



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:23 PM UTC

PDB ID : 1XYG / pdb_00001xyg
Title : X-RAY STRUCTURE OF GENE PRODUCT FROM ARABIDOPSIS
THALIANA AT2G19940
Authors : Wesenberg, G.E.; Phillips Jr., G.N.; Bitto, E.; Bingman, C.A.; Allard, S.T.M.;
Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2004-11-09
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

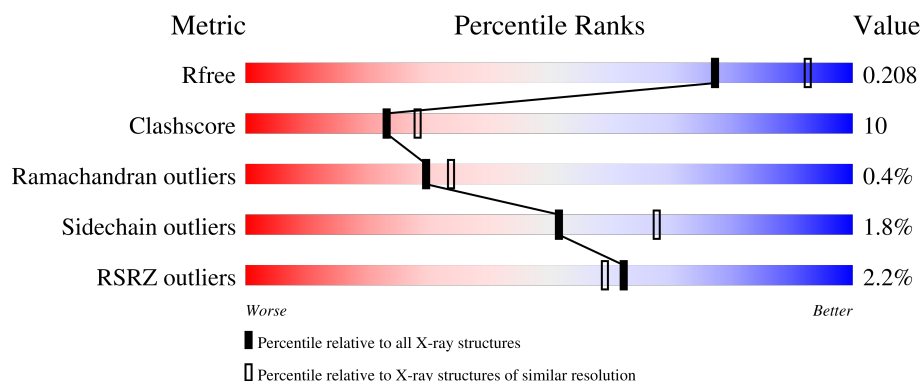
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	2% 73% 23% .
1	B	359	% 74% 21% ..
1	C	359	3% 66% 28% ..
1	D	359	3% 77% 18% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11676 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 putative N-acetyl-gamma-glutamyl-phosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	B	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	C	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			
1	D	345	Total	C	N	O	S	0	0	0
			2680	1700	467	501	12			

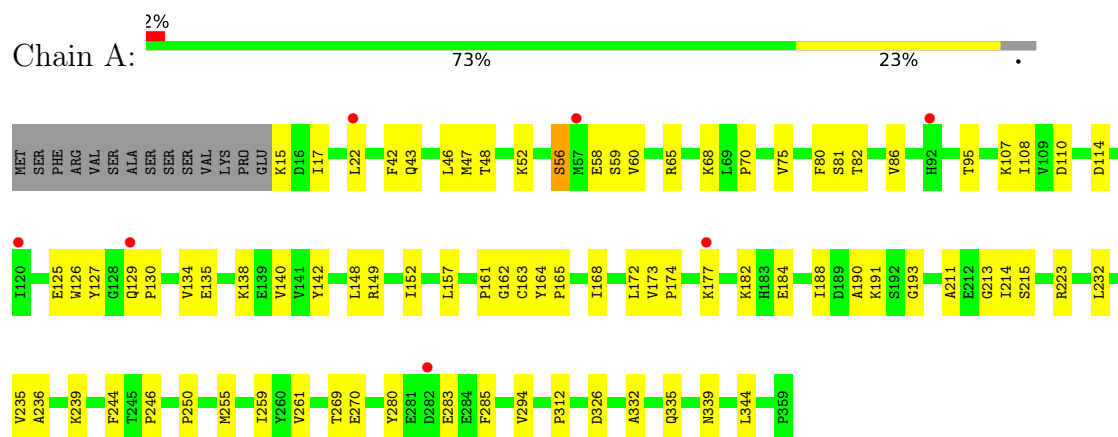
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	262	Total	O	0	0
			262	262		
2	B	227	Total	O	0	0
			227	227		
2	C	226	Total	O	0	0
			226	226		
2	D	241	Total	O	0	0
			241	241		

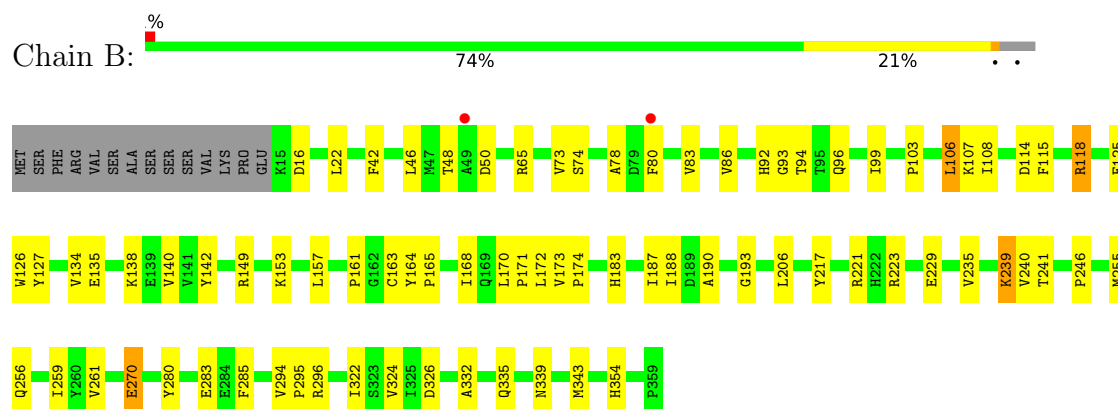
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

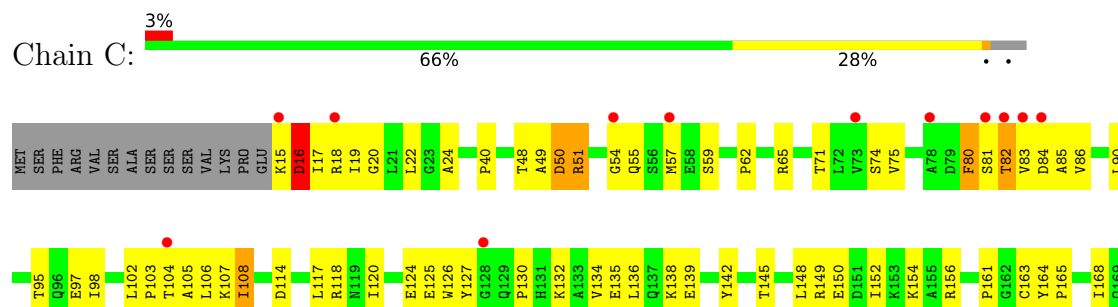
- Molecule 1: putative N-acetyl-gamma-glutamyl-phosphate reductase

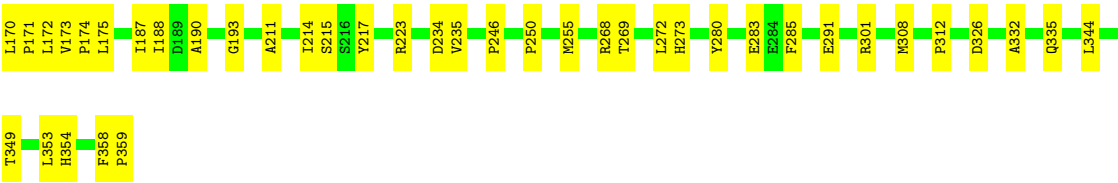


- Molecule 1: putative N-acetyl-gamma-glutamyl-phosphate reductase

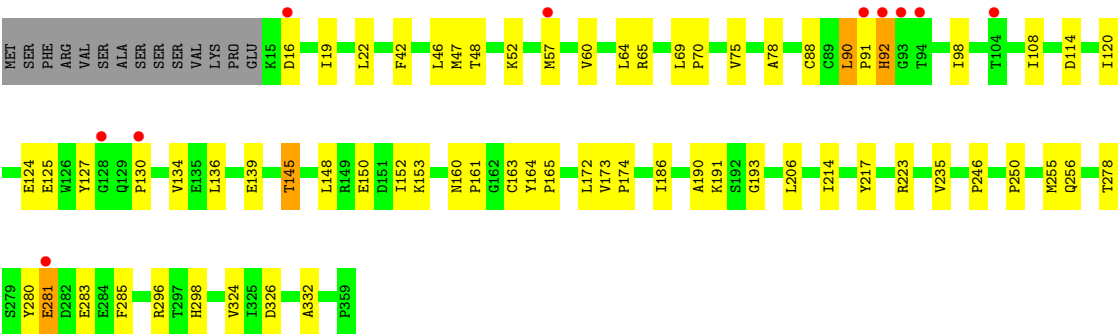
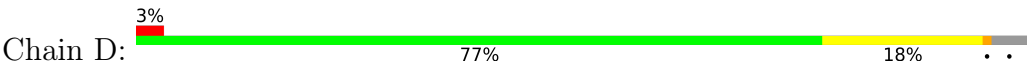


- Molecule 1: putative N-acetyl-gamma-glutamyl-phosphate reductase





- Molecule 1: putative N-acetyl-gamma-glutamyl-phosphate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.60Å 107.07Å 85.75Å 90.00° 118.88° 90.00°	Depositor
Resolution (Å)	27.54 – 2.19 27.54 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.9 (27.54-2.19) 92.9 (27.54-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.208 0.187 , 0.208	Depositor DCC
R_{free} test set	3240 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.018 for h,-k,-h-l 0.017 for -h-l,-k,l 0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11676	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	1/2734 (0.0%)	1.00	14/3709 (0.4%)
1	B	0.41	0/2734	0.97	11/3709 (0.3%)
1	C	0.41	0/2734	1.01	19/3709 (0.5%)
1	D	0.42	0/2734	0.98	13/3709 (0.4%)
All	All	0.42	1/10936 (0.0%)	0.99	57/14836 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	LYS	N-CA	5.34	1.52	1.45

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	HIS	N-CA-C	-8.12	97.78	109.96
1	C	172	LEU	N-CA-C	7.50	119.53	111.36
1	D	172	LEU	N-CA-C	7.33	119.35	111.36
1	B	172	LEU	N-CA-C	7.32	119.33	111.36
1	A	326	ASP	N-CA-C	-7.05	97.76	108.96
1	A	172	LEU	N-CA-C	7.03	119.02	111.36
1	C	326	ASP	N-CA-C	-6.88	98.01	108.96
1	B	114	ASP	N-CA-C	6.80	120.68	112.38
1	A	81	SER	N-CA-C	-6.64	105.16	113.20
1	C	80	PHE	N-CA-C	6.57	120.91	113.02
1	D	326	ASP	N-CA-C	-6.54	97.87	108.41
1	B	326	ASP	N-CA-C	-6.50	97.95	108.41
1	A	285	PHE	N-CA-C	6.50	121.20	113.28
1	A	58	GLU	N-CA-C	-6.46	104.65	112.54
1	C	50	ASP	N-CA-C	6.38	117.90	111.07
1	C	114	ASP	N-CA-C	6.33	120.11	112.38
1	D	19	ILE	N-CA-C	6.30	117.67	108.53
1	D	114	ASP	N-CA-C	6.25	120.01	112.38
1	B	285	PHE	N-CA-C	6.24	120.89	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	ILE	N-CA-C	6.24	116.84	108.11
1	C	16	ASP	N-CA-C	6.18	123.97	110.80
1	C	285	PHE	N-CA-C	6.17	120.81	113.28
1	A	108	ILE	N-CA-C	6.14	116.70	108.11
1	C	17	ILE	N-CA-C	6.09	117.07	108.36
1	D	16	ASP	N-CA-C	5.95	120.40	113.20
1	D	285	PHE	N-CA-C	5.90	120.47	113.28
1	C	82	THR	N-CA-C	-5.86	106.26	113.41
1	C	95	THR	N-CA-C	5.81	118.49	111.40
1	C	105	ALA	N-CA-C	-5.71	106.53	112.93
1	B	107	LYS	N-CA-C	-5.68	100.02	109.46
1	C	81	SER	N-CA-C	-5.66	106.60	112.93
1	B	108	ILE	N-CA-C	5.65	116.02	108.11
1	D	145	THR	N-CA-C	5.59	120.53	111.37
1	A	294	VAL	N-CA-C	5.56	113.38	107.76
1	C	145	THR	N-CA-C	5.51	120.41	111.37
1	D	108	ILE	N-CA-C	5.40	115.67	108.11
1	B	294	VAL	N-CA-C	5.39	113.21	107.76
1	A	56	SER	N-CA-C	-5.37	102.53	110.48
1	D	134	VAL	N-CA-C	5.35	115.98	110.36
1	A	114	ASP	N-CA-C	5.33	119.27	112.34
1	C	134	VAL	N-CA-C	5.32	115.95	110.36
1	B	193	GLY	N-CA-C	-5.31	105.75	112.54
1	B	16	ASP	N-CA-C	5.29	116.73	111.07
1	A	17	ILE	N-CA-C	5.28	115.56	108.17
1	B	134	VAL	N-CA-C	5.26	115.88	110.36
1	C	120	ILE	N-CA-C	5.24	115.45	110.42
1	C	19	ILE	N-CA-C	5.23	116.11	108.53
1	D	193	GLY	N-CA-C	-5.21	105.86	112.54
1	C	193	GLY	N-CA-C	-5.19	105.89	112.54
1	A	211	ALA	N-CA-C	5.16	117.52	110.24
1	B	94	THR	N-CA-C	-5.11	107.02	114.12
1	C	211	ALA	N-CA-C	5.10	117.43	110.24
1	A	134	VAL	N-CA-C	5.03	115.64	110.36
1	A	107	LYS	N-CA-C	-5.01	101.14	109.46
1	D	90	LEU	CA-C-N	5.01	124.91	119.85
1	D	90	LEU	C-N-CA	5.01	124.91	119.85
1	A	193	GLY	N-CA-C	-5.00	106.13	112.54

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	2680	0	2718	57	0
1	B	2680	0	2718	56	0
1	C	2680	0	2718	78	0
1	D	2680	0	2718	42	0
2	A	262	0	0	5	0
2	B	227	0	0	6	0
2	C	226	0	0	4	0
2	D	241	0	0	6	0
All	All	11676	0	10872	223	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 10.

All (223) 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:C:51:ARG:H	1:C:51:ARG:HD2	1.16	1.11
1:A:135:GLU:OE1	1:A:138:LYS:HE2	1.69	0.93
1:B:103:PRO:HG2	1:B:106:LEU:HD22	1.54	0.88
1:C:118:ARG:HH22	1:C:234:ASP:CG	1.82	0.87
1:A:177:LYS:HG3	1:A:235:VAL:CG2	2.05	0.85
1:D:90:LEU:HB3	1:D:91:PRO:HD2	1.58	0.85
1:A:48:THR:HG21	1:A:75:VAL:HG22	1.60	0.84
1:A:215:SER:HB3	1:D:296:ARG:HG3	1.63	0.79
1:C:15:LYS:HD3	1:C:40:PRO:O	1.86	0.76
1:C:48:THR:HG21	1:C:75:VAL:HG22	1.67	0.76
1:B:22:LEU:HA	1:B:48:THR:OG1	1.86	0.75
1:C:15:LYS:HG2	1:C:16:ASP:H	1.52	0.75
1:C:71:THR:OG1	2:C:533:HOH:O	2.04	0.75
1:C:118:ARG:NH2	1:C:234:ASP:OD2	2.20	0.73
1:C:22:LEU:HD11	1:C:80:PHE:HE2	1.53	0.73
1:C:51:ARG:H	1:C:51:ARG:CD	1.94	0.73
1:A:239:LYS:HE3	2:A:608:HOH:O	1.89	0.73
1:D:75:VAL:HG23	2:D:401:HOH:O	1.88	0.72
1:B:73:VAL:HG12	1:B:74:SER:N	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:VAL:HG13	1:D:235:VAL:HG21	1.72	0.71
1:C:22:LEU:HA	1:C:48:THR:HB	1.74	0.70
1:B:173:VAL:HG13	1:B:235:VAL:HG21	1.73	0.69
1:B:22:LEU:HD11	1:B:80:PHE:HE1	1.56	0.69
1:A:163:CYS:SG	1:A:255:MET:HE1	2.33	0.69
1:C:22:LEU:HD11	1:C:80:PHE:CE2	2.28	0.69
1:C:161:PRO:HG2	1:C:335:GLN:NE2	2.09	0.67
1:D:52:LYS:HD3	1:D:60:VAL:HG22	1.76	0.67
1:C:150:GLU:O	1:C:154:LYS:HE2	1.95	0.67
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.29	0.66
1:D:278:THR:HA	2:D:442:HOH:O	1.96	0.66
1:A:52:LYS:HD3	1:A:60:VAL:HG22	1.77	0.66
1:A:48:THR:HG21	1:A:75:VAL:CG2	2.26	0.65
1:A:177:LYS:HG3	1:A:235:VAL:HG23	1.78	0.65
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.31	0.65
1:A:232:LEU:O	1:A:235:VAL:HG12	1.96	0.65
1:A:215:SER:CB	1:D:296:ARG:HG3	2.27	0.64
1:C:22:LEU:HD13	1:C:86:VAL:CG1	2.28	0.64
1:C:51:ARG:HD2	1:C:51:ARG:N	2.00	0.64
1:D:22:LEU:HA	1:D:48:THR:OG1	1.97	0.64
1:B:163:CYS:SG	1:B:255:MET:HE1	2.38	0.64
1:A:177:LYS:HG3	1:A:235:VAL:HG21	1.81	0.63
1:B:50:ASP:OD1	1:B:74:SER:HA	1.98	0.63
1:A:15:LYS:HD2	1:A:43:GLN:HB2	1.81	0.63
1:B:168:ILE:O	1:B:171:PRO:HD2	1.98	0.63
1:A:22:LEU:HD11	1:A:80:PHE:CE1	2.34	0.63
1:C:50:ASP:OD1	1:C:74:SER:HA	1.99	0.62
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.80	0.62
1:D:150:GLU:HA	1:D:153:LYS:HD3	1.81	0.62
1:A:215:SER:HB3	1:D:296:ARG:CG	2.30	0.61
1:C:83:VAL:HG12	1:C:85:ALA:H	1.65	0.61
1:C:135:GLU:O	1:C:138:LYS:HG2	2.01	0.60
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.84	0.60
1:B:173:VAL:HB	1:B:174:PRO:HD3	1.84	0.60
1:B:296:ARG:CG	1:C:215:SER:HB3	2.32	0.60
1:D:163:CYS:SG	1:D:255:MET:HE1	2.41	0.60
1:A:48:THR:HG22	2:A:555:HOH:O	2.01	0.60
1:C:168:ILE:O	1:C:171:PRO:HD2	2.01	0.60
1:C:97:GLU:OE1	1:C:132:LYS:HD3	2.02	0.60
1:C:80:PHE:HB3	1:C:106:LEU:HD11	1.82	0.59
1:A:161:PRO:HG2	1:A:335:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:O	1:C:83:VAL:HG13	2.02	0.59
1:A:47:MET:HE2	1:A:70:PRO:HD2	1.85	0.59
1:B:73:VAL:HG12	1:B:74:SER:H	1.68	0.59
1:C:124:GLU:HG2	1:C:130:PRO:HA	1.85	0.58
1:C:103:PRO:HG2	1:C:106:LEU:HG	1.85	0.58
1:B:296:ARG:HG3	1:C:215:SER:HB3	1.86	0.58
1:C:48:THR:CG2	1:C:75:VAL:HG22	2.32	0.58
1:B:46:LEU:HD21	1:B:78:ALA:HB1	1.85	0.57
1:A:140:VAL:HG22	1:A:157:LEU:HD23	1.86	0.57
1:D:22:LEU:HD12	1:D:88:CYS:SG	2.45	0.57
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.87	0.56
1:B:168:ILE:HD13	1:B:188:ILE:HD13	1.87	0.56
1:B:22:LEU:HD11	1:B:80:PHE:CE1	2.40	0.56
1:B:118:ARG:HH11	1:B:118:ARG:HB2	1.70	0.56
1:B:73:VAL:CG1	1:B:74:SER:N	2.67	0.56
1:C:175:LEU:HD22	1:C:272:LEU:HD22	1.88	0.56
1:C:163:CYS:SG	1:C:255:MET:HE1	2.45	0.56
1:B:140:VAL:HG22	1:B:157:LEU:HD23	1.86	0.55
1:C:83:VAL:HG11	1:C:85:ALA:O	2.07	0.55
1:C:173:VAL:HB	1:C:174:PRO:HD3	1.88	0.55
1:C:127:TYR:CE1	1:C:223:ARG:HD3	2.42	0.55
1:C:83:VAL:CG1	1:C:85:ALA:O	2.55	0.55
1:C:142:TYR:CZ	1:C:161:PRO:HB3	2.42	0.55
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.89	0.54
1:B:221:ARG:HD3	2:B:478:HOH:O	2.08	0.54
1:A:177:LYS:CG	1:A:235:VAL:HG23	2.38	0.54
1:A:22:LEU:HD13	1:A:86:VAL:CG1	2.37	0.53
1:D:173:VAL:HB	1:D:174:PRO:HD3	1.91	0.53
1:B:83:VAL:O	1:B:106:LEU:HD11	2.08	0.53
1:B:270:GLU:CD	1:B:270:GLU:H	2.16	0.53
1:B:206:LEU:HA	1:D:206:LEU:HA	1.90	0.53
1:B:239:LYS:HD3	1:B:240:VAL:N	2.23	0.53
1:D:47:MET:CE	1:D:69:LEU:HB3	2.38	0.53
1:D:127:TYR:CE1	1:D:223:ARG:HD3	2.45	0.52
1:C:149:ARG:NH2	1:C:283:GLU:OE2	2.42	0.52
1:D:47:MET:HE1	1:D:69:LEU:HB3	1.90	0.52
1:B:73:VAL:CG1	1:B:74:SER:H	2.23	0.52
1:D:47:MET:HE2	1:D:70:PRO:HD2	1.92	0.52
1:B:161:PRO:HG2	1:B:335:GLN:NE2	2.24	0.52
1:C:22:LEU:HD13	1:C:86:VAL:HG11	1.92	0.52
1:C:22:LEU:HD13	1:C:86:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:HD13	1:C:98:ILE:HD12	1.92	0.51
1:B:153:LYS:HD2	2:B:555:HOH:O	2.10	0.51
1:C:102:LEU:HD12	1:C:108:ILE:HD13	1.92	0.51
1:C:15:LYS:HG2	1:C:16:ASP:OD1	2.10	0.51
1:D:190:ALA:C	1:D:191:LYS:HD2	2.36	0.51
1:B:22:LEU:HD13	1:B:86:VAL:CG1	2.40	0.51
1:A:95:THR:HG21	1:A:110:ASP:CG	2.36	0.50
1:D:280:TYR:HD1	1:D:283:GLU:HG3	1.76	0.50
1:B:125:GLU:HG3	1:B:126:TRP:CD1	2.46	0.50
1:C:54:GLY:C	2:C:533:HOH:O	2.55	0.50
1:D:217:TYR:O	1:D:246:PRO:HD2	2.12	0.50
1:A:56:SER:O	1:A:59:SER:HB2	2.12	0.50
1:A:82:THR:HG22	1:A:82:THR:O	2.11	0.50
1:A:190:ALA:C	1:A:191:LYS:HD2	2.36	0.50
1:A:135:GLU:OE1	1:A:138:LYS:CE	2.53	0.49
1:A:168:ILE:HD13	1:A:188:ILE:HD13	1.94	0.49
1:A:270:GLU:H	1:A:270:GLU:CD	2.21	0.49
1:C:16:ASP:OD1	1:C:16:ASP:N	2.44	0.49
1:C:15:LYS:CG	1:C:16:ASP:H	2.25	0.49
1:A:164:TYR:HB2	1:A:165:PRO:HD3	1.93	0.49
1:D:136:LEU:O	1:D:139:GLU:HG2	2.12	0.49
1:B:127:TYR:CE1	1:B:223:ARG:HD3	2.48	0.49
1:D:46:LEU:HD21	1:D:78:ALA:HB1	1.95	0.49
1:A:164:TYR:CE1	1:A:190:ALA:HB1	2.47	0.48
1:B:280:TYR:HD1	1:B:283:GLU:HG3	1.78	0.48
1:C:168:ILE:HD13	1:C:188:ILE:HD13	1.94	0.48
1:C:349:THR:HB	1:C:353:LEU:HD21	1.94	0.48
1:C:24:ALA:HB1	1:C:57:MET:HE1	1.96	0.48
1:C:55:GLN:HG2	1:C:59:SER:OG	2.14	0.48
1:A:174:PRO:HG3	2:A:584:HOH:O	2.13	0.48
1:D:150:GLU:O	1:D:153:LYS:HG2	2.14	0.48
1:C:280:TYR:HD1	1:C:283:GLU:HG3	1.78	0.47
1:A:149:ARG:NH2	1:A:283:GLU:OE2	2.45	0.47
1:B:256:GLN:HB2	1:B:324:VAL:HG12	1.95	0.47
1:B:99:ILE:HD12	1:B:115:PHE:HE2	1.79	0.47
1:B:164:TYR:CE1	1:B:190:ALA:HB1	2.48	0.47
1:B:135:GLU:O	1:B:138:LYS:HG3	2.14	0.47
1:B:239:LYS:HE3	2:B:480:HOH:O	2.14	0.47
1:A:46:LEU:HD12	2:A:427:HOH:O	2.14	0.47
1:D:150:GLU:HA	1:D:153:LYS:CD	2.44	0.47
1:C:62:PRO:HD2	2:C:400:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG21	1:A:110:ASP:OD2	2.14	0.46
1:B:149:ARG:NH2	1:B:283:GLU:OE2	2.48	0.46
1:A:127:TYR:CE1	1:A:223:ARG:HD3	2.50	0.46
1:B:106:LEU:HD13	2:B:535:HOH:O	2.16	0.46
1:B:296:ARG:HG3	1:C:215:SER:CB	2.45	0.46
1:C:214:ILE:HG22	1:C:250:PRO:HD3	1.97	0.46
1:D:124:GLU:OE2	1:D:130:PRO:HA	2.15	0.46
1:B:217:TYR:O	1:B:246:PRO:HD2	2.15	0.46
2:C:378:HOH:O	1:D:64:LEU:HD23	2.16	0.46
1:D:256:GLN:HB2	1:D:324:VAL:HG12	1.98	0.46
1:C:20:GLY:N	1:C:83:VAL:HG11	2.31	0.45
1:A:280:TYR:HD1	1:A:283:GLU:HG3	1.82	0.45
1:B:339:ASN:O	1:B:343:MET:HG3	2.16	0.45
1:D:64:LEU:HD21	2:D:450:HOH:O	2.16	0.45
1:B:170:LEU:HB2	1:B:171:PRO:HD3	1.98	0.45
1:B:296:ARG:HG2	1:C:215:SER:HB3	1.97	0.45
1:A:42:PHE:CZ	1:A:344:LEU:HD12	2.51	0.45
1:B:22:LEU:HD13	1:B:86:VAL:HG13	1.97	0.45
1:A:235:VAL:HG13	1:A:236:ALA:N	2.31	0.45
1:B:96:GLN:HG3	2:B:433:HOH:O	2.16	0.45
1:B:187:ILE:HD12	1:C:187:ILE:HD12	1.99	0.45
1:B:229:GLU:OE2	1:B:241:THR:HA	2.17	0.45
1:A:68:LYS:HD2	1:A:68:LYS:N	2.32	0.45
1:C:83:VAL:HG12	1:C:85:ALA:N	2.30	0.45
1:A:125:GLU:HG3	1:A:126:TRP:N	2.32	0.44
1:A:48:THR:CG2	2:A:555:HOH:O	2.62	0.44
1:A:22:LEU:HD13	1:A:86:VAL:HG13	1.99	0.44
1:B:295:PRO:HG2	1:B:322:ILE:CG2	2.48	0.44
1:C:170:LEU:HB2	1:C:171:PRO:HD3	2.00	0.44
1:C:269:THR:HG21	1:C:312:PRO:HA	1.99	0.44
1:C:15:LYS:HG2	1:C:16:ASP:N	2.26	0.44
1:C:173:VAL:HG13	1:C:235:VAL:HG21	1.99	0.44
1:D:90:LEU:HB3	1:D:91:PRO:CD	2.40	0.44
1:A:177:LYS:CG	1:A:235:VAL:CG2	2.86	0.44
1:B:259:ILE:HG22	1:B:261:VAL:HG13	2.00	0.44
1:D:148:LEU:O	1:D:152:ILE:HG13	2.18	0.43
1:B:168:ILE:C	1:B:171:PRO:HD2	2.42	0.43
1:D:164:TYR:CE1	1:D:190:ALA:HB1	2.54	0.43
1:D:186:ILE:HB	2:D:413:HOH:O	2.17	0.43
1:A:129:GLN:HA	1:A:130:PRO:HD3	1.89	0.43
1:C:354:HIS:CD2	1:C:354:HIS:H	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:O	1:C:152:ILE:HG13	2.19	0.43
1:D:120:ILE:O	1:D:124:GLU:HG3	2.19	0.43
1:C:83:VAL:HG12	1:C:84:ASP:N	2.34	0.42
1:A:213:GLY:C	1:D:298:HIS:CE1	2.97	0.42
1:D:214:ILE:HG22	1:D:250:PRO:HD3	2.01	0.42
1:C:168:ILE:C	1:C:171:PRO:HD2	2.44	0.42
1:D:90:LEU:HD13	1:D:98:ILE:HD12	2.01	0.42
1:A:22:LEU:HD13	1:A:86:VAL:HG11	2.00	0.42
1:B:239:LYS:HD3	1:B:239:LYS:C	2.42	0.42
1:C:136:LEU:O	1:C:139:GLU:HG2	2.19	0.42
1:C:217:TYR:O	1:C:246:PRO:HD2	2.19	0.42
1:D:160:ASN:HA	1:D:161:PRO:HD3	1.95	0.42
1:C:268:ARG:HG3	1:C:268:ARG:HH11	1.85	0.42
1:C:125:GLU:HG3	1:C:126:TRP:N	2.33	0.42
1:D:281:GLU:HB3	2:D:590:HOH:O	2.20	0.42
1:A:22:LEU:HA	1:A:48:THR:HB	2.01	0.42
1:D:281:GLU:HB2	2:D:442:HOH:O	2.19	0.42
1:A:191:LYS:HD2	1:A:191:LYS:N	2.35	0.42
1:A:259:ILE:HG22	1:A:261:VAL:HG13	2.02	0.41
1:C:104:THR:O	1:C:156:ARG:HD2	2.19	0.41
1:C:24:ALA:HB1	1:C:57:MET:CE	2.50	0.41
1:C:125:GLU:HG3	1:C:126:TRP:CD1	2.55	0.41
1:C:171:PRO:HG3	1:C:308:MET:HE2	2.02	0.41
1:A:244:PHE:CE2	1:A:246:PRO:HG3	2.56	0.41
1:C:164:TYR:CE1	1:C:190:ALA:HB1	2.56	0.41
1:D:42:PHE:N	1:D:42:PHE:CD1	2.85	0.41
1:A:148:LEU:O	1:A:152:ILE:HG13	2.21	0.41
1:A:214:ILE:HG22	1:A:250:PRO:HD3	2.03	0.41
1:C:18:ARG:HD3	1:C:82:THR:O	2.21	0.41
1:C:269:THR:HG21	1:C:312:PRO:CA	2.50	0.41
1:B:93:GLY:HA2	2:B:432:HOH:O	2.21	0.40
1:C:358:PHE:HA	1:C:359:PRO:C	2.46	0.40
1:C:273:HIS:CD2	1:C:291:GLU:HG3	2.56	0.40
1:C:301:ARG:NH2	1:C:359:PRO:OXT	2.54	0.40
1:A:162:GLY:C	1:A:165:PRO:HD2	2.46	0.40
1:A:269:THR:HG21	1:A:312:PRO:HA	2.03	0.40
1:A:152:ILE:HD13	1:A:339:ASN:OD1	2.21	0.40
1:B:135:GLU:HA	1:B:138:LYS:HE3	2.03	0.40
1:B:42:PHE:N	1:B:42:PHE:CD1	2.88	0.40
1:B:354:HIS:CD2	1:B:354:HIS:H	2.38	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	343/359 (96%)	329 (96%)	13 (4%)	1 (0%)	36	42
1	B	343/359 (96%)	327 (95%)	15 (4%)	1 (0%)	36	42
1	C	343/359 (96%)	324 (94%)	17 (5%)	2 (1%)	21	23
1	D	343/359 (96%)	330 (96%)	12 (4%)	1 (0%)	36	42
All	All	1372/1436 (96%)	1310 (96%)	57 (4%)	5 (0%)	30	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	49	ALA
1	B	332	ALA
1	C	332	ALA
1	D	332	ALA
1	A	332	ALA

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	295/308 (96%)	293 (99%)	2 (1%)	76	87
1	B	295/308 (96%)	288 (98%)	7 (2%)	43	58
1	C	295/308 (96%)	289 (98%)	6 (2%)	48	64
1	D	295/308 (96%)	289 (98%)	6 (2%)	48	64
All	All	1180/1232 (96%)	1159 (98%)	21 (2%)	51	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	184	GLU
1	B	65	ARG
1	B	92	HIS
1	B	106	LEU
1	B	118	ARG
1	B	183	HIS
1	B	239	LYS
1	B	270	GLU
1	C	16	ASP
1	C	51	ARG
1	C	65	ARG
1	C	107	LYS
1	C	117	LEU
1	C	344	LEU
1	D	57	MET
1	D	65	ARG
1	D	92	HIS
1	D	125	GLU
1	D	145	THR
1	D	281	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	273	HIS
1	A	274	GLN
1	A	299	ASN
1	B	92	HIS
1	B	205	ASN
1	B	237	GLN
1	B	256	GLN
1	B	273	HIS
1	B	354	HIS
1	C	274	GLN
1	C	354	HIS
1	D	55	GLN
1	D	129	GLN
1	D	274	GLN
1	D	354	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	345/359 (96%)	0.08	7 (2%) 65 62	20, 34, 61, 73	0
1	B	345/359 (96%)	0.06	2 (0%) 85 83	19, 34, 65, 103	1 (0%)
1	C	345/359 (96%)	0.15	12 (3%) 47 44	21, 35, 69, 93	1 (0%)
1	D	345/359 (96%)	0.05	10 (2%) 53 50	20, 34, 61, 100	0
All	All	1380/1436 (96%)	0.09	31 (2%) 62 59	19, 34, 65, 103	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	92	HIS	3.5
1	D	91	PRO	3.5
1	D	128	GLY	3.2
1	D	93	GLY	3.2
1	C	83	VAL	2.9
1	D	94	THR	2.8
1	A	92	HIS	2.7
1	C	73	VAL	2.7
1	C	82	THR	2.6
1	C	15	LYS	2.6
1	D	281	GLU	2.6
1	A	129	GLN	2.6
1	A	177	LYS	2.5
1	C	57	MET	2.5
1	C	81	SER	2.4
1	D	104	THR	2.4
1	C	84	ASP	2.4
1	A	120	ILE	2.4
1	C	104	THR	2.3
1	C	18	ARG	2.3
1	B	49	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	128	GLY	2.2
1	C	54	GLY	2.2
1	D	130	PRO	2.2
1	D	16	ASP	2.2
1	C	78	ALA	2.2
1	A	282	ASP	2.2
1	B	80	PHE	2.1
1	A	57	MET	2.0
1	D	57	MET	2.0
1	A	22	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.