Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 08:34 PM EDT

PDB ID	:	1EGA
Title	:	CRYSTAL STRUCTURE OF A WIDELY CONSERVED GTPASE ERA
Authors	:	Chen, X.; Ji, X.
Deposited on	:	1998-12-01
Resolution	:	2.40 Å(reported)

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

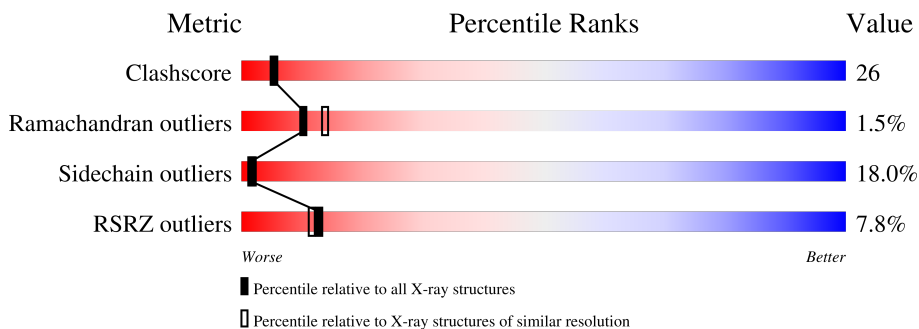|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.40 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	Percentile Ranks	Value
Clashscore		26
Ramachandran outliers		1.5%
Sidechain outliers		18.0%
RSRZ outliers		7.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures
⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	301	5% 54% / 35% / 8% ·
1	B	301	10% 49% / 37% / 10% · ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4790 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 PROTEIN (GTP-BINDING PROTEIN ERA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total 2306	C 1460	N 410	O 426	S 10	36	0	0
1	B	293	Total 2310	C 1462	N 411	O 427	S 10	36	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
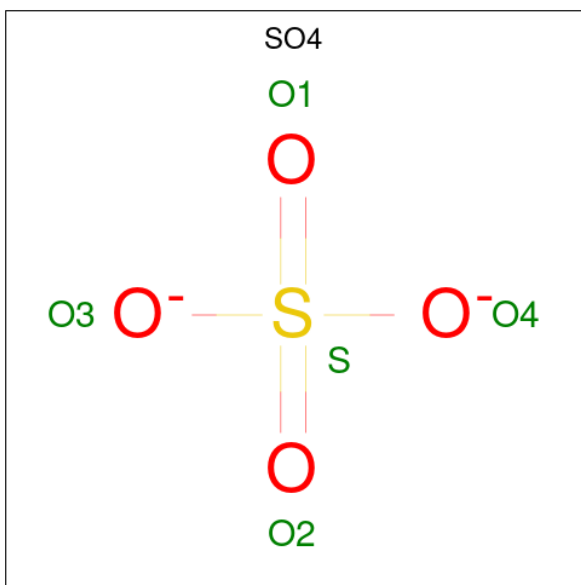
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total 85	O 85	0	0
3	B	64	Total 64	O 64	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: PROTEIN (GTP-BINDING PROTEIN ERA)
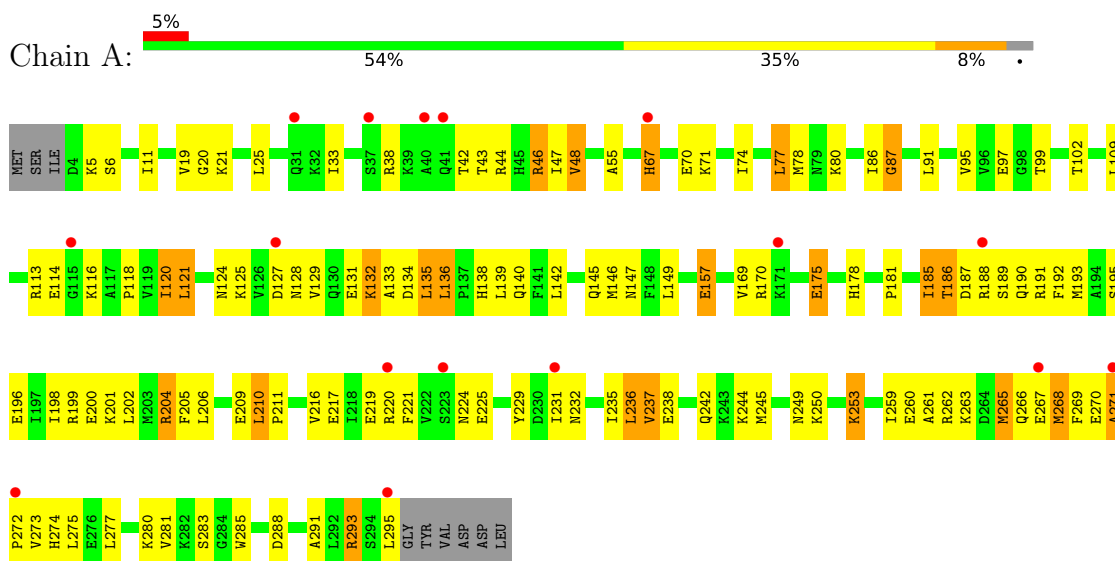
• Molecule 1: PROTEIN (GTP-BINDING PROTEIN ERA)
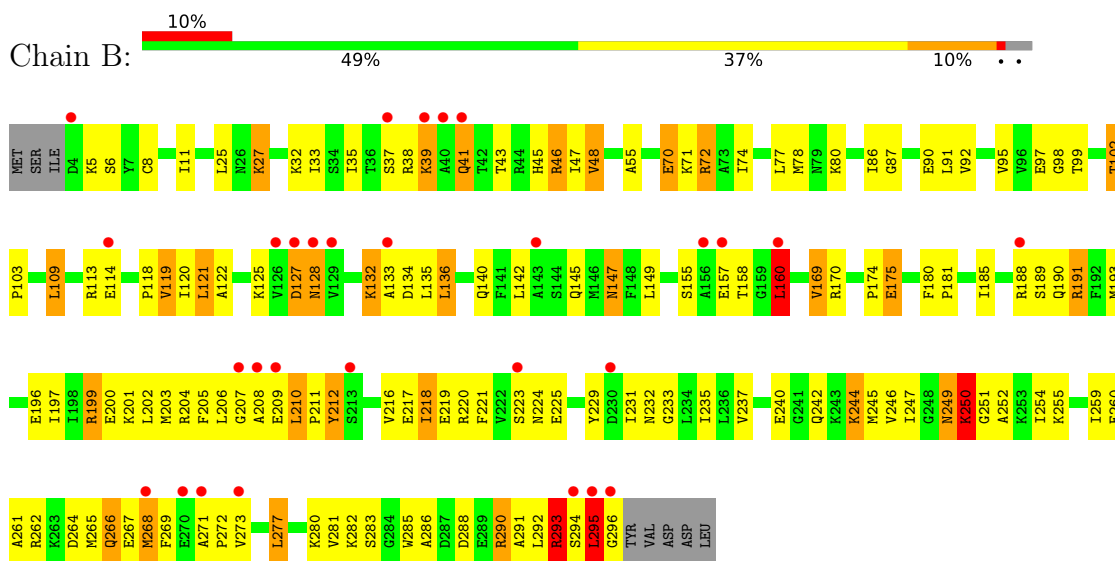
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.79Å 67.56Å 87.29Å 90.00° 115.82° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 24.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	82.9 (8.00-2.40) 95.0 (24.91-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.243 , 0.298 0.250 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.096 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4790	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.49	0/2344	0.72	0/3161
1	B	0.50	0/2348	0.78	3/3166 (0.1%)
All	All	0.50	0/4692	0.75	3/6327 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	293	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	B	188	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	B	295	LEU	O-C-N	-5.53	113.80	123.20

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	2306	0	2364	103	0
1	B	2310	0	2367	143	0
2	A	15	0	0	1	0
2	B	10	0	0	0	0
3	A	85	0	0	5	0
3	B	64	0	0	3	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4790	0	4731	244	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 26.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ALA:HB1	1:B:272:PRO:HD2	1.54	0.88
1:B:197:ILE:HD11	1:B:268:MET:HG2	1.59	0.83
1:B:231:ILE:HG21	1:B:265:MET:HE1	1.62	0.79
1:B:202:LEU:HD21	1:B:235:ILE:HD13	1.62	0.79
1:B:39:LYS:HG3	1:B:41:GLN:HG2	1.64	0.79
1:B:193:MET:SD	1:B:268:MET:CE	2.71	0.79
1:B:155:SER:HB3	1:B:158:THR:HB	1.66	0.78
1:A:237:VAL:HG21	1:A:242:GLN:HB3	1.66	0.77
1:B:193:MET:SD	1:B:268:MET:HE2	2.25	0.77
1:A:193:MET:SD	1:A:268:MET:HE3	2.25	0.76
1:A:259:ILE:HG13	1:A:260:GLU:N	2.00	0.75
1:B:32:LYS:HE2	1:B:212:TYR:HA	1.66	0.75
1:A:231:ILE:HD13	1:A:265:MET:CE	2.17	0.74
1:A:261:ALA:O	1:A:265:MET:HG3	1.88	0.74
1:B:118:PRO:HB2	1:B:149:LEU:HD12	1.69	0.73
1:A:190:GLN:HG2	1:A:193:MET:HE3	1.71	0.73
1:A:206:LEU:HD12	1:A:210:LEU:HD23	1.70	0.73
1:A:25:LEU:HD22	1:A:48:VAL:HG13	1.69	0.72
1:A:118:PRO:HB2	1:A:149:LEU:HD12	1.73	0.71
1:B:27:LYS:HG3	3:B:448:HOH:O	1.91	0.70
1:A:46:ARG:HG2	1:A:70:GLU:HG2	1.73	0.70
1:B:261:ALA:O	1:B:265:MET:HG3	1.92	0.69
1:B:191:ARG:NH1	1:B:218:ILE:HG22	2.09	0.68
1:A:262:ARG:NH1	1:A:274:HIS:HA	2.08	0.68
1:B:46:ARG:HG2	1:B:70:GLU:HG2	1.75	0.68
1:B:285:TRP:CZ2	1:B:293:ARG:HD2	2.29	0.68
1:B:102:THR:HG22	1:B:103:PRO:CD	2.24	0.67
1:B:128:ASN:N	1:B:128:ASN:HD22	1.92	0.67
1:A:186:THR:HB	3:A:350:HOH:O	1.95	0.66
1:B:132:LYS:NZ	1:B:133:ALA:HA	2.11	0.66
1:B:205:PHE:CZ	1:B:260:GLU:HG3	2.30	0.66
1:B:264:ASP:O	1:B:268:MET:HB3	1.95	0.66
1:B:155:SER:CB	1:B:158:THR:HB	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HE2	1:A:175:GLU:CD	2.16	0.65
1:A:221:PHE:CD2	1:A:231:ILE:HG12	2.31	0.65
1:A:193:MET:SD	1:A:268:MET:CE	2.84	0.65
1:B:240:GLU:HG3	1:B:244:LYS:HE2	1.77	0.65
1:B:265:MET:O	1:B:269:PHE:HB2	1.96	0.64
1:A:25:LEU:CD2	1:A:48:VAL:HG13	2.28	0.63
1:A:285:TRP:CZ2	1:A:293:ARG:HD2	2.32	0.63
1:B:295:LEU:HG	1:B:296:GLY:N	2.13	0.63
1:A:70:GLU:O	1:A:74:ILE:HG13	1.99	0.62
1:B:193:MET:SD	1:B:268:MET:HE1	2.39	0.62
1:A:229:TYR:HB2	1:A:273:VAL:HG12	1.82	0.62
1:B:99:THR:O	1:B:99:THR:HG22	2.00	0.62
1:A:157:GLU:HB3	3:A:348:HOH:O	2.00	0.61
1:B:6:SER:HA	1:B:55:ALA:HB1	1.82	0.61
1:B:189:SER:O	1:B:193:MET:HG3	2.01	0.61
1:B:220:ARG:HB3	1:B:232:ASN:HB2	1.84	0.60
1:B:46:ARG:CG	1:B:70:GLU:HG2	2.31	0.60
1:A:77:LEU:HD11	1:A:186:THR:HG23	1.84	0.59
1:A:231:ILE:HG21	1:A:265:MET:HE1	1.84	0.59
1:B:25:LEU:HD22	1:B:48:VAL:HG13	1.83	0.59
1:B:70:GLU:O	1:B:74:ILE:HG13	2.02	0.59
1:A:19:VAL:CG1	1:A:95:VAL:HG12	2.33	0.59
1:B:268:MET:HE2	1:B:269:PHE:HE1	1.68	0.59
1:B:127:ASP:C	1:B:128:ASN:HD22	2.06	0.59
1:B:5:LYS:HE2	1:B:175:GLU:CD	2.24	0.58
1:A:237:VAL:HG21	1:A:242:GLN:CB	2.33	0.58
1:B:264:ASP:HA	1:B:267:GLU:HG2	1.84	0.58
1:A:196:GLU:O	1:A:200:GLU:HG3	2.04	0.58
1:A:259:ILE:HG13	1:A:260:GLU:H	1.68	0.58
1:B:95:VAL:HG22	1:B:122:ALA:HB3	1.86	0.58
1:A:219:GLU:CG	1:A:232:ASN:HB3	2.34	0.58
1:B:91:LEU:HD12	1:B:118:PRO:O	2.04	0.57
1:A:67:HIS:HB2	1:A:70:GLU:OE1	2.05	0.57
1:B:109:LEU:HD11	1:B:145:GLN:HB3	1.86	0.57
1:B:293:ARG:C	1:B:295:LEU:H	2.08	0.56
1:B:196:GLU:O	1:B:200:GLU:HG3	2.06	0.56
1:A:219:GLU:HG2	1:A:232:ASN:HB3	1.86	0.56
1:B:219:GLU:HG2	1:B:232:ASN:HB3	1.87	0.56
1:B:191:ARG:HH11	1:B:218:ILE:HG22	1.69	0.56
1:B:264:ASP:HA	1:B:267:GLU:CG	2.36	0.56
1:A:132:LYS:NZ	1:A:133:ALA:HA	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ILE:HD11	1:A:149:LEU:HD13	1.86	0.55
1:B:199:ARG:HH21	1:B:203:MET:HE2	1.72	0.55
1:A:99:THR:HG22	1:A:99:THR:O	2.05	0.55
1:B:292:LEU:O	1:B:295:LEU:HD23	2.06	0.55
1:A:189:SER:O	1:A:193:MET:HG3	2.07	0.55
1:B:91:LEU:HD11	1:B:120:ILE:HD13	1.89	0.54
1:B:259:ILE:HG13	1:B:260:GLU:N	2.23	0.54
1:B:268:MET:HE3	1:B:268:MET:O	2.06	0.54
1:A:262:ARG:HH12	1:A:274:HIS:HA	1.72	0.54
1:B:266:GLN:CD	1:B:272:PRO:HA	2.27	0.54
1:A:266:GLN:O	1:A:269:PHE:O	2.25	0.54
1:B:128:ASN:N	1:B:128:ASN:ND2	2.55	0.54
1:B:33:ILE:HD11	1:B:210:LEU:HD11	1.89	0.54
1:A:253:LYS:HE3	3:A:396:HOH:O	2.08	0.54
1:B:136:LEU:HD22	1:B:140:GLN:HE21	1.73	0.54
1:B:288:ASP:O	1:B:291:ALA:HB3	2.08	0.54
1:B:102:THR:HG22	1:B:103:PRO:HD2	1.89	0.53
1:B:286:ALA:O	1:B:290:ARG:HB2	2.08	0.53
1:B:136:LEU:HD22	1:B:140:GLN:NE2	2.24	0.53
1:B:132:LYS:HZ2	1:B:133:ALA:HA	1.74	0.53
1:B:120:ILE:HD11	1:B:149:LEU:HD13	1.90	0.53
1:B:249:ASN:HD22	1:B:249:ASN:C	2.12	0.53
1:B:281:VAL:HG12	1:B:283:SER:H	1.74	0.53
1:B:249:ASN:C	1:B:251:GLY:H	2.13	0.52
1:A:99:THR:HA	1:A:138:HIS:CD2	2.45	0.52
1:B:221:PHE:CD2	1:B:231:ILE:HD12	2.44	0.52
1:A:231:ILE:HD13	1:A:265:MET:HE1	1.88	0.52
1:B:102:THR:HG22	1:B:103:PRO:HD3	1.90	0.52
1:B:25:LEU:CD2	1:B:48:VAL:HG13	2.40	0.52
1:B:266:GLN:OE1	1:B:273:VAL:HG22	2.10	0.52
1:B:90:GLU:HG3	1:B:174:PRO:HD3	1.92	0.52
1:B:267:GLU:HG3	1:B:268:MET:H	1.75	0.52
1:A:187:ASP:OD2	1:A:192:PHE:HB2	2.10	0.51
1:B:250:LYS:HE3	1:B:252:ALA:HB2	1.93	0.51
1:A:25:LEU:HD22	1:A:48:VAL:CG1	2.39	0.51
1:A:149:LEU:HD23	1:A:149:LEU:O	2.10	0.51
1:B:109:LEU:O	1:B:113:ARG:HG3	2.10	0.51
1:B:32:LYS:HD2	1:B:212:TYR:CD1	2.46	0.51
1:A:80:LYS:HE3	3:A:332:HOH:O	2.10	0.51
1:A:78:MET:HB3	1:A:80:LYS:HG3	1.93	0.51
1:A:210:LEU:HD22	1:A:211:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD11	1:A:186:THR:CG2	2.42	0.50
1:B:11:ILE:HD13	1:B:169:VAL:HG13	1.92	0.50
1:B:193:MET:HA	3:B:326:HOH:O	2.11	0.50
1:B:249:ASN:C	1:B:249:ASN:ND2	2.65	0.50
1:B:45:HIS:HD2	1:B:47:ILE:HB	1.77	0.50
1:B:249:ASN:ND2	1:B:250:LYS:HB3	2.26	0.50
1:B:219:GLU:CG	1:B:232:ASN:HB3	2.42	0.50
1:A:47:ILE:HD11	1:A:74:ILE:HG23	1.94	0.50
1:B:267:GLU:HG3	1:B:268:MET:N	2.27	0.50
1:B:92:VAL:HB	1:B:119:VAL:HB	1.93	0.50
1:A:55:ALA:O	1:A:178:HIS:HE1	1.95	0.49
1:B:33:ILE:HD11	1:B:210:LEU:CD1	2.42	0.49
1:A:71:LYS:HG2	1:A:86:ILE:HB	1.92	0.49
1:B:72:ARG:HG2	1:B:72:ARG:HH11	1.76	0.49
1:B:249:ASN:O	1:B:250:LYS:HG2	2.11	0.49
1:A:198:ILE:HB	1:A:216:VAL:HG11	1.93	0.49
1:B:39:LYS:HG3	1:B:41:GLN:CG	2.39	0.49
1:A:11:ILE:HD13	1:A:169:VAL:HG13	1.93	0.49
1:A:91:LEU:HD11	1:A:120:ILE:HD13	1.93	0.49
1:A:202:LEU:HD21	1:A:235:ILE:HD13	1.93	0.49
1:B:216:VAL:HG12	1:B:217:GLU:N	2.28	0.49
1:B:121:LEU:HD11	1:B:142:LEU:HD13	1.94	0.49
1:A:71:LYS:HE2	1:A:87:GLY:O	2.12	0.49
1:A:46:ARG:CG	1:A:70:GLU:HG2	2.43	0.48
1:A:136:LEU:HD22	1:A:140:GLN:HE21	1.78	0.48
1:B:25:LEU:HD22	1:B:48:VAL:CG1	2.43	0.48
1:B:293:ARG:O	1:B:295:LEU:N	2.46	0.48
1:A:136:LEU:HD22	1:A:140:GLN:NE2	2.28	0.48
1:B:233:GLY:HA3	1:B:277:LEU:HD12	1.95	0.48
1:B:247:ILE:HA	1:B:254:ILE:HB	1.95	0.48
1:A:288:ASP:O	1:A:291:ALA:HB3	2.14	0.48
1:B:99:THR:O	1:B:99:THR:CG2	2.62	0.47
1:A:21:LYS:HE2	2:A:302:SO4:O3	2.14	0.47
1:A:19:VAL:HG12	1:A:95:VAL:HG12	1.97	0.47
1:A:262:ARG:CZ	1:A:275:LEU:H	2.27	0.47
1:B:35:ILE:HD11	1:B:199:ARG:HG3	1.97	0.47
1:B:170:ARG:HE	1:B:170:ARG:HB2	1.47	0.47
1:A:33:ILE:HD11	1:A:210:LEU:HD11	1.97	0.47
1:B:11:ILE:CD1	1:B:169:VAL:HG13	2.45	0.47
1:B:147:ASN:C	1:B:147:ASN:HD22	2.17	0.47
1:A:262:ARG:NH2	1:A:275:LEU:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ALA:HB1	1:B:272:PRO:CD	2.35	0.46
1:B:45:HIS:CD2	1:B:47:ILE:HB	2.50	0.46
1:A:121:LEU:HD11	1:A:142:LEU:HD13	1.98	0.46
1:A:236:LEU:HA	1:A:280:LYS:O	2.15	0.46
1:B:109:LEU:O	1:B:109:LEU:HD22	2.15	0.46
1:B:205:PHE:HZ	1:B:260:GLU:HG3	1.75	0.46
1:B:210:LEU:C	1:B:210:LEU:HD23	2.36	0.46
1:A:190:GLN:OE1	1:A:269:PHE:CD1	2.69	0.46
1:A:190:GLN:HB3	1:A:269:PHE:CE1	2.51	0.46
1:A:80:LYS:HG2	1:B:181:PRO:HA	1.98	0.45
1:A:120:ILE:CD1	1:A:149:LEU:HD13	2.46	0.45
1:A:135:LEU:HD22	1:A:139:LEU:HG	1.98	0.45
1:B:190:GLN:HG2	1:B:193:MET:HE3	1.97	0.45
1:B:201:LYS:HA	1:B:201:LYS:HD3	1.72	0.45
1:A:99:THR:O	1:A:99:THR:CG2	2.65	0.45
1:B:266:GLN:O	1:B:269:PHE:O	2.35	0.45
1:A:237:VAL:CG2	1:A:238:GLU:N	2.80	0.45
1:B:72:ARG:HG2	1:B:72:ARG:NH1	2.32	0.45
1:B:218:ILE:HG21	1:B:221:PHE:HB2	1.99	0.45
1:A:20:GLY:HA3	1:A:124:ASN:ND2	2.32	0.44
1:B:33:ILE:CG1	1:B:210:LEU:HD11	2.47	0.44
1:B:210:LEU:HA	1:B:211:PRO:HD3	1.64	0.44
1:B:266:GLN:OE1	1:B:266:GLN:HA	2.17	0.44
1:A:280:LYS:HB2	1:A:285:TRP:CZ3	2.52	0.44
1:B:250:LYS:CE	1:B:252:ALA:HB2	2.47	0.44
1:B:285:TRP:CE2	1:B:293:ARG:HD2	2.52	0.44
1:A:237:VAL:CG2	1:A:242:GLN:HB3	2.41	0.44
1:B:132:LYS:HZ1	1:B:133:ALA:HA	1.82	0.44
1:B:43:THR:OG1	1:B:46:ARG:HA	2.18	0.44
1:A:47:ILE:HB	1:A:186:THR:HG21	2.00	0.44
1:A:170:ARG:HE	1:A:170:ARG:HB2	1.47	0.43
1:B:87:GLY:HA3	3:B:371:HOH:O	2.18	0.43
1:A:97:GLU:HG3	1:A:125:LYS:CD	2.47	0.43
1:A:120:ILE:HD12	1:A:149:LEU:HB3	1.99	0.43
1:B:218:ILE:HG22	1:B:218:ILE:O	2.19	0.43
1:A:237:VAL:HG23	1:A:242:GLN:OE1	2.17	0.43
1:A:266:GLN:HG2	1:A:272:PRO:HA	2.01	0.43
1:B:266:GLN:OE1	1:B:272:PRO:HA	2.18	0.43
1:A:193:MET:HG2	3:A:320:HOH:O	2.17	0.43
1:B:206:LEU:HD11	1:B:246:VAL:HG22	2.00	0.43
1:B:293:ARG:C	1:B:295:LEU:N	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:O	1:A:70:GLU:HA	2.19	0.43
1:B:39:LYS:C	1:B:41:GLN:H	2.21	0.43
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.80	0.43
1:A:185:ILE:H	1:A:185:ILE:HG12	1.63	0.43
1:B:160:LEU:HD22	1:B:160:LEU:HA	1.87	0.43
1:A:132:LYS:C	1:A:134:ASP:H	2.23	0.42
1:A:281:VAL:HG12	1:A:283:SER:H	1.83	0.42
1:A:11:ILE:CD1	1:A:169:VAL:HG13	2.49	0.42
1:A:201:LYS:NZ	1:A:204:ARG:NH2	2.67	0.42
1:A:210:LEU:CD2	1:A:211:PRO:HD2	2.49	0.42
1:A:265:MET:HE3	1:A:265:MET:HB3	1.90	0.42
1:B:207:GLY:O	1:B:208:ALA:HB3	2.19	0.42
1:B:132:LYS:C	1:B:134:ASP:H	2.22	0.42
1:B:202:LEU:O	1:B:206:LEU:HB2	2.19	0.42
1:B:268:MET:HE2	1:B:269:PHE:CE1	2.51	0.42
1:B:218:ILE:HD12	1:B:218:ILE:HA	1.91	0.42
1:B:120:ILE:CD1	1:B:149:LEU:HD13	2.49	0.42
1:B:120:ILE:HD12	1:B:149:LEU:HB3	2.02	0.42
1:B:147:ASN:C	1:B:147:ASN:ND2	2.72	0.42
1:B:208:ALA:C	1:B:210:LEU:N	2.73	0.42
1:B:210:LEU:HG	1:B:211:PRO:HD2	2.01	0.42
1:B:262:ARG:HG3	1:B:273:VAL:HG23	2.01	0.42
1:B:45:HIS:CD2	1:B:47:ILE:H	2.38	0.42
1:B:71:LYS:HG2	1:B:86:ILE:HB	2.00	0.42
1:B:266:GLN:OE1	1:B:273:VAL:N	2.53	0.42
1:B:280:LYS:HB2	1:B:285:TRP:CZ3	2.55	0.42
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.90	0.41
1:B:37:SER:O	1:B:38:ARG:HG2	2.20	0.41
1:B:145:GLN:NE2	1:B:145:GLN:HA	2.34	0.41
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.86	0.41
1:A:205:PHE:HB3	1:A:253:LYS:HD2	2.02	0.41
1:A:181:PRO:HA	1:B:80:LYS:HG2	2.02	0.41
1:B:33:ILE:HD12	1:B:203:MET:HE2	2.01	0.41
1:A:38:ARG:HD2	1:A:38:ARG:HA	1.93	0.41
1:A:145:GLN:O	1:A:146:MET:HB3	2.21	0.41
1:A:42:THR:HG22	1:A:43:THR:O	2.20	0.41
1:B:78:MET:HG3	1:B:180:PHE:CE1	2.55	0.41
1:B:97:GLU:HG3	1:B:125:LYS:HD3	2.01	0.41
1:A:6:SER:HA	1:A:55:ALA:HB1	2.02	0.41
1:A:209:GLU:HG2	1:A:245:MET:SD	2.60	0.41
1:B:237:VAL:O	1:B:282:LYS:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PRO:HB3	1:B:242:GLN:CD	2.41	0.40
1:A:190:GLN:HB3	1:A:269:PHE:CZ	2.57	0.40
1:A:193:MET:SD	1:A:268:MET:HE1	2.62	0.40
1:A:270:GLU:O	1:A:271:ALA:HB2	2.22	0.40
1:A:231:ILE:HD13	1:A:265:MET:HE2	2.01	0.40
1:B:264:ASP:O	1:B:268:MET:N	2.49	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	290/301 (96%)	262 (90%)	23 (8%)	5 (2%)	9	11
1	B	291/301 (97%)	258 (89%)	29 (10%)	4 (1%)	11	15
All	All	581/602 (96%)	520 (90%)	52 (9%)	9 (2%)	10	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	LYS
1	B	294	SER
1	A	113	ARG
1	A	87	GLY
1	B	98	GLY
1	B	160	LEU
1	A	250	LYS
1	A	129	VAL
1	A	271	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	250/258 (97%)	207 (83%)	43 (17%)	2	2
1	B	250/258 (97%)	203 (81%)	47 (19%)	1	1
All	All	500/516 (97%)	410 (82%)	90 (18%)	1	2

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	48	VAL
1	A	67	HIS
1	A	77	LEU
1	A	102	THR
1	A	109	LEU
1	A	114	GLU
1	A	116	LYS
1	A	120	ILE
1	A	121	LEU
1	A	127	ASP
1	A	128	ASN
1	A	131	GLU
1	A	132	LYS
1	A	135	LEU
1	A	136	LEU
1	A	147	ASN
1	A	157	GLU
1	A	175	GLU
1	A	185	ILE
1	A	186	THR
1	A	188	ARG
1	A	191	ARG
1	A	195	SER
1	A	199	ARG
1	A	204	ARG
1	A	210	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	217	GLU
1	A	220	ARG
1	A	224	ASN
1	A	225	GLU
1	A	236	LEU
1	A	237	VAL
1	A	244	LYS
1	A	249	ASN
1	A	253	LYS
1	A	263	LYS
1	A	265	MET
1	A	267	GLU
1	A	268	MET
1	A	277	LEU
1	A	293	ARG
1	A	295	LEU
1	B	8	CYS
1	B	27	LYS
1	B	39	LYS
1	B	41	GLN
1	B	46	ARG
1	B	48	VAL
1	B	70	GLU
1	B	72	ARG
1	B	77	LEU
1	B	102	THR
1	B	109	LEU
1	B	114	GLU
1	B	119	VAL
1	B	121	LEU
1	B	127	ASP
1	B	128	ASN
1	B	132	LYS
1	B	135	LEU
1	B	136	LEU
1	B	147	ASN
1	B	157	GLU
1	B	160	LEU
1	B	169	VAL
1	B	175	GLU
1	B	185	ILE
1	B	191	ARG

Continued from previous page...

Mol	Chain	Res	Type
1	B	199	ARG
1	B	204	ARG
1	B	209	GLU
1	B	210	LEU
1	B	212	TYR
1	B	218	ILE
1	B	223	SER
1	B	224	ASN
1	B	225	GLU
1	B	229	TYR
1	B	244	LYS
1	B	245	MET
1	B	249	ASN
1	B	250	LYS
1	B	255	LYS
1	B	266	GLN
1	B	268	MET
1	B	277	LEU
1	B	290	ARG
1	B	293	ARG
1	B	295	LEU

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	79	ASN
1	A	130	GLN
1	A	140	GLN
1	A	147	ASN
1	A	161	ASN
1	A	172	HIS
1	A	178	HIS
1	B	41	GLN
1	B	45	HIS
1	B	51	HIS
1	B	110	ASN
1	B	128	ASN
1	B	140	GLN
1	B	147	ASN
1	B	172	HIS
1	B	249	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	SO4	B	303	-	4,4,4	0.67	0	6,6,6	1.95	2 (33%)
2	SO4	A	305	-	4,4,4	0.59	0	6,6,6	0.40	0
2	SO4	B	304	-	4,4,4	0.29	0	6,6,6	0.42	0
2	SO4	A	302	-	4,4,4	0.61	0	6,6,6	1.02	0
2	SO4	A	303	-	4,4,4	0.45	0	6,6,6	0.43	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	303	SO4	O4-S-O3	3.55	124.21	109.06
2	B	303	SO4	O3-S-O1	-2.61	95.69	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	SO4	1	0

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	287/301 (95%)	0.11	16 (5%)	24	23	18, 40, 89, 100	0
1	B	288/301 (95%)	0.31	29 (10%)	7	6	16, 45, 95, 100	0
All	All	575/602 (95%)	0.21	45 (7%)	13	11	16, 42, 92, 100	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	SER	8.1
1	B	37	SER	8.0
1	A	37	SER	7.4
1	B	213	SER	6.3
1	B	209	GLU	6.3
1	B	271	ALA	5.9
1	B	133	ALA	5.9
1	B	273	VAL	5.1
1	B	39	LYS	4.8
1	B	208	ALA	4.7
1	B	126	VAL	4.6
1	A	295	LEU	4.5
1	A	223	SER	4.3
1	B	114	GLU	4.3
1	A	220	ARG	3.9
1	B	156	ALA	3.7
1	B	129	VAL	3.7
1	A	272	PRO	3.7
1	B	294	SER	3.6
1	A	127	ASP	3.5
1	B	296	GLY	3.5
1	B	41	GLN	3.5
1	B	4	ASP	3.4
1	A	271	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	143	ALA	3.2
1	A	40	ALA	3.2
1	A	41	GLN	3.0
1	A	188	ARG	2.8
1	A	67	HIS	2.8
1	B	157	GLU	2.7
1	A	115	GLY	2.6
1	B	230	ASP	2.6
1	B	268	MET	2.6
1	A	231	ILE	2.6
1	B	40	ALA	2.5
1	B	188	ARG	2.5
1	B	295	LEU	2.5
1	A	171	LYS	2.3
1	B	127	ASP	2.3
1	B	207	GLY	2.3
1	A	267	GLU	2.3
1	B	128	ASN	2.2
1	B	160	LEU	2.2
1	B	270	GLU	2.1
1	A	31	GLN	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 monosaccharides 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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	304	5/5	0.82	0.17	98,99,100,100	0
2	SO4	A	305	5/5	0.96	0.16	67,70,81,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	SO4	A	303	5/5	0.98	0.13	56,67,69,74	0
2	SO4	B	303	5/5	0.99	0.09	23,43,59,61	0
2	SO4	A	302	5/5	0.99	0.11	16,38,43,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.