

Full wwPDB X-ray Structure Validation Report (i)

May 17, 2023 – 07:29 pm BST

PDB ID	:	7ZUV
Title	:	Crystal structure of Chlamydomonas reinhardtii chloroplastic sedoheptulose-
		1,7-bisphosphatase in reducing conditions
Authors	:	Le Moigne, T.; Robert, G.Q.; Lemaire, S.D.; Henri, J.
Deposited on	:	2022-05-13
Resolution	:	3.11 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
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)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 3.11 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))
Bc	130704	1292 (3 14-3 10)
	141014	
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	А	331	.% 7 9%	14%	• 6%
1	В	331	% • 82%	12%	6%
1	С	331	77%	13% •	9%
1	D	331	% 8 0%	13%	6%
1	Ε	331	78%	11% ·	9%



Mol	Chain	Length	Quality of chain		
1	F	331	3% 82%	11%	6%
1	G	331	2% 77%	14%	9%
1	Н	331	75%	16%	• 8%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18714 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	210	Total	С	Ν	0	S	0	0	0
1	А	310	2363	1503	391	448	21	0	0	0
1	р	211	Total	С	Ν	0	S	0	0	0
1	D	311	2372	1509	393	449	21	0	0	0
1	С	300	Total	С	Ν	0	S	0	0	0
1	U	302	2309	1471	383	435	20	0	0	0
1	а	210	Total	С	Ν	0	S	0	0	0
1	D	310	2363	1503	391	448	21	0	0	0
1	F	201	Total	С	Ν	0	S	0	0	0
1	Ľ	301	2299	1465	381	433	20	0	0	0
1	Б	210	Total	С	Ν	0	S	0	0	0
1	Г	310	2363	1503	391	448	21	0	0	0
1	С	201	Total	С	Ν	0	S	0	0	0
1	G	301	2297	1464	381	431	21	0	0	0
1	ц	206	Total	С	Ν	0	S	0	0	0
1	п	300	2338	1489	387	441	21	U		

• Molecule 1 is a protein called FBPase domain-containing protein.

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	61	MET	-	initiating methionine	UNP A0A2K3DY10
А	62	HIS	-	expression tag	UNP A0A2K3DY10
А	63	HIS	-	expression tag	UNP A0A2K3DY10
А	64	HIS	-	expression tag	UNP A0A2K3DY10
А	65	HIS	-	expression tag	UNP A0A2K3DY10
А	66	HIS	-	expression tag	UNP A0A2K3DY10
А	67	HIS	-	expression tag	UNP A0A2K3DY10
А	68	HIS	-	expression tag	UNP A0A2K3DY10
А	69	MET	-	expression tag	UNP A0A2K3DY10
В	61	MET	-	initiating methionine	UNP A0A2K3DY10
В	62	HIS	-	expression tag	UNP A0A2K3DY10
В	63	HIS	-	expression tag	UNP A0A2K3DY10
В	64	HIS	-	expression tag	UNP A0A2K3DY10



1 Z U V	7ZI	UV
---------	-----	----

Chain	Residue	Modelled	Actual	Comment	Reference
В	65	HIS	-	expression tag	UNP A0A2K3DY10
В	66	HIS	_	expression tag	UNP A0A2K3DY10
В	67	HIS	-	expression tag	UNP A0A2K3DY10
В	68	HIS	_	expression tag	UNP A0A2K3DY10
В	69	MET	-	expression tag	UNP A0A2K3DY10
С	61	MET	-	initiating methionine	UNP A0A2K3DY10
С	62	HIS	-	expression tag	UNP A0A2K3DY10
С	63	HIS	-	expression tag	UNP A0A2K3DY10
С	64	HIS	-	expression tag	UNP A0A2K3DY10
С	65	HIS	-	expression tag	UNP A0A2K3DY10
С	66	HIS	-	expression tag	UNP A0A2K3DY10
С	67	HIS	-	expression tag	UNP A0A2K3DY10
С	68	HIS	-	expression tag	UNP A0A2K3DY10
С	69	MET	-	expression tag	UNP A0A2K3DY10
D	61	MET	-	initiating methionine	UNP A0A2K3DY10
D	62	HIS	-	expression tag	UNP A0A2K3DY10
D	63	HIS	-	expression tag	UNP A0A2K3DY10
D	64	HIS	-	expression tag	UNP A0A2K3DY10
D	65	HIS	-	expression tag	UNP A0A2K3DY10
D	66	HIS	-	expression tag	UNP A0A2K3DY10
D	67	HIS	-	expression tag	UNP A0A2K3DY10
D	68	HIS	-	expression tag	UNP A0A2K3DY10
D	69	MET	-	expression tag	UNP A0A2K3DY10
E	61	MET	-	initiating methionine	UNP A0A2K3DY10
Е	62	HIS	-	expression tag	UNP A0A2K3DY10
Е	63	HIS	-	expression tag	UNP A0A2K3DY10
E	64	HIS	-	expression tag	UNP A0A2K3DY10
E	65	HIS	-	expression tag	UNP A0A2K3DY10
E	66	HIS	-	expression tag	UNP A0A2K3DY10
E	67	HIS	-	expression tag	UNP A0A2K3DY10
E	68	HIS	-	expression tag	UNP A0A2K3DY10
E	69	MET	-	expression tag	UNP A0A2K3DY10
F	61	MET	-	initiating methionine	UNP A0A2K3DY10
F	62	HIS	-	expression tag	UNP A0A2K3DY10
F	63	HIS	-	expression tag	UNP A0A2K3DY10
F	64	HIS	-	expression tag	UNP A0A2K3DY10
F	65	HIS	-	expression tag	UNP A0A2K3DY10
F	66	HIS	-	expression tag	UNP A0A2K3DY10
F	67	HIS	-	expression tag	UNP A0A2K3DY10
F	68	HIS	-	expression tag	UNP A0A2K3DY10
F	69	MET	-	expression tag	UNP A0A2K3DY10
G	61	MET	-	initiating methionine	UNP A0A2K3DY10



Chain	Residue	Modelled	Actual	Comment	Reference
G	62	HIS	-	expression tag	UNP A0A2K3DY10
G	63	HIS	-	expression tag	UNP A0A2K3DY10
G	64	HIS	-	expression tag	UNP A0A2K3DY10
G	65	HIS	-	expression tag	UNP A0A2K3DY10
G	66	HIS	-	expression tag	UNP A0A2K3DY10
G	67	HIS	-	expression tag	UNP A0A2K3DY10
G	68	HIS	-	expression tag	UNP A0A2K3DY10
G	69	MET	-	expression tag	UNP A0A2K3DY10
Н	61	MET	-	initiating methionine	UNP A0A2K3DY10
Н	62	HIS	-	expression tag	UNP A0A2K3DY10
Н	63	HIS	-	expression tag	UNP A0A2K3DY10
Н	64	HIS	-	expression tag	UNP A0A2K3DY10
Н	65	HIS	-	expression tag	UNP A0A2K3DY10
Н	66	HIS	-	expression tag	UNP A0A2K3DY10
Н	67	HIS	-	expression tag	UNP A0A2K3DY10
Н	68	HIS	-	expression tag	UNP A0A2K3DY10
Н	69	MET	-	expression tag	UNP A0A2K3DY10

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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: FBPase domain-containing protein









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	53.77Å 163.46Å 172.76Å	Deperitor
a, b, c, α , β , γ	90.00° 91.94° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	48.54 - 3.11	Depositor
Resolution (A)	48.54 - 3.11	EDS
% Data completeness	99.5 (48.54-3.11)	Depositor
(in resolution range)	99.4(48.54-3.11)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.33 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D.	0.195 , 0.231	Depositor
Π, Π_{free}	0.196 , 0.232	DCC
R_{free} test set	1984 reflections (3.71%)	wwPDB-VP
Wilson B-factor $(Å^2)$	68.5	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33 , 45.4	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18714	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	
			# Z > 5	RMSZ	# Z > 5
1	А	0.31	0/2412	0.50	0/3264
1	В	0.29	0/2421	0.49	0/3275
1	С	0.29	0/2355	0.50	0/3184
1	D	0.27	0/2412	0.50	0/3264
1	Ε	0.30	0/2346	0.51	0/3173
1	F	0.28	0/2412	0.49	0/3264
1	G	0.28	0/2343	0.49	0/3168
1	Н	0.29	0/2386	0.49	0/3227
All	All	0.29	0/19087	0.50	0/25819

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2363	0	2340	26	0
1	В	2372	0	2353	27	0
1	С	2309	0	2298	37	0
1	D	2363	0	2340	21	0
1	Е	2299	0	2289	32	0



	J	1	1			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2363	0	2340	21	0
1	G	2297	0	2287	32	0
1	Н	2338	0	2318	38	0
2	А	5	0	0	0	0
2	G	5	0	0	0	0
All	All	18714	0	18565	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 6.

All (223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:344:GLY:HA2	1:C:379:TYR:OH	1.78	0.84
1:G:261:PRO:HB2	1:G:264:LEU:HD13	1.64	0.79
1:C:114:THR:HG23	1:C:124:ASN:HD21	1.46	0.79
1:E:261:PRO:HB2	1:E:264:LEU:HD13	1.64	0.79
1:D:293:MET:HE1	1:D:325:GLU:HB3	1.64	0.79
1:A:261:PRO:HB2	1:A:264:LEU:HD13	1.72	0.72
1:D:261:PRO:HB2	1:D:264:LEU:HD13	1.75	0.69
1:G:182:ILE:HB	1:G:187:PHE:HB2	1.75	0.69
1:H:266:ALA:HB1	1:H:313:SER:HB3	1.73	0.68
1:A:228:LYS:HA	1:A:335:LYS:HE3	1.76	0.67
1:E:182:ILE:HB	1:E:187:PHE:HB2	1.77	0.67
1:C:182:ILE:HB	1:C:187:PHE:HB2	1.75	0.67
1:C:265:ARG:HH21	1:H:284:LYS:HD2	1.59	0.67
1:E:307:VAL:HG22	1:E:370:GLU:HB3	1.77	0.66
1:G:322:ILE:HA	1:G:326:VAL:HB	1.78	0.66
1:E:334:GLU:O	1:E:335:LYS:HB2	1.94	0.66
1:G:266:ALA:C	1:G:268:PHE:H	2.00	0.65
1:G:266:ALA:HB1	1:G:313:SER:HB3	1.80	0.64
1:C:265:ARG:NH1	1:C:315:THR:OG1	2.30	0.64
1:G:256:GLY:HA3	1:G:305:LYS:HD2	1.80	0.64
1:C:345:LYS:O	1:C:347:VAL:HG13	1.99	0.63
1:F:251:THR:HA	1:F:336:ALA:HA	1.80	0.63
1:D:251:THR:HA	1:D:336:ALA:HA	1.82	0.62
1:A:269:ASP:HB2	1:A:314:PRO:HD2	1.82	0.62
1:B:83:GLU:O	1:B:86:VAL:HG12	2.01	0.60
1:E:331:LEU:O	1:E:335:LYS:HB2	2.02	0.60
1:B:287:LEU:HD21	1:F:287:LEU:HD11	1.84	0.60
1:C:329:LEU:HD23	1:C:332:LEU:HD12	1.83	0.60



	A L C	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:197:PRO:HD3	1:D:210:VAL:HG13	1.83	0.59
1:G:266:ALA:C	1:G:268:PHE:N	2.56	0.58
1:H:342:CYS:HB3	1:H:352:ILE:HG13	1.85	0.58
1:H:269:ASP:HB2	1:H:314:PRO:HD2	1.84	0.58
1:C:265:ARG:NH2	1:H:284:LYS:HD2	2.18	0.58
1:A:351:ASP:HB3	1:B:159:VAL:HG12	1.85	0.58
1:E:343:ASP:O	1:E:345:LYS:HG2	2.03	0.57
1:A:157:GLU:OE1	1:A:321:ARG:NH2	2.36	0.57
1:E:197:PRO:HD3	1:E:210:VAL:HG13	1.85	0.57
1:B:219:PRO:HG3	1:F:217:TYR:O	2.05	0.57
1:F:197:PRO:HD3	1:F:210:VAL:HG13	1.87	0.57
1:F:261:PRO:HB2	1:F:264:LEU:HD13	1.85	0.57
1:H:261:PRO:HB2	1:H:264:LEU:HD13	1.87	0.57
1:H:126:PHE:HB2	1:H:136:VAL:HG22	1.87	0.56
1:B:269:ASP:N	1:B:269:ASP:OD1	2.37	0.56
1:E:266:ALA:HB1	1:E:313:SER:HB3	1.87	0.55
1:E:342:CYS:SG	1:E:343:ASP:N	2.79	0.55
1:H:268:PHE:C	1:H:270:ASN:H	2.11	0.54
1:H:293:MET:HE1	1:H:325:GLU:HB3	1.88	0.54
1:E:363:ILE:HG12	1:E:365:TYR:CZ	2.41	0.54
1:H:182:ILE:HB	1:H:187:PHE:HB2	1.88	0.54
1:D:111:LYS:O	1:D:124:ASN:ND2	2.40	0.54
1:D:269:ASP:OD1	1:D:269:ASP:N	2.40	0.54
1:A:182:ILE:HB	1:A:187:PHE:HB2	1.90	0.53
1:F:363:ILE:HG12	1:F:365:TYR:CZ	2.44	0.53
1:G:313:SER:N	1:G:316:THR:HG22	2.24	0.53
1:B:190:GLY:HA3	1:B:294:VAL:HG11	1.90	0.53
1:C:269:ASP:OD1	1:C:269:ASP:N	2.38	0.53
1:B:197:PRO:HD3	1:B:210:VAL:HG13	1.89	0.53
1:B:261:PRO:HB2	1:B:264:LEU:HD13	1.89	0.53
1:F:182:ILE:HB	1:F:187:PHE:HB2	1.91	0.53
1:A:344:GLY:HA2	1:A:379:TYR:OH	2.09	0.53
1:A:266:ALA:C	1:A:268:PHE:H	2.13	0.52
1:E:265:ARG:HD3	1:E:265:ARG:O	2.10	0.52
1:E:227:LEU:O	1:E:335:LYS:HE3	2.09	0.52
1:C:197:PRO:HD3	1:C:210:VAL:HG13	1.91	0.52
1:C:261:PRO:HB2	1:C:264:LEU:HD13	1.92	0.52
1:C:363:ILE:HG12	1:C:365:TYR:CZ	2.45	0.52
1:H:279:PHE:CE1	1:H:283:GLU:HG3	2.45	0.52
1:E:343:ASP:HB2	1:E:352:ILE:HD12	1.92	0.52
1:D:363:ILE:HG12	1:D:365:TYR:CZ	2.44	0.51



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:363:ILE:HG12	1:G:365:TYR:CZ	2.44	0.51	
1:C:265:ARG:NE	1:C:316:THR:OG1	2.44	0.51	
1:D:83:GLU:O	1:D:86:VAL:HG12	2.10	0.51	
1:E:322:ILE:HA	1:E:326:VAL:HB	1.92	0.51	
1:D:288:ARG:HH12	1:D:303:LYS:HE3	1.76	0.50	
1:B:287:LEU:HD11	1:F:287:LEU:HD21	1.94	0.50	
1:E:265:ARG:HD3	1:E:268:PHE:CD1	2.47	0.50	
1:G:313:SER:H	1:G:316:THR:HG22	1.75	0.50	
1:H:256:GLY:HA3	1:H:305:LYS:HD2	1.93	0.50	
1:A:197:PRO:HD3	1:A:210:VAL:HG13	1.92	0.50	
1:B:290:THR:HG22	1:F:290:THR:HG22	1.93	0.50	
1:G:196:TRP:CE2	1:G:209:GLN:HG2	2.47	0.50	
1:C:220:ARG:NH1	1:H:115:ALA:O	2.45	0.49	
1:D:322:ILE:HA	1:D:326:VAL:HB	1.93	0.49	
1:E:196:TRP:CD1	1:E:204:ILE:HD12	2.47	0.49	
1:A:129:GLU:HG3	1:A:131:LEU:HD23	1.94	0.49	
1:F:322:ILE:HA	1:F:326:VAL:HB	1.93	0.49	
1:B:89:THR:O	1:B:95:ARG:NH1	2.45	0.49	
1:E:333:ILE:C	1:E:334:GLU:O	2.48	0.49	
1:G:269:ASP:OD2	1:G:315:THR:OG1	2.27	0.49	
1:C:111:LYS:O	1:C:124:ASN:ND2	2.45	0.49	
1:C:319:LYS:O	1:C:321:ARG:NH1	2.45	0.49	
1:H:363:ILE:HG13	1:H:364:CYS:N	2.28	0.49	
1:G:363:ILE:HG13	1:G:364:CYS:N	2.28	0.49	
1:A:89:THR:O	1:A:95:ARG:NH1	2.45	0.48	
1:B:266:ALA:HB1	1:B:313:SER:HB3	1.93	0.48	
1:B:305:LYS:HE2	1:B:305:LYS:HB2	1.70	0.48	
1:B:363:ILE:HG12	1:B:365:TYR:CZ	2.48	0.48	
1:F:106:ARG:HH12	1:H:242:GLY:HA3	1.79	0.48	
1:B:153:LEU:HB2	1:B:171:CYS:SG	2.54	0.48	
1:E:307:VAL:HG22	1:E:370:GLU:CB	2.43	0.48	
1:D:153:LEU:HB2	1:D:171:CYS:SG	2.54	0.48	
1:E:157:GLU:HG3	1:E:321:ARG:NH2	2.28	0.48	
1:H:268:PHE:O	1:H:270:ASN:N	2.47	0.48	
1:B:180:SER:HA	1:B:183:VAL:HG23	1.95	0.48	
1:H:153:LEU:HB2	1:H:171:CYS:SG	2.54	0.48	
1:A:181:SER:O	1:A:182:ILE:HG23	2.14	0.47	
1:H:261:PRO:HD2	1:H:289:TYR:HB2	1.96	0.47	
1:A:133:VAL:HA	1:A:136:VAL:HG12	1.96	0.47	
1:C:153:LEU:HB2	1:C:171:CYS:SG	2.54	0.47	
1:C:342:CYS:SG	1:C:343:ASP:N	2.88	0.47	



	i agem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:307:VAL:CG2 1:E:370:GLU:HB		2.45	0.47	
1:G:83:GLU:O	1:G:86:VAL:HG12	2.14	0.47	
1:G:269:ASP:OD2	1:G:313:SER:OG	2.25	0.47	
1:A:222:VAL:HG13	1:A:235:GLU:HG3	1.95	0.47	
1:E:269:ASP:OD2	1:E:315:THR:HG23	2.15	0.47	
1:F:179:GLY:HA3	1:F:189:VAL:HG12	1.95	0.47	
1:F:321:ARG:HD3	1:F:360:ARG:HD3	1.95	0.47	
1:A:384:ARG:HD2	1:B:161:GLU:HG2	1.96	0.47	
1:C:363:ILE:HG13	1:C:364:CYS:N	2.30	0.47	
1:G:117:CYS:HA	1:G:122:CYS:HA	1.95	0.47	
1:H:197:PRO:HD3	1:H:210:VAL:HG13	1.95	0.47	
1:H:342:CYS:HB2	1:H:349:ALA:HB2	1.95	0.47	
1:A:83:GLU:O	1:A:86:VAL:HG12	2.15	0.46	
1:E:331:LEU:O	1:E:334:GLU:O	2.33	0.46	
1:H:117:CYS:HA	1:H:122:CYS:HA	1.96	0.46	
1:H:363:ILE:HG12	1:H:365:TYR:CZ	2.51	0.46	
1:D:363:ILE:HG13	1:D:364:CYS:N	2.30	0.46	
1:H:266:ALA:HB1	1:H:313:SER:CB	2.42	0.46	
1:C:230:ALA:O	1:C:335:LYS:NZ	2.32	0.46	
1:F:266:ALA:HB1	1:F:313:SER:HB3	1.98	0.46	
1:G:269:ASP:OD1	1:G:269:ASP:N	2.47	0.46	
1:B:304:GLU:O	1:B:305:LYS:HG3	2.16	0.46	
1:F:305:LYS:HB2	1:F:305:LYS:HE2	1.73	0.46	
1:F:335:LYS:O	1:F:336:ALA:HB3	2.16	0.46	
1:F:363:ILE:HG13	1:F:364:CYS:N	2.30	0.46	
1:B:363:ILE:HG13	1:B:364:CYS:N	2.31	0.45	
1:E:153:LEU:HB2	1:E:171:CYS:SG	2.56	0.45	
1:G:266:ALA:CB	1:G:313:SER:HB3	2.45	0.45	
1:C:322:ILE:HA	1:C:326:VAL:HB	1.97	0.45	
1:H:269:ASP:OD2	1:H:315:THR:OG1	2.30	0.45	
1:C:322:ILE:HG22	1:C:327:ALA:HB2	1.97	0.45	
1:C:342:CYS:HB2	1:C:363:ILE:HD12	1.97	0.45	
1:E:363:ILE:HG13	1:E:364:CYS:N	2.31	0.45	
1:E:339:ALA:HB2	1:E:368:ILE:HD13	1.98	0.45	
1:F:257:LYS:HB3	1:F:285:TYR:HA	1.99	0.45	
1:H:266:ALA:C	1:H:268:PHE:N	2.68	0.45	
1:F:253:ILE:HG22	1:F:367:SER:HB3	1.99	0.45	
1:C:83:GLU:O	1:C:86:VAL:HG12	2.17	0.45	
1:A:343:ASP:HB3	1:A:345:LYS:HD2	1.98	0.44	
1:G:279:PHE:CZ	1:G:283:GLU:HG3	2.52	0.44	
1:H:334:GLU:C	1:H:336:ALA:H	2.21	0.44	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:343:ASP:HB2	1:C:352:ILE:HD12	1.99	0.44
1:E:265:ARG:O	1:E:268:PHE:HD1	2.00	0.44
1:F:184:ASP:N	1:F:184:ASP:OD1	2.50	0.44
1:A:106:ARG:HG3	1:A:238:LEU:HD21	1.98	0.44
1:D:128:ASP:OD1	1:D:128:ASP:N	2.47	0.44
1:G:115:ALA:HB1	1:G:122:CYS:HB3	1.99	0.44
1:H:269:ASP:OD1	1:H:269:ASP:N	2.44	0.44
1:D:180:SER:HA	1:D:183:VAL:HG23	1.99	0.44
1:G:184:ASP:OD1	1:G:184:ASP:N	2.51	0.44
1:B:179:GLY:O	1:B:182:ILE:HG12	2.18	0.44
1:C:287:LEU:HD21	1:H:287:LEU:HD11	2.00	0.44
1:C:317:LYS:HE3	1:C:317:LYS:HB2	1.72	0.44
1:H:83:GLU:O	1:H:86:VAL:HG12	2.18	0.44
1:G:264:LEU:HD11	1:G:277:ILE:HG13	2.00	0.44
1:H:276:LEU:O	1:H:279:PHE:HB3	2.18	0.44
1:A:363:ILE:HG13	1:A:364:CYS:N	2.33	0.43
1:C:184:ASP:N	1:C:184:ASP:OD1	2.50	0.43
1:H:205:THR:O	1:H:208:GLU:HG2	2.19	0.43
1:A:119:GLY:C	1:A:121:ALA:H	2.22	0.43
1:D:213:GLY:HA3	1:D:225:ILE:HG22	2.00	0.43
1:A:196:TRP:CD1	1:A:204:ILE:HD12	2.54	0.43
1:G:153:LEU:HB2	1:G:171:CYS:SG	2.58	0.43
1:H:102:ALA:HB1	1:H:244:TRP:NE1	2.34	0.43
1:C:322:ILE:HG12	1:C:361:THR:CG2	2.49	0.43
1:H:116:SER:HB3	1:H:123:VAL:HG22	2.01	0.43
1:H:293:MET:CE	1:H:325:GLU:HB3	2.48	0.43
1:E:268:PHE:CE1	1:E:269:ASP:HB2	2.54	0.43
1:B:183:VAL:HG22	1:B:189:VAL:HG11	2.00	0.43
1:H:267:THR:HB	1:H:274:GLU:HG3	2.00	0.43
1:H:344:GLY:O	1:H:379:TYR:CE1	2.72	0.43
1:G:199:ASP:OD1	1:G:199:ASP:N	2.52	0.42
1:G:308:PHE:HD2	1:G:365:TYR:HD2	1.67	0.42
1:A:363:ILE:HG12	1:A:365:TYR:CZ	2.54	0.42
1:G:197:PRO:HD3	1:G:210:VAL:HG13	2.00	0.42
1:G:305:LYS:HE2	1:G:305:LYS:HB2	1.82	0.42
1:B:307:VAL:HG22	1:B:370:GLU:HB3	2.01	0.42
1:A:184:ASP:N	1:A:184:ASP:OD1	2.52	0.42
1:C:342:CYS:HB2	1:C:363:ILE:CD1	2.50	0.42
1:D:223:PHE:HB2	1:D:244:TRP:CZ3	2.54	0.42
1:H:268:PHE:C	1:H:270:ASN:N	2.73	0.42
1:F:153:LEU:HB2	1:F:171:CYS:SG	2.60	0.42



A 4 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:184:ASP:N	1:B:184:ASP:OD1	2.54	0.41
1:D:345:LYS:O	1:D:347:VAL:HG13	2.20	0.41
1:E:343:ASP:CB	1:E:352:ILE:HD12	2.50	0.41
1:A:322:ILE:HD11	1:A:361:THR:HB	2.02	0.41
1:D:190:GLY:HA3	1:D:294:VAL:HG11	2.02	0.41
1:E:213:GLY:HA3	1:E:225:ILE:HG22	2.01	0.41
1:B:101:MET:HE3	1:B:172:VAL:HG11	2.02	0.41
1:C:179:GLY:O	1:C:183:VAL:HG13	2.20	0.41
1:C:372:ARG:HH11	1:C:385:PHE:HB3	1.85	0.41
1:D:184:ASP:OD1	1:D:184:ASP:N	2.51	0.41
1:E:264:LEU:HD12	1:E:267:THR:HG21	2.02	0.41
1:B:320:LEU:O	1:B:360:ARG:HA	2.20	0.41
1:C:264:LEU:HD12	1:C:264:LEU:HA	1.92	0.41
1:D:85:LEU:O	1:D:95:ARG:HD3	2.21	0.41
1:G:134:ASP:OD1	1:G:134:ASP:N	2.51	0.41
1:G:264:LEU:HD12	1:G:264:LEU:HA	1.82	0.41
1:G:263:ASN:ND2	1:G:319:LYS:HE3	2.36	0.41
1:C:266:ALA:C	1:C:268:PHE:H	2.24	0.41
1:G:154:ALA:HB3	1:G:165:MET:HE3	2.02	0.41
1:A:322:ILE:HA	1:A:326:VAL:HB	2.02	0.41
1:D:126:PHE:CD2	1:D:139:LYS:HD3	2.55	0.41
1:G:102:ALA:HB1	1:G:244:TRP:NE1	2.36	0.41
1:B:199:ASP:OD1	1:B:199:ASP:N	2.52	0.41
1:C:342:CYS:SG	1:C:361:THR:OG1	2.69	0.41
1:C:201:LEU:HD23	1:C:201:LEU:HA	1.83	0.40
1:E:334:GLU:O	1:E:335:LYS:CB	2.64	0.40
1:A:266:ALA:C	1:A:268:PHE:N	2.73	0.40
1:B:101:MET:CE	1:B:172:VAL:HG11	2.51	0.40
1:C:321:ARG:HE	1:C:321:ARG:HB2	1.68	0.40
1:E:159:VAL:O	1:E:161:GLU:N	2.49	0.40
1:H:79:ASP:HB2	1:H:83:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	308/331~(93%)	292~(95%)	14 (4%)	2(1%)	25 59
1	В	309/331~(93%)	296~(96%)	12~(4%)	1 (0%)	41 73
1	С	296/331~(89%)	282~(95%)	13~(4%)	1 (0%)	41 73
1	D	308/331~(93%)	293~(95%)	13~(4%)	2(1%)	25 59
1	Ε	297/331~(90%)	282~(95%)	14~(5%)	1 (0%)	41 73
1	F	308/331~(93%)	290 (94%)	17~(6%)	1 (0%)	41 73
1	G	295/331~(89%)	282~(96%)	12~(4%)	1 (0%)	41 73
1	Н	302/331~(91%)	280 (93%)	19 (6%)	3 (1%)	15 48
All	All	2423/2648~(92%)	2297~(95%)	114 (5%)	12 (0%)	29 63

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

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Е	116	SER
1	F	343	ASP
1	Н	269	ASP
1	С	179	GLY
1	G	179	GLY
1	D	343	ASP
1	Н	335	LYS
1	D	267	THR
1	Н	343	ASP
1	В	267	THR
1	A	179	GLY
1	А	182	ILE

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		Outliers	Percentiles	
1	А	253/270~(94%)	247~(98%)	6 (2%)	49 75	



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	254/270~(94%)	252~(99%)	2(1%)	81 92
1	С	248/270~(92%)	245~(99%)	3~(1%)	71 87
1	D	253/270~(94%)	249~(98%)	4 (2%)	62 84
1	Ε	246/270~(91%)	240~(98%)	6(2%)	49 75
1	F	253/270~(94%)	246~(97%)	7 (3%)	43 72
1	G	247/270~(92%)	242 (98%)	5(2%)	55 79
1	Н	251/270~(93%)	243~(97%)	8 (3%)	39 69
All	All	2005/2160~(93%)	1964 (98%)	41 (2%)	55 79

Continued from previous page...

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	130	GLN
1	А	180	SER
1	А	220	ARG
1	А	265	ARG
1	А	269	ASP
1	А	321	ARG
1	В	220	ARG
1	В	321	ARG
1	С	220	ARG
1	С	265	ARG
1	С	321	ARG
1	D	130	GLN
1	D	181	SER
1	D	220	ARG
1	D	265	ARG
1	Е	220	ARG
1	Е	268	PHE
1	Е	321	ARG
1	Е	335	LYS
1	Е	343	ASP
1	Е	345	LYS
1	F	130	GLN
1	F	220	ARG
1	F	263	ASN
1	F	265	ARG
1	F	273	TYR
1	F	321	ARG
1	F	345	LYS



Mol	Chain	Res	Type
1	G	220	ARG
1	G	229	ASP
1	G	265	ARG
1	G	269	ASP
1	G	284	LYS
1	Н	220	ARG
1	Н	265	ARG
1	Н	267	THR
1	Н	268	PHE
1	Н	269	ASP
1	Н	274	GLU
1	Н	321	ARG
1	Н	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	Turne	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Tink	В	ond leng	gths	В	ond ang	gles
	туре		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2														
2	SO4	A	401	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0														
2	SO4	G	401	-	4,4,4	0.13	0	$6,\!6,\!6$	0.06	0														

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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 $>$	#RS	SRZ:	>2	$OWAB(Å^2)$	Q < 0.9
1	А	310/331~(93%)	-0.26	3~(0%)	82	69	30, 50, 84, 118	0
1	В	311/331~(93%)	-0.13	2 (0%)	89	79	35, 49, 91, 124	0
1	С	302/331~(91%)	-0.08	1 (0%)	94	89	45, 64, 88, 113	0
1	D	310/331~(93%)	-0.12	4 (1%)	77	60	48, 67, 96, 126	0
1	Е	301/331~(90%)	-0.08	1 (0%)	94	89	49, 66, 92, 107	0
1	F	310/331~(93%)	0.00	10 (3%)	47	26	48, 71, 102, 121	0
1	G	301/331~(90%)	0.12	7 (2%)	60	39	52, 77, 104, 119	0
1	Н	306/331~(92%)	0.40	17 (5%)	24	11	50, 82, 110, 134	0
All	All	2451/2648~(92%)	-0.02	45 (1%)	68	48	30, 67, 101, 134	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	128	ASP	4.4
1	В	128	ASP	4.3
1	Н	201	LEU	4.3
1	D	129	GLU	4.0
1	Н	129	GLU	3.8
1	G	357	CYS	3.6
1	Н	169	GLY	3.6
1	Н	200	LYS	3.4
1	Н	126	PHE	3.2
1	А	120	THR	3.1
1	Н	381	THR	3.0
1	F	129	GLU	2.9
1	F	118	ALA	2.9
1	Н	165	MET	2.9
1	Е	357	CYS	2.8
1	F	122	CYS	2.7



120 V	$7\mathrm{Z}$	U	V
-------	---------------	---	---

Mol	Chain	Res	Type	RSRZ
1	G	166	GLY	2.6
1	В	127	GLY	2.6
1	Н	385	PHE	2.6
1	Н	380	GLY	2.6
1	F	F 120 THR		2.5
1	F 316 THR		2.5	
1	D 127 GLY		2.4	
1	Н	368	ILE	2.4
1	Н	151	CYS	2.4
1	F	128	ASP	2.4
1	А	129	GLU	2.4
1	F	315	THR	2.3
1	D	128	ASP	2.3
1	G	201	LEU	2.2
1	Н	323	LEU	2.2
1	G	283	GLU	2.2
1	А	130	GLN	2.2
1	G	368	ILE	2.2
1	Н	206	GLY	2.2
1	F	123	VAL	2.1
1	С	124	ASN	2.1
1	F	269	ASP	2.1
1	G	165	MET	2.1
1	Н	357	CYS	2.0
1	D	118	ALA	2.0
1	G	200	LYS	2.0
1	Н	273	TYR	2.0
1	F	130	GLN	2.0
1	Н	152	LYS	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 monosaccharides in this entry.



6.4 Ligands (i)

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	SO4	G	401	5/5	0.89	0.22	85,90,106,111	0
2	SO4	А	401	5/5	0.97	0.11	79,89,92,99	0

6.5 Other polymers (i)

There are no such residues in this entry.

