381:ILE:CD1	2.15	0.75
1:B:358:PHE:CE2	1:B:383:ILE:HD13	2.21	0.75
1:B:354:LEU:CD1	1:B:397:MET:HG2	2.17	0.74
1:A:12:LYS:H	1:A:55:HIS:HD2	1.33	0.73
1:B:338:ARG:HD2	1:B:410:TYR:OXT	1.89	0.73
1:B:92:ASP:O	1:B:96:LYS:HG3	1.88	0.73
1:A:354:LEU:CD2	1:A:381:ILE:HD11	2.20	0.72
1:B:88:GLN:H	1:B:88:GLN:HE21	0.83	0.72
1:A:214:ASN:HB2	1:A:215:PRO:HD2	1.73	0.71
1:B:342:HIS:HD2	1:B:344:HIS:ND1	1.89	0.70
1:A:342:HIS:HD2	1:A:344:HIS:ND1	1.90	0.69
1:B:332:LEU:HD12	1:B:333:PRO:HD2	1.75	0.69
1:A:341:MET:CE	1:A:343:ILE:HG13	2.25	0.67
1:B:110:ARG:HH12	1:B:169:LEU:HD21	1.59	0.67
1:A:96:LYS:HE3	1:A:375:GLN:NE2	2.09	0.67
1:A:185:LYS:O	1:A:187:PRO:HD3	1.95	0.67
1:B:125:ARG:HD3	1:B:147:PHE:O	1.94	0.66
1:B:12:LYS:N	1:B:55:HIS:HD2	1.86	0.65
1:B:103:ASN:O	1:B:311:LYS:HE3	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:332:LEU:HD12	1:A:333:PRO:HD2	1.77	0.65
1:A:159:TYR:CE2	1:A:164:THR:HG22	2.32	0.64
1:A:272:THR:HG22	1:A:273:ASN:N	2.12	0.64
1:A:290:THR:HB	1:A:293:ILE:HD11	1.80	0.63
1:B:214:ASN:C	1:B:214:ASN:HD22	2.01	0.62
1:A:120:LEU:C	1:A:120:LEU:HD12	2.20	0.62
1:B:76:LEU:HD23	1:B:99:ILE:HD13	1.80	0.62
1:B:237:ASN:ND2	1:B:239:SER:OG	2.30	0.61
1:A:213:GLU:OE1	1:A:240:ARG:HD2	2.00	0.61
1:A:172:SER:HB3	1:B:172:SER:HB3	1.83	0.60
1:B:7:GLU:HG2	1:B:7:GLU:O	2.01	0.60
1:B:108:ASN:HB3	1:B:300:ALA:HB1	1.82	0.59
1:A:96:LYS:HE3	1:A:375:GLN:HE22	1.66	0.59
1:B:79:ILE:HB	1:B:101:VAL:HG22	1.83	0.59
1:B:12:LYS:N	1:B:55:HIS:CD2	2.60	0.59
1:A:246:ILE:HD12	1:A:267:PRO:CD	2.32	0.59
1:B:6:LEU:N	1:B:7:GLU:HB3	2.17	0.58
1:B:354:LEU:HD21	1:B:381:ILE:HD11	1.85	0.58
1:A:133:LYS:O	1:A:138:VAL:HG12	2.03	0.58
1:A:66:THR:HG22	1:A:69:VAL:HG23	1.86	0.58
1:A:239:SER:OG	1:A:240:ARG:N	2.33	0.58
1:B:17:GLU:OE1	1:B:62:ARG:HB2	2.04	0.58
1:B:115:LEU:O	1:B:119:GLU:HG3	2.04	0.58
1:A:341:MET:HB2	1:A:409:LEU:HD11	1.85	0.57
1:A:338:ARG:HD2	1:A:410:TYR:OXT	2.03	0.57
1:A:272:THR:HG22	1:A:274:SER:H	1.69	0.57
1:B:66:THR:HG22	1:B:69:VAL:HG23	1.84	0.57
1:A:354:LEU:CD2	1:A:381:ILE:CD1	2.82	0.57
1:A:341:MET:HE1	1:A:343:ILE:HG13	1.87	0.57
1:B:110:ARG:NH1	1:B:169:LEU:HD21	2.19	0.56
1:B:341:MET:CG	1:B:409:LEU:HD21	2.28	0.56
1:B:185:LYS:H	1:B:193:GLN:HE22	1.53	0.56
1:B:373:SER:O	1:B:374:ALA:C	2.43	0.56
1:B:245:ASP:OD1	1:B:247:PRO:HD2	2.06	0.56
1:A:341:MET:HG2	1:A:378:TYR:HE1	1.72	0.55
1:A:342:HIS:CE1	1:A:403:THR:OG1	2.60	0.55
1:A:122:LEU:HD12	1:B:122:LEU:HD12	1.88	0.55
1:B:342:HIS:CD2	1:B:344:HIS:ND1	2.73	0.55
1:A:341:MET:HE3	1:A:343:ILE:HG13	1.89	0.54
1:B:108:ASN:HD21	2:B:550:NAI:H5N	1.73	0.54
1:B:332:LEU:O	1:B:339:ARG:NH1	2.36	0.54
1:A:120:LEU:HD12	1:A:121:LEU:N	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:THR:HG22	1:A:273:ASN:H	1.70	0.53
1:B:22:LYS:HA	1:B:25:GLU:HG2	1.91	0.53
1:A:12:LYS:H	1:A:55:HIS:CD2	2.22	0.53
1:B:224:LYS:O	1:B:227:SER:OG	2.27	0.53
1:B:160:GLY:O	1:B:164:THR:CG2	2.53	0.53
1:A:316:SER:HA	1:A:407:ARG:HH22	1.72	0.53
1:B:338:ARG:NH1	1:B:387:GLU:HG2	2.24	0.53
1:A:342:HIS:HE1	1:A:403:THR:OG1	1.92	0.52
1:A:221:MET:HB2	1:A:244:VAL:HG22	1.90	0.52
1:B:22:LYS:HG3	1:B:302:GLU:HG3	1.92	0.52
1:B:123:LEU:HD11	1:B:262:ALA:HB2	1.90	0.52
1:A:341:MET:HB2	1:A:409:LEU:CD1	2.39	0.52
1:A:143:ALA:HB2	1:B:296:SER:HB3	1.90	0.52
1:A:339:ARG:HD3	1:A:380:VAL:HG11	1.89	0.52
1:B:116:VAL:HG13	1:B:236:ILE:HD13	1.92	0.52
1:A:327:PHE:HZ	1:A:343:ILE:HD13	1.75	0.52
1:A:64:HIS:HD2	1:A:88:GLN:HB2	1.74	0.51
1:A:53:ASP:HA	1:A:75:LYS:HE3	1.93	0.51
1:B:341:MET:HE3	1:B:407:ARG:NH1	2.25	0.51
1:B:52:ARG:HA	1:B:73:ALA:HA	1.91	0.51
1:B:347:ARG:NH1	1:B:401:PRO:HB2	2.25	0.51
1:A:21:GLN:O	1:A:25:GLU:HG3	2.11	0.50
1:B:125:ARG:HB3	1:B:125:ARG:HH11	1.77	0.50
1:B:20:HIS:CE1	1:B:302:GLU:HB2	2.47	0.50
1:A:27:LEU:HA	1:A:313:ILE:HD11	1.93	0.50
1:B:127:VAL:N	1:B:128:PRO:CD	2.75	0.50
1:A:43:ASP:O	1:A:44:ASP:C	2.49	0.49
1:A:65:LEU:HD23	1:A:79:ILE:HD13	1.93	0.49
1:B:298:GLN:HA	1:B:298:GLN:NE2	2.28	0.49
1:B:249:LEU:HD23	1:B:281:LEU:HD11	1.94	0.49
1:B:409:LEU:HD23	1:B:409:LEU:N	2.28	0.49
1:A:332:LEU:HB3	1:A:339:ARG:NH1	2.29	0.48
1:A:354:LEU:HD21	1:A:381:ILE:HD12	1.94	0.48
1:A:316:SER:O	1:A:407:ARG:NH2	2.46	0.48
1:A:159:TYR:CZ	1:A:164:THR:HG22	2.48	0.48
1:A:179:PHE:CZ	1:A:193:GLN:HB2	2.48	0.48
1:A:339:ARG:HD3	1:A:380:VAL:HG12	1.92	0.48
1:B:214:ASN:HB2	1:B:215:PRO:HD2	1.96	0.48
1:B:156:ILE:O	1:B:179:PHE:HA	2.14	0.48
1:A:300:ALA:HA	1:A:303:ASN:HD22	1.79	0.47
1:A:131:ASN:HA	1:B:289:LEU:O	2.14	0.47
1:B:6:LEU:HA	1:B:7:GLU:C	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:133:LYS:HG2	1:A:138:VAL:CG1	2.40	0.47
1:B:341:MET:CE	1:B:378:TYR:OH	2.63	0.47
1:B:187:PRO:HB3	1:B:191:ALA:O	2.15	0.47
1:B:108:ASN:C	1:B:108:ASN:HD22	2.19	0.46
1:A:150:ARG:NH1	1:B:110:ARG:HG2	2.30	0.46
1:A:343:ILE:HG12	1:A:378:TYR:CD1	2.50	0.46
1:B:221:MET:HB2	1:B:244:VAL:HG22	1.97	0.46
1:A:133:LYS:CG	1:A:138:VAL:CG1	2.94	0.46
1:B:370:LEU:HG	1:B:371:GLN:N	2.29	0.46
1:B:7:GLU:O	1:B:7:GLU:CG	2.64	0.46
1:B:22:LYS:HE3	1:B:25:GLU:OE1	2.15	0.46
1:B:78:ALA:HA	1:B:99:ILE:HG23	1.97	0.45
1:A:200:LEU:C	1:A:200:LEU:HD23	2.37	0.45
1:A:66:THR:CG2	1:A:69:VAL:HG23	2.47	0.45
1:B:336:VAL:HG11	1:B:366:ALA:CB	2.46	0.45
1:A:119:GLU:HG2	1:A:288:LEU:HD13	1.99	0.45
1:A:52:ARG:HE	1:A:52:ARG:HB3	1.65	0.45
1:B:157:ILE:HB	1:B:209:LEU:HD23	1.98	0.45
1:A:341:MET:CG	1:A:378:TYR:HE1	2.30	0.45
1:A:27:LEU:HD12	1:A:313:ILE:HD11	1.99	0.45
1:B:66:THR:HG23	1:B:69:VAL:H	1.81	0.44
1:B:14:LEU:O	1:B:15:LEU:HD23	2.16	0.44
1:B:370:LEU:HD12	1:B:378:TYR:O	2.18	0.44
1:B:354:LEU:CD2	1:B:381:ILE:HD11	2.45	0.44
1:A:11:ILE:O	1:A:34:ASN:HB3	2.18	0.44
1:A:341:MET:O	1:A:341:MET:HE2	2.18	0.44
1:A:343:ILE:HG12	1:A:378:TYR:HD1	1.83	0.44
1:A:246:ILE:HD12	1:A:267:PRO:HD3	1.99	0.44
1:B:123:LEU:HB3	1:B:234:LEU:HD13	1.99	0.44
1:A:107:SER:HB3	1:A:303:ASN:HB3	1.99	0.43
1:A:8:LYS:HB3	1:A:31:GLY:O	2.18	0.43
1:A:272:THR:CG2	1:A:273:ASN:N	2.80	0.43
1:B:199:ASP:O	1:B:203:MET:HG3	2.18	0.43
1:A:270:PRO:HG2	1:B:139:TRP:CG	2.53	0.43
1:A:115:LEU:HD22	1:A:294:GLY:HA2	1.99	0.43
1:B:334:LEU:N	1:B:334:LEU:HD12	2.33	0.43
1:A:123:LEU:HB3	1:A:234:LEU:HD22	2.00	0.43
1:A:337:GLY:HA3	1:A:383:ILE:O	2.18	0.43
1:B:347:ARG:NH1	1:B:401:PRO:CB	2.81	0.43
1:B:214:ASN:O	1:B:216:SER:N	2.51	0.43
1:A:95:ALA:O	1:A:376:MET:CE	2.66	0.43
1:A:20:HIS:ND1	1:A:22:LYS:HG3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:47:LEU:O	1:B:51:ILE:HG22	2.19	0.43
1:B:356:LYS:O	1:B:360:GLU:HG3	2.18	0.42
1:B:121:LEU:O	1:B:125:ARG:HG2	2.19	0.42
1:B:86:THR:C	1:B:88:GLN:NE2	2.72	0.42
1:A:27:LEU:HD13	1:A:309:ALA:HB1	2.01	0.42
1:A:342:HIS:CD2	1:A:344:HIS:ND1	2.79	0.42
1:B:59:LEU:HD12	1:B:63:THR:HB	2.02	0.42
1:B:338:ARG:CD	1:B:410:TYR:OXT	2.64	0.42
1:B:338:ARG:O	1:B:382:ASP:HA	2.19	0.42
1:A:270:PRO:HG2	1:B:139:TRP:CD2	2.55	0.41
1:A:341:MET:HE2	1:A:341:MET:C	2.40	0.41
1:B:291:PRO:O	1:B:292:HIS:C	2.59	0.41
1:B:180:TYR:HE2	1:B:195:GLN:O	2.03	0.41
1:B:66:THR:HG22	1:B:69:VAL:CG2	2.50	0.41
1:A:334:LEU:HD12	1:A:334:LEU:N	2.36	0.41
1:A:344:HIS:CG	1:A:350:VAL:HG11	2.55	0.41
1:A:24:LEU:H	1:A:24:LEU:HD12	1.86	0.41
1:A:95:ALA:O	1:A:376:MET:HE1	2.21	0.41
1:A:341:MET:HG2	1:A:378:TYR:CE1	2.54	0.41
1:A:66:THR:HG23	1:A:69:VAL:H	1.86	0.41
1:B:102:PHE:HB3	1:B:311:LYS:HD2	2.03	0.41
1:B:179:PHE:CZ	1:B:193:GLN:HB2	2.55	0.41
1:B:8:LYS:C	1:B:10:LYS:H	2.24	0.41
1:B:269:GLU:O	1:B:270:PRO:C	2.59	0.40
1:B:181:ASP:HB3	1:B:183:GLU:O	2.21	0.40
1:A:332:LEU:HA	1:A:333:PRO:HD2	1.82	0.40
1:A:162:ILE:HD12	2:A:450:NAI:O5D	2.22	0.40
1:B:340:LEU:HD22	1:B:397:MET:SD	2.61	0.40
1:A:129:GLU:HA	1:A:285:ASP:HB3	2.04	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	403/410 (98%)	376 (93%)	25 (6%)	2 (0%)	38	57
1	B	403/410 (98%)	374 (93%)	27 (7%)	2 (0%)	38	57
All	All	806/820 (98%)	750 (93%)	52 (6%)	4 (0%)	38	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	ASP
1	A	73	ALA
1	B	8	LYS
1	B	215	PRO

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	324/328 (99%)	306 (94%)	18 (6%)	30	49
1	B	324/328 (99%)	302 (93%)	22 (7%)	22	37
All	All	648/656 (99%)	608 (94%)	40 (6%)	26	43

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

Mol	Chain	Res	Type
1	A	6	LEU
1	A	96	LYS
1	A	97	ARG
1	A	125	ARG
1	A	150	ARG
1	A	165	GLN
1	A	224	LYS
1	A	230	LYS
1	A	240	ARG
1	A	274	SER
1	A	307	GLU
1	A	327	PHE
1	A	336	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	339	ARG
1	A	340	LEU
1	A	341	MET
1	A	369	TYR
1	A	391	GLU
1	B	6	LEU
1	B	22	LYS
1	B	43	ASP
1	B	49	GLU
1	B	50	SER
1	B	52	ARG
1	B	88	GLN
1	B	108	ASN
1	B	173	LEU
1	B	203	MET
1	B	214	ASN
1	B	230	LYS
1	B	253	LEU
1	B	256	LYS
1	B	306	LEU
1	B	323	SER
1	B	327	PHE
1	B	336	VAL
1	B	339	ARG
1	B	369	TYR
1	B	395	GLN
1	B	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	64	HIS
1	A	87	ASN
1	A	303	ASN
1	A	335	HIS
1	A	342	HIS
1	A	375	GLN
1	A	395	GLN
1	B	55	HIS
1	B	88	GLN
1	B	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	193	GLN
1	B	214	ASN
1	B	237	ASN
1	B	298	GLN
1	B	342	HIS
1	B	395	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 ligands are 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	NAI	A	450	-	48,48,48	1.71	8 (16%)	73,73,73	1.83	12 (16%)
3	SER	A	451	-	6,6,6	1.04	1 (16%)	7,7,7	1.93	2 (28%)
3	SER	A	551	-	6,6,6	0.93	1 (16%)	7,7,7	1.65	2 (28%)
2	NAI	B	550	-	48,48,48	1.80	7 (14%)	73,73,73	1.78	13 (17%)

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	NAI	A	450	-	-	0/30/72/72	0/3/5/5
3	SER	A	451	-	-	0/6/6/6	0/0/0/0
3	SER	A	551	-	-	0/6/6/6	0/0/0/0
2	NAI	B	550	-	-	0/30/72/72	0/3/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	550	NAI	O7N-C7N	6.49	1.41	1.24
2	A	450	NAI	O7N-C7N	5.78	1.39	1.24
2	A	450	NAI	C4N-C3N	-5.56	1.39	1.50
2	B	550	NAI	C4N-C3N	-5.53	1.39	1.50
2	B	550	NAI	C4N-C5N	-4.37	1.39	1.49
2	A	450	NAI	C4N-C5N	-4.25	1.39	1.49
2	B	550	NAI	C2A-N3A	3.38	1.38	1.32
2	A	450	NAI	C2A-N3A	3.35	1.38	1.32
2	B	550	NAI	C6N-C5N	3.00	1.39	1.33
2	B	550	NAI	C2N-C3N	2.88	1.40	1.34
2	A	450	NAI	C2A-N1A	2.77	1.39	1.33
2	A	450	NAI	C6N-C5N	2.64	1.38	1.33
2	B	550	NAI	C2A-N1A	2.52	1.38	1.33
2	A	450	NAI	C2N-C3N	2.48	1.39	1.34
3	A	551	SER	OXT-C	-2.16	1.22	1.30
2	A	450	NAI	O4D-C4D	-2.12	1.40	1.45
3	A	451	SER	OXT-C	-2.04	1.23	1.30

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	NAI	N3A-C2A-N1A	-11.04	119.48	128.71
2	B	550	NAI	N3A-C2A-N1A	-9.60	120.69	128.71
2	B	550	NAI	N3A-C4A-N9A	4.31	133.21	125.43
2	B	550	NAI	PN-O3-PA	-3.92	120.19	131.68
3	A	451	SER	OXT-C-O	-3.76	115.56	124.07
2	A	450	NAI	N3A-C4A-N9A	3.45	131.66	125.43
3	A	551	SER	OXT-C-O	-3.38	116.43	124.07
2	A	450	NAI	C3N-C7N-N7N	3.24	123.72	117.48
3	A	451	SER	OXT-C-CA	2.84	123.25	116.88
2	A	450	NAI	C5N-C4N-C3N	2.75	120.06	112.60
2	A	450	NAI	O7N-C7N-C3N	-2.71	115.42	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	550	NAI	N7A-C8A-N9A	-2.67	106.82	114.36
2	B	550	NAI	C8A-N9A-C4A	2.66	108.93	106.90
2	B	550	NAI	C5A-C4A-N3A	-2.65	119.94	125.70
2	B	550	NAI	C4A-C5A-N7A	-2.56	107.33	109.52
2	B	550	NAI	C5N-C4N-C3N	2.50	119.37	112.60
2	A	450	NAI	PN-O3-PA	-2.42	124.60	131.68
3	A	551	SER	OXT-C-CA	2.41	122.29	116.88
2	B	550	NAI	O4D-C1D-N1N	2.35	113.04	108.05
2	B	550	NAI	O3-PN-O5D	-2.31	93.07	103.41
2	A	450	NAI	C3N-C2N-N1N	-2.28	119.81	123.05
2	A	450	NAI	N7A-C8A-N9A	-2.27	107.93	114.36
2	B	550	NAI	C4N-C3N-C2N	-2.24	118.95	121.68
2	A	450	NAI	C2A-N3A-C4A	2.17	120.18	114.01
2	B	550	NAI	C2A-N3A-C4A	2.09	119.97	114.01
2	B	550	NAI	C8A-N7A-C5A	2.09	110.06	103.58
2	A	450	NAI	C4A-C5A-N7A	-2.05	107.77	109.52
2	A	450	NAI	O4D-C1D-C2D	-2.03	101.95	106.60
2	A	450	NAI	C5A-C4A-N3A	-2.01	121.32	125.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	405/410 (98%)	-0.16	5 (1%) 75 76	30, 43, 59, 80	4 (0%)
1	B	405/410 (98%)	-0.04	8 (1%) 62 63	31, 45, 61, 89	4 (0%)
All	All	810/820 (98%)	-0.10	13 (1%) 68 70	30, 44, 60, 89	8 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	TYR	5.7
1	A	410	TYR	3.5
1	B	155	GLY	2.8
1	B	182	ILE	2.6
1	B	52	ARG	2.6
1	B	45	GLU	2.4
1	A	118	GLY	2.3
1	A	122	LEU	2.2
1	B	157	ILE	2.2
1	B	118	GLY	2.1
1	A	334	LEU	2.1
1	B	209	LEU	2.1
1	A	7	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SER	A	551	7/7	0.23	3.26	37,38,54,58	0
3	SER	A	451	7/7	0.22	2.66	25,31,41,45	0
2	NAI	A	450	44/44	0.15	0.32	30,40,46,52	0
2	NAI	B	550	44/44	0.17	0.07	33,48,55,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.