

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8183
Title	:	Crystal Structure of phosphinothricin dehydrogenase
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Deposited on	:	2023-02-03
Resolution	:	2.62 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 2.62 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	422	3% 	14%	
		122	0270	1470	
1	В	422	80%	16%	•••
1	С	422	8%	17%	•••
1	D	422	64% 12% •	24%	
1	Е	422	85%	12%	••
1	F	422	85%	13%	•



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18861 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	Λ	410	Total	С	Ν	0	\mathbf{S}	0	0	0
1	Л	410	3173	2005	539	609	20	0	0	0
1	Р	408	Total	С	Ν	0	S	0	0	0
1	D	400	3157	1995	536	606	20	0	0	0
1	C	410	Total	С	Ν	0	S	0	0	0
		410	3173	2005	539	609	20	0	0	0
1	Л	200	Total	С	Ν	0	S	0	0	0
1	D	522	2511	1592	430	470	19	0	0	U
1	Б	415	Total	С	Ν	0	S	0	0	0
	Г	415	3212	2028	545	619	20	0	0	0
1	1 E	413	Total	С	Ν	0	S	0	0	0
			3195	2017	543	615	20	0	U	

• Molecule 1 is a protein called Glutamate dehydrogenase.

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	138	GLY	ALA	conflict	UNP A0A3N9UCW8
А	141	MET	VAL	conflict	UNP A0A3N9UCW8
А	339	ALA	VAL	conflict	UNP A0A3N9UCW8
А	369	TYR	VAL	conflict	UNP A0A3N9UCW8
А	409	LEU	-	expression tag	UNP A0A3N9UCW8
А	410	GLU	-	expression tag	UNP A0A3N9UCW8
А	411	HIS	-	expression tag	UNP A0A3N9UCW8
А	412	HIS	-	expression tag	UNP A0A3N9UCW8
А	413	HIS	-	expression tag	UNP A0A3N9UCW8
А	414	HIS	-	expression tag	UNP A0A3N9UCW8
А	415	HIS	-	expression tag	UNP A0A3N9UCW8
А	416	HIS	-	expression tag	UNP A0A3N9UCW8
В	138	GLY	ALA	conflict	UNP A0A3N9UCW8
В	141	MET	VAL	conflict	UNP A0A3N9UCW8
В	339	ALA	VAL	conflict	UNP A0A3N9UCW8
В	369	TYR	VAL	conflict	UNP A0A3N9UCW8
В	409	LEU	-	expression tag	UNP A0A3N9UCW8



Chain	Residue	Modelled	Actual	Comment	Reference
В	410	GLU	-	expression tag	UNP A0A3N9UCW8
В	411	HIS	-	expression tag	UNP A0A3N9UCW8
В	412	HIS	-	expression tag	UNP A0A3N9UCW8
В	413	HIS	-	expression tag	UNP A0A3N9UCW8
В	414	HIS	-	expression tag	UNP A0A3N9UCW8
В	415	HIS	-	expression tag	UNP A0A3N9UCW8
В	416	HIS	-	expression tag	UNP A0A3N9UCW8
С	138	GLY	ALA	conflict	UNP A0A3N9UCW8
С	141	MET	VAL	conflict	UNP A0A3N9UCW8
С	339	ALA	VAL	conflict	UNP A0A3N9UCW8
С	369	TYR	VAL	conflict	UNP A0A3N9UCW8
С	409	LEU	-	expression tag	UNP A0A3N9UCW8
С	410	GLU	-	expression tag	UNP A0A3N9UCW8
С	411	HIS	-	expression tag	UNP A0A3N9UCW8
С	412	HIS	-	expression tag	UNP A0A3N9UCW8
С	413	HIS	-	expression tag	UNP A0A3N9UCW8
С	414	HIS	-	expression tag	UNP A0A3N9UCW8
С	415	HIS	-	expression tag	UNP A0A3N9UCW8
С	416	HIS	-	expression tag	UNP A0A3N9UCW8
D	138	GLY	ALA	conflict	UNP A0A3N9UCW8
D	141	MET	VAL	conflict	UNP A0A3N9UCW8
D	339	ALA	VAL	conflict	UNP A0A3N9UCW8
D	369	TYR	VAL	conflict	UNP A0A3N9UCW8
D	409	LEU	-	expression tag	UNP A0A3N9UCW8
D	410	GLU	-	expression tag	UNP A0A3N9UCW8
D	411	HIS	-	expression tag	UNP A0A3N9UCW8
D	412	HIS	-	expression tag	UNP A0A3N9UCW8
D	413	HIS	-	expression tag	UNP A0A3N9UCW8
D	414	HIS	-	expression tag	UNP A0A3N9UCW8
D	415	HIS	-	expression tag	UNP A0A3N9UCW8
D	416	HIS	-	expression tag	UNP A0A3N9UCW8
F	138	GLY	ALA	conflict	UNP A0A3N9UCW8
F	141	MET	VAL	conflict	UNP A0A3N9UCW8
F	339	ALA	VAL	conflict	UNP A0A3N9UCW8
F	369	TYR	VAL	conflict	UNP A0A3N9UCW8
F	409	LEU	-	expression tag	UNP A0A3N9UCW8
F	410	GLU	-	expression tag	UNP A0A3N9UCW8
F	411	HIS	-	expression tag	UNP A0A3N9UCW8
F	412	HIS	-	expression tag	UNP A0A3N9UCW8
F	413	HIS	-	expression tag	UNP A0A3N9UCW8
F	414	HIS	-	expression tag	UNP A0A3N9UCW8
F	415	HIS	-	expression tag	UNP A0A3N9UCW8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	416	HIS	-	expression tag	UNP A0A3N9UCW8
Е	138	GLY	ALA	conflict	UNP A0A3N9UCW8
E	141	MET	VAL	conflict	UNP A0A3N9UCW8
Е	339	ALA	VAL	conflict	UNP A0A3N9UCW8
E	369	TYR	VAL	conflict	UNP A0A3N9UCW8
Е	409	LEU	-	expression tag	UNP A0A3N9UCW8
Е	410	GLU	-	expression tag	UNP A0A3N9UCW8
E	411	HIS	-	expression tag	UNP A0A3N9UCW8
Е	412	HIS	-	expression tag	UNP A0A3N9UCW8
E	413	HIS	-	expression tag	UNP A0A3N9UCW8
E	414	HIS	-	expression tag	UNP A0A3N9UCW8
Ē	415	HIS	-	expression tag	UNP A0A3N9UCW8
E	416	HIS	-	expression tag	UNP A0A3N9UCW8

• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	68	Total O 68 68	0	0
3	В	84	Total O 84 84	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	56	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 56 & 56 \end{array}$	0	0
3	D	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0
3	F	97	Total O 97 97	0	0
3	Ε	84	Total O 84 84	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: Glutamate dehydrogenase

• Molecule 1: Glutamate dehydrogenase











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	95.13Å 126.67Å 223.74Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	48.22 - 2.62	Depositor
Resolution (A)	48.22 - 2.62	EDS
% Data completeness	99.1 (48.22-2.62)	Depositor
(in resolution range)	99.1 (48.22-2.62)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.16 (at 2.61 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.198 , 0.250	Depositor
n, n_{free}	0.199 , 0.251	DCC
R_{free} test set	4027 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	38.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.35 , 45.6	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18861	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.07% 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: EDO

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	
10101	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/3230	0.48	0/4369
1	В	0.25	0/3214	0.48	0/4347
1	С	0.25	0/3230	0.48	0/4369
1	D	0.25	0/2558	0.47	0/3447
1	Ε	0.25	0/3252	0.48	0/4399
1	F	0.26	0/3269	0.49	0/4422
All	All	0.25	0/18753	0.48	0/25353

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	3173	0	3167	40	0
1	В	3157	0	3150	41	0
1	С	3173	0	3167	41	0
1	D	2511	0	2520	31	0
1	Е	3195	0	3184	34	0
1	F	3212	0	3201	35	0
2	F	4	0	6	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	68	0	0	1	0
3	В	84	0	0	2	0
3	С	56	0	0	2	0
3	D	47	0	0	2	0
3	Е	84	0	0	2	0
3	F	97	0	0	2	0
All	All	18861	0	18395	214	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 (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:31:ARG:NH1	1:B:55:GLN:OE1	2.20	0.74
1:C:243:ASP:HB2	1:C:247:LEU:HD13	1.70	0.73
1:D:35:VAL:HG21	1:D:125:ALA:HB1	1.70	0.73
1:D:31:ARG:NH1	1:D:55:GLN:OE1	2.23	0.72
1:E:213:PHE:O	1:E:256:ARG:NH1	2.23	0.71
1:A:31:ARG:NH1	1:A:55:GLN:OE1	2.24	0.71
1:A:255:ARG:HD2	1:E:381:THR:HG23	1.74	0.70
1:F:81:LEU:HA	1:F:84:TRP:CD1	2.28	0.69
1:C:31:ARG:NH1	1:C:55:GLN:OE1	2.26	0.69
1:C:143:THR:HA	1:C:147:ILE:HD12	1.75	0.69
1:F:31:ARG:NH1	1:F:55:GLN:OE1	2.24	0.68
1:B:81:LEU:HB3	1:B:100:LYS:HE3	1.76	0.68
1:A:255:ARG:HD3	1:A:265:LEU:HD13	1.76	0.67
1:A:366:LYS:NZ	1:F:356:GLU:OE2	2.24	0.67
1:F:300:ILE:O	1:F:324:ARG:NH2	2.28	0.66
1:C:307:GLU:OE2	1:C:387:ARG:NH2	2.22	0.66
1:F:73:VAL:HG13	1:F:104:ILE:HG12	1.78	0.66
1:C:397:ARG:NH2	3:C:501:HOH:O	2.30	0.65
1:E:257:ASP:HB3	1:E:261:THR:H	1.61	0.64
1:E:318:THR:HG21	1:E:387:ARG:HE	1.63	0.64
1:C:231:VAL:HB	1:C:249:ILE:HD11	1.79	0.64
1:A:294:ALA:HB2	1:A:316:GLU:HG3	1.81	0.63
1:A:254:ASP:OD2	1:E:382:ARG:NH1	2.32	0.62
1:C:273:GLN:NE2	3:C:503:HOH:O	2.30	0.62
1:E:293:THR:O	1:E:295:GLU:N	2.28	0.62
1:B:397:ARG:NH2	3:B:501:HOH:O	2.27	0.61
1:D:92:VAL:HG23	1:D:94:LEU:HG	1.82	0.61



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:70:HIS:HB3	1:B:73:VAL:HG23	1.84	0.60	
1:B:279:ASP:HA	1:B:301:LYS:HB2	1.84	0.60	
1:A:190:ILE:HD13	1:A:365:TYR:HA	1.83	0.59	
1:C:64:LYS:HD2	1:C:136:ILE:HB	1.85	0.59	
1:D:382:ARG:HB3	1:D:382:ARG:HH11	1.68	0.59	
1:E:92:VAL:HG23	1:E:94:LEU:HG	1.85	0.59	
1:B:15:LYS:NZ	3:B:506:HOH:O	2.35	0.58	
1:C:190:ILE:HD13	1:C:365:TYR:HA	1.86	0.58	
1:F:92:VAL:HG23	1:F:94:LEU:HG	1.86	0.58	
1:B:180:ARG:HA	1:B:341:VAL:HG11	1.86	0.57	
1:C:81:LEU:HB3	1:C:100:LYS:HE3	1.85	0.57	
1:C:191:VAL:HG21	1:C:334:ALA:HA	1.87	0.57	
1:D:190:ILE:HD12	1:D:365:TYR:HA	1.87	0.57	
1:B:253:LEU:HA	1:B:256:ARG:HD3	1.87	0.56	
1:C:306:VAL:HA	1:C:329:VAL:HB	1.87	0.56	
1:B:311:GLY:N	1:B:312:PRO:HD3	2.20	0.56	
1:F:88:LYS:NZ	3:F:602:HOH:O	2.39	0.56	
1:C:225:SER:HB3	1:C:249:ILE:HD13	1.87	0.56	
1:B:356:GLU:OE1	1:B:356:GLU:N	2.36	0.55	
1:C:32:LEU:HD22	1:C:79:LYS:HD3	1.88	0.55	
1:C:321:LEU:HD22	1:C:326:ILE:HD12	1.89	0.55	
1:B:240:ALA:HB3	1:B:270:ILE:HG13	1.88	0.55	
1:A:180:ARG:NH1	1:A:345:GLU:OE1	2.40	0.55	
1:E:319:LYS:O	1:E:323:GLU:HG2	2.06	0.55	
1:E:231:VAL:HB	1:E:249:ILE:HD11	1.89	0.55	
1:A:266:PHE:O	1:A:268:ASN:N	2.39	0.55	
1:D:81:LEU:HB3	1:D:100:LYS:HG2	1.88	0.55	
1:F:199:ARG:NH2	1:F:325:GLY:O	2.41	0.54	
1:D:191:VAL:HG11	1:D:329:VAL:HG21	1.89	0.54	
1:D:382:ARG:HB3	1:D:382:ARG:NH1	2.23	0.54	
1:A:287:ALA:HB2	1:A:308:ALA:HB3	1.89	0.54	
1:F:65:GLY:HA3	1:F:99:GLY:O	2.08	0.54	
1:A:32:LEU:HD22	1:A:79:LYS:HD3	1.89	0.53	
1:A:201:ILE:HD13	1:A:281:ASP:HB3	1.90	0.53	
1:A:143:THR:HA	1:A:147:ILE:HD12	1.90	0.53	
1:E:292:ILE:HB	1:E:313:THR:HB	1.89	0.53	
1:C:393:VAL:HG22	1:C:396:ARG:HH22	1.74	0.53	
1:D:319:LYS:NZ	3:D:506:HOH:O	2.40	0.53	
1:E:65:GLY:HA3	1:E:99:GLY:O	2.08	0.53	
1:B:65:GLY:HA3	1:B:99:GLY:O	2.09	0.53	
1:F:65:GLY:O	1:F:137:PRO:HA	2.09	0.53	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:298:HIS:O	1:F:324:ARG:NH1	2.42	0.52
1:A:300:ILE:HD11	1:A:326:ILE:HD13	1.91	0.52
1:E:314:THR:O	1:E:318:THR:HG23	2.08	0.52
1:B:143:THR:HA	1:B:147:ILE:HD12	1.92	0.52
1:D:203:ILE:HG23	1:D:204:LYS:HD3	1.91	0.52
1:B:32:LEU:HD22	1:B:79:LYS:HD3	1.92	0.52
1:C:292:ILE:HG22	1:C:317:ALA:HB1	1.91	0.51
1:E:64:LYS:HD2	1:E:136:ILE:HB	1.91	0.51
1:F:84:TRP:HZ3	1:F:391:TYR:HH	1.59	0.51
1:A:63:THR:HG22	1:A:135:ASP:OD1	2.10	0.51
1:A:92:VAL:HG23	1:A:94:LEU:HG	1.93	0.51
1:D:2:PHE:HA	1:D:80:ALA:HB2	1.93	0.50
1:D:64:LYS:HD2	1:D:136:ILE:HB	1.91	0.50
1:C:278:LEU:O	1:C:301:LYS:HB3	2.11	0.50
1:C:287:ALA:HA	1:C:309:ALA:CB	2.42	0.50
1:F:240:ALA:HB3	1:F:270:ILE:HG13	1.94	0.50
1:B:13:LEU:HD11	1:B:26:LEU:HD12	1.94	0.49
1:C:257:ASP:OD1	1:C:258:SER:N	2.44	0.49
1:F:36:ARG:NH1	3:F:606:HOH:O	2.45	0.49
1:E:382:ARG:NH2	3:E:508:HOH:O	2.45	0.49
1:B:56:HIS:CD2	1:B:83:MET:HG2	2.48	0.49
1:A:144:ASN:O	1:A:148:MET:HG2	2.13	0.49
1:F:320:ILE:O	1:F:324:ARG:HG3	2.13	0.49
1:C:92:VAL:HG23	1:C:94:LEU:HG	1.93	0.49
1:C:357:GLU:O	1:C:361:GLN:HG3	2.13	0.49
1:C:287:ALA:HA	1:C:309:ALA:HB1	1.93	0.49
1:E:191:VAL:HG11	1:E:329:VAL:HG11	1.95	0.49
1:C:293:THR:HG22	1:C:294:ALA:H	1.77	0.49
1:B:92:VAL:HG12	1:B:367:LYS:HD2	1.95	0.48
1:D:65:GLY:HA3	1:D:99:GLY:O	2.12	0.48
1:C:65:GLY:HA3	1:C:99:GLY:O	2.12	0.48
1:E:198:LYS:HD2	1:E:376:TYR:CE1	2.49	0.48
1:F:208:VAL:HG22	1:F:282:ILE:HB	1.94	0.48
1:E:293:THR:HG22	1:E:314:THR:HG23	1.96	0.48
1:C:63:THR:HG23	1:C:99:GLY:HA3	1.95	0.47
1:F:124:ARG:NE	1:F:154:GLU:OE2	2.47	0.47
1:A:157:ARG:HD3	1:D:124:ARG:NH1	2.29	0.47
1:B:306:VAL:HA	1:B:329:VAL:HB	1.96	0.47
1:E:356:GLU:CD	1:E:356:GLU:H	2.17	0.47
1:F:70:HIS:O	1:F:73:VAL:HG12	2.13	0.47
1:E:199:ARG:NH2	1:E:325:GLY:O	2.28	0.47



Interatomic Clash						
Atom-1	Atom-2	distance (Å)	overlap (Å)			
1:A:157:ARG:HD3	1:D:124:ARG:HH11	1.80	0.47			
1:E:311:GLY:N	1:E:312:PRO:HD3	2.30	0.47			
1:D:69:PHE:N	3:D:501:HOH:O	2.27	0.47			
1:D:70:HIS:HB3	1:D:73:VAL:HG23	1.97	0.47			
1:F:144:ASN:O	1:F:148:MET:HG2	2.15	0.47			
1:A:65:GLY:HA3	1:A:99:GLY:O	2.13	0.47			
1:A:310:ASN:O	1:A:310:ASN:ND2	2.48	0.47			
1:B:178:LYS:HB3	1:B:357:GLU:HG2	1.97	0.47			
1:F:292:ILE:HG22	1:F:317:ALA:HB1	1.96	0.47			
1:B:144:ASN:O	1:B:148:MET:HG2	2.15	0.46			
1:F:120:ARG:O	1:F:124:ARG:HG3	2.15	0.46			
1:E:292:ILE:HG22	1:E:317:ALA:HB1	1.98	0.46			
1:A:240:ALA:HB3	1:A:270:ILE:HG23	1.97	0.46			
1:C:55:GLN:HG2	1:C:63:THR:HG21	1.97	0.46			
1:D:331:ASP:OD1	1:D:331:ASP:N	2.49	0.46			
1:D:376:TYR:HA	1:D:386:MET:HE2	1.98	0.46			
1:B:28:GLU:HB2	1:D:36:ARG:HD2	1.98	0.46			
1:A:178:LYS:HB3	1:A:357:GLU:HG2	1.98	0.46			
1:B:252:LEU:O	1:B:256:ARG:HB3	2.16	0.46			
1:B:65:GLY:O	1:B:137:PRO:HA	2.16	0.46			
1:C:65:GLY:O	1:C:137:PRO:HA	2.16	0.46			
1:D:170:LYS:O	1:D:180:ARG:NH2	2.49	0.46			
1:E:321:LEU:HD22	1:E:326:ILE:HD13	1.97	0.46			
1:F:84:TRP:HZ3	1:F:391:TYR:OH	1.99	0.46			
1:B:2:PHE:HZ	1:B:28:GLU:HG2	1.81	0.45			
1:D:388:LEU:HA	1:D:391:TYR:CD2	2.51	0.45			
1:B:358:GLU:O	1:B:362:GLU:HG2	2.16	0.45			
1:A:16:LEU:HD22	1:A:396:ARG:HH11	1.82	0.45			
1:A:29:PRO:HA	1:A:56:HIS:HA	1.98	0.45			
1:F:81:LEU:HB3	1:F:100:LYS:HG2	1.98	0.45			
1:C:187:GLY:O	1:C:191:VAL:HG23	2.16	0.45			
1:C:192:ILE:HG12	1:C:306:VAL:HG21	1.98	0.45			
1:F:63:THR:HG22	1:F:135:ASP:OD1	2.16	0.45			
1:F:64:LYS:HD2	1:F:136:ILE:HB	1.99	0.45			
1:B:318:THR:HG23	1:B:328:LEU:HD23	1.99	0.45			
1:A:134:LYS:HG2	1:F:161:PHE:HB3	1.98	0.45			
1:E:307:GLU:OE2	1:E:313:THR:HG23	2.17	0.45			
1:D:368:MET:HE2	1:D:368:MET:HA	1.98	0.44			
1:B:356:GLU:H	1:B:356:GLU:CD	2.20	0.44			
1:B:221:ALA:HB1	1:B:249:ILE:HD12	1.99	0.44			
1:B:316:GLU:H	1:B:316:GLU:HG3	1.48	0.44			



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:E:15:LYS:HD2	1:E:388:LEU:HD21	1.99	0.44	
1:E:356:GLU:OE1	1:E:356:GLU:N	2.46	0.44	
1:D:190:ILE:HG21	1:D:368:MET:HB2	1.99	0.44	
1:F:73:VAL:HA	1:F:77:GLU:OE1	2.18	0.44	
1:E:191:VAL:CG1	1:E:329:VAL:HG11	2.48	0.44	
1:C:316:GLU:HA	1:C:319:LYS:HB3	2.00	0.44	
1:F:87:LEU:HB2	1:F:332:VAL:HG21	1.99	0.44	
1:B:191:VAL:HG13	1:B:372:PHE:CD1	2.52	0.43	
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.87	0.43	
1:E:235:SER:HB3	1:E:275:LEU:HD13	1.99	0.43	
1:A:124:ARG:NH1	1:D:157:ARG:HG3	2.33	0.43	
1:B:300:ILE:HD11	1:B:326:ILE:HD13	1.99	0.43	
1:D:32:LEU:HD22	1:D:79:LYS:HD3	2.00	0.43	
1:D:185:ALA:HB1	1:D:219:PHE:CD1	2.54	0.43	
1:E:65:GLY:O	1:E:137:PRO:HA	2.18	0.43	
1:A:57:SER:O	1:A:97:GLY:HA3	2.18	0.43	
1:B:190:ILE:HD13	1:B:365:TYR:HA	2.01	0.43	
1:F:356:GLU:H	1:F:356:GLU:HG2	1.73	0.43	
1:B:300:ILE:O	1:B:300:ILE:HG13	2.19	0.43	
1:D:314:THR:N	1:D:317:ALA:HB3	2.34	0.43	
1:D:387:ARG:NH1	1:D:391:TYR:OH	2.50	0.43	
1:A:63:THR:HG23	1:A:99:GLY:HA3	2.01	0.43	
1:A:300:ILE:HD12	1:A:302:ALA:H	1.84	0.43	
1:F:297:ALA:HA	1:F:300:ILE:HD12	2.01	0.43	
1:E:182:ARG:O	1:E:186:GLU:HB2	2.19	0.43	
1:B:283:LEU:O	1:B:305:VAL:HA	2.19	0.43	
1:C:171:PRO:HD2	1:C:174:LEU:HD12	2.00	0.43	
1:B:2:PHE:HA	1:B:80:ALA:HB2	2.01	0.42	
1:B:331:ASP:OD1	1:B:331:ASP:N	2.52	0.42	
1:D:53:ARG:HD2	1:D:53:ARG:HA	1.86	0.42	
1:E:124:ARG:NH1	3:E:511:HOH:O	2.52	0.42	
1:A:279:ASP:HA	1:A:301:LYS:HB3	2.02	0.42	
1:A:316:GLU:HG2	1:A:317:ALA:N	2.34	0.42	
1:A:318:THR:HG23	1:A:328:LEU:HD23	2.00	0.42	
1:E:66:GLY:HA2	1:E:138:GLY:H	1.85	0.42	
1:A:65:GLY:O	1:A:137:PRO:HA	2.19	0.42	
1:E:144:ASN:O	1:E:148:MET:HG2	2.20	0.42	
1:C:358:GLU:OE1	1:C:358:GLU:N	2.45	0.42	
1:F:15:LYS:HE3	1:F:384:ILE:HG21	2.01	0.42	
1:A:300:ILE:HG12	1:A:321:LEU:HD21	2.01	0.42	
1:A:70:HIS:HB3	1:A:73:VAL:HG23	2.02	0.42	



Atom 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:178:LYS:NZ	3:A:513:HOH:O	2.53	0.42
1:B:88:LYS:HG2	1:B:332:VAL:HG23	2.02	0.42
1:A:13:LEU:HD11	1:A:26:LEU:HD12	2.02	0.41
1:A:15:LYS:HD2	1:A:388:LEU:HD21	2.02	0.41
1:E:68:ARG:HB3	1:E:140:ASP:HB3	2.02	0.41
1:F:63:THR:HG23	1:F:99:GLY:HA3	2.03	0.41
1:E:307:GLU:OE2	1:E:387:ARG:NH2	2.40	0.41
1:C:144:ASN:O	1:C:148:MET:HG2	2.20	0.41
1:F:81:LEU:HD23	1:F:84:TRP:HD1	1.86	0.41
1:B:220:LEU:O	1:B:224:MET:HG2	2.21	0.41
1:C:15:LYS:HD2	1:C:15:LYS:HA	1.86	0.41
1:C:152:MET:HE1	1:C:174:LEU:HD22	2.03	0.41
1:D:15:LYS:HE3	1:D:15:LYS:HB3	1.94	0.41
1:C:207:ARG:HA	1:C:230:LYS:O	2.21	0.41
1:F:153:ASP:O	1:F:157:ARG:HG2	2.20	0.41
1:B:64:LYS:HD2	1:B:136:ILE:HB	2.03	0.40
1:C:135:ASP:O	1:C:137:PRO:HD3	2.20	0.40
1:F:35:VAL:HG21	1:F:125:ALA:HB1	2.02	0.40
1:C:92:VAL:HA	1:C:371:SER:OG	2.21	0.40
1:C:192:ILE:HG23	1:C:282:ILE:HG21	2.03	0.40
1:B:284:VAL:HG22	1:B:306:VAL:HB	2.04	0.40
1:A:235:SER:HA	1:A:240:ALA:HA	2.04	0.40
1:C:292:ILE:HB	1:C:313:THR:HG22	2.03	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.

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	Perce	ntiles
1	А	408/422~(97%)	394 (97%)	12 (3%)	2 (0%)	29	50
1	В	406/422~(96%)	396 (98%)	10 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	С	408/422~(97%)	393~(96%)	14 (3%)	1 (0%)	47	69
1	D	318/422~(75%)	312 (98%)	6(2%)	0	100	100
1	Ε	411/422~(97%)	396~(96%)	15 (4%)	0	100	100
1	F	413/422~(98%)	403 (98%)	10 (2%)	0	100	100
All	All	2364/2532~(93%)	2294 (97%)	67 (3%)	3~(0%)	51	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	310	ASN
1	А	262	VAL
1	А	311	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	337/348~(97%)	330~(98%)	7 (2%)	53	76
1	В	335/348~(96%)	326~(97%)	9(3%)	44	69
1	С	337/348~(97%)	326~(97%)	11 (3%)	38	62
1	D	265/348~(76%)	255~(96%)	10 (4%)	33	57
1	Ε	339/348~(97%)	333~(98%)	6 (2%)	59	79
1	F	341/348~(98%)	332 (97%)	9(3%)	46	70
All	All	1954/2088~(94%)	1902 (97%)	52 (3%)	44	69

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	63	THR
1	А	92	VAL
1	А	159	ASP
1	А	265	LEU



Mol	Chain	Res	Type
1	А	300	ILE
1	А	316	GLU
1	А	380	THR
1	В	47	GLN
1	В	60	VAL
1	В	78	VAL
1	В	92	VAL
1	В	159	ASP
1	В	189	THR
1	В	288	ILE
1	В	300	ILE
1	В	316	GLU
1	С	14	ASN
1	С	35	VAL
1	С	47	GLN
1	С	63	THR
1	С	92	VAL
1	С	159	ASP
1	С	243	ASP
1	С	245	ASN
1	С	255	ARG
1	С	270	ILE
1	С	272	ASN
1	D	7	GLU
1	D	35	VAL
1	D	47	GLN
1	D	159	ASP
1	D	181	ASP
1	D	191	VAL
1	D	203	ILE
1	D	369	TYR
1	D	395	VAL
1	D	403	ARG
1	F	4	SER
1	F	35	VAL
1	F	63	THR
1	F	78	VAL
1	F	159	ASP
1	F	191	VAL
1	F	209	VAL
1	F	213	PHE
1	F	410	GLU



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Mol	Chain	Res	Type
1	Ε	35	VAL
1	Ε	159	ASP
1	Ε	191	VAL
1	Е	209	VAL
1	Е	213	PHE
1	Ε	313	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	Ε	47	GLN

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)

1 ligand is 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 Cl		Chain	Chain Rea		Bond lengths			Bond angles		
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	EDO	F	501	-	3,3,3	0.48	0	$2,\!2,\!2$	0.36	0



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	EDO	F	501	-	-	0/1/1/1	-

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 >	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	410/422~(97%)	0.01	11 (2%) 54 49	25, 41, 87, 124	0
1	В	408/422~(96%)	-0.25	0 100 100	27, 43, 66, 87	0
1	С	410/422~(97%)	0.26	33 (8%) 12 9	26, 50, 113, 141	0
1	D	322/422~(76%)	0.71	58 (18%) 1 0	29, 47, 113, 154	0
1	Е	413/422~(97%)	-0.23	0 100 100	26, 40, 64, 91	0
1	F	415/422~(98%)	-0.31	2 (0%) 91 89	23, 37, 55, 87	0
All	All	2378/2532~(93%)	0.00	104 (4%) 34 28	23, 42, 97, 154	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	205	GLY	8.3
1	D	196	ALA	7.8
1	D	214	GLY	7.2
1	D	212	GLY	6.5
1	D	200	ASN	6.4
1	D	326	ILE	6.2
1	С	245	ASN	6.0
1	D	224	MET	5.9
1	D	213	PHE	5.9
1	D	190	ILE	5.9
1	D	203	ILE	5.9
1	С	-1	LEU	5.8
1	D	207	ARG	5.8
1	D	329	VAL	5.7
1	D	206	ALA	5.6
1	D	327	LEU	5.6
1	D	209	VAL	5.6
1	D	208	VAL	5.4
1	D	210	ILE	5.4



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Mol	Chain	Res	Type	RSRZ
1	D	201	ILE	5.3
1	D	211	GLN	5.1
1	D	322	THR	4.9
1	С	265	LEU	4.8
1	D	204	LYS	4.8
1	D	191	VAL	4.8
1	D	198	LYS	4.7
1	D	217	GLY	4.7
1	D	195	ALA	4.4
1	D	323	GLU	4.3
1	С	266	PHE	4.3
1	D	218	SER	4.2
1	С	303	THR	4.2
1	D	318	THR	4.1
1	С	227	LEU	4.0
1	D	202	ASP	4.0
1	D	328	LEU	4.0
1	А	-1	LEU	3.8
1	D	223	PHE	3.8
1	А	259	PHE	3.8
1	С	304	ILE	3.7
1	D	324	ARG	3.6
1	D	222	LYS	3.6
1	D	197	LYS	3.5
1	D	316	GLU	3.5
1	С	264	THR	3.4
1	D	221	ALA	3.4
1	С	267	GLU	3.3
1	А	258	SER	3.3
1	С	274	GLU	3.2
1	С	200	ASN	3.2
1	D	220	LEU	3.2
1	D	314	THR	3.1
1	D	369	TYR	3.1
1	А	203	ILE	3.1
1	D	-1	LEU	3.0
1	С	204	LYS	3.0
1	D	193	GLN	3.0
1	С	279	ASP	3.0
1	D	325	GLY	2.9
1	С	202	ASP	2.9
1	С	268	ASN	2.9



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Mol	Chain	Res	Type	RSRZ	
1	С	203	ILE	2.9	
1	D	321	LEU	2.9	
1	D	194	GLU	2.9	
1	С	322	THR	2.9	
1	D	365	TYR	2.8	
1	С	249	ILE	2.8	
1	D	334	ALA	2.8	
1	С	246	GLY	2.8	
1	D	320	ILE	2.8	
1	С	233	GLY	2.8	
1	С	262	VAL	2.7	
1	С	255	ARG	2.7	
1	D	319	LYS	2.6	
1	С	260	GLY	2.6	
1	D	182	ARG	2.6	
1	С	198	LYS	2.5	
1	D	199	ARG	2.5	
1	С	230	LYS	2.4	
1	D	376	TYR	2.4	
1	А	270	ILE	2.4	
1	С	272	ASN	2.4	
1	С	206	ALA	2.4	
1	А	262	VAL	2.4	
1	А	202	ASP	2.4	
1	А	301	LYS	2.4	
1	D	372	PHE	2.4	
1	D	192	ILE	2.3	
1	С	308	ALA	2.3	
1	D	215	ASN	2.3	
1	А	267	GLU	2.3	
1	С	284	VAL	2.3	
1	С	325	GLY	2.3	
1	D	330	PRO	2.2	
1	F	-4	ALA	2.2	
1	А	204	LYS	2.2	
1	С	278	LEU	2.2	
1	D	225	SER	2.1	
1	С	327	LEU	2.1	
1	D	386	MET	2.1	
1	F	203	ILE	2.1	
1	С	248	ASP	2.1	
1	D	189	THR	2.1	



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Mol	Chain	Res	Type	RSRZ	
1	А	212	GLY	2.1	

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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
2	EDO	F	501	4/4	0.95	0.28	27,28,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.

