



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:24 PM UTC

PDB ID : 8I83 / pdb_00008i83
Title : Crystal Structure of phosphinothricin dehydrogenase
Authors : Cheng, F.; Xue, Y.P.; Zheng, Y.G.; Zou, S.P.
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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
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

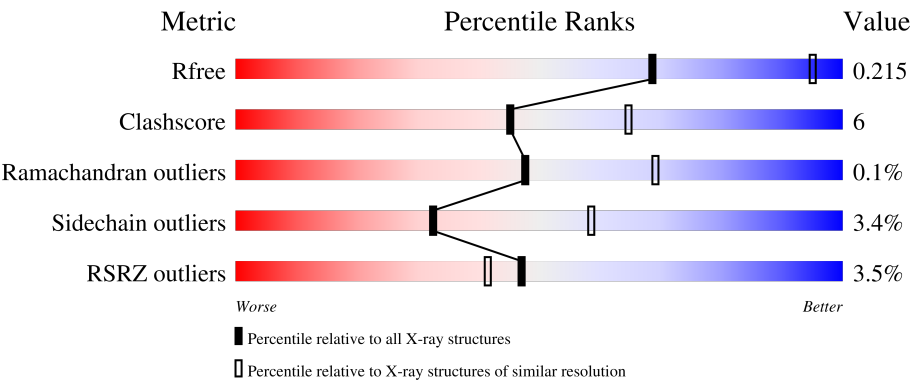
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 $\leq 5\%$. 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	422	2% 81% 15% ..
1	B	422	% 79% 17% ..
1	C	422	6% 79% 18% ..
1	D	422	9% 63% 11% 24%
1	E	422	% 84% 14% .

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Mol	Chain	Length	Quality of chain
1	F	422	 86% 12% ..

2 Entry composition

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.

- Molecule 1 is a protein called Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3173	2005	539	609	20			
1	B	408	Total	C	N	O	S	0	0	0
			3157	1995	536	606	20			
1	C	410	Total	C	N	O	S	0	0	0
			3173	2005	539	609	20			
1	D	322	Total	C	N	O	S	0	0	0
			2511	1592	430	470	19			
1	F	415	Total	C	N	O	S	0	0	0
			3212	2028	545	619	20			
1	E	413	Total	C	N	O	S	0	0	0
			3195	2017	543	615	20			

There are 72 discrepancies between the modelled and reference sequences:

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

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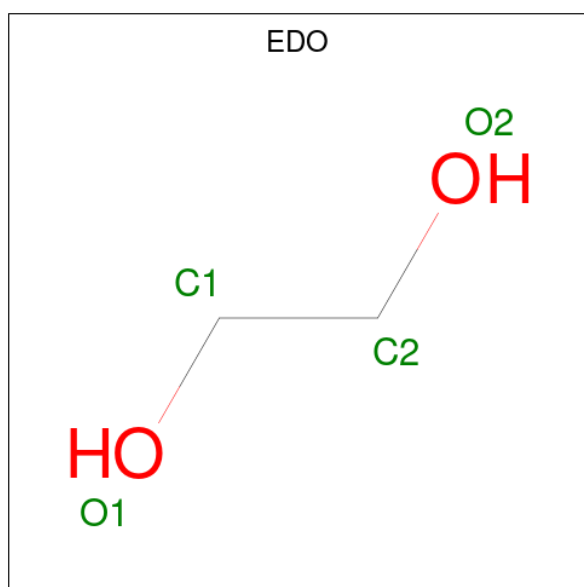
Chain	Residue	Modelled	Actual	Comment	Reference
B	410	GLU	-	expression tag	UNP A0A3N9UCW8
B	411	HIS	-	expression tag	UNP A0A3N9UCW8
B	412	HIS	-	expression tag	UNP A0A3N9UCW8
B	413	HIS	-	expression tag	UNP A0A3N9UCW8
B	414	HIS	-	expression tag	UNP A0A3N9UCW8
B	415	HIS	-	expression tag	UNP A0A3N9UCW8
B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

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	84	Total	O	0	0
			84	84		

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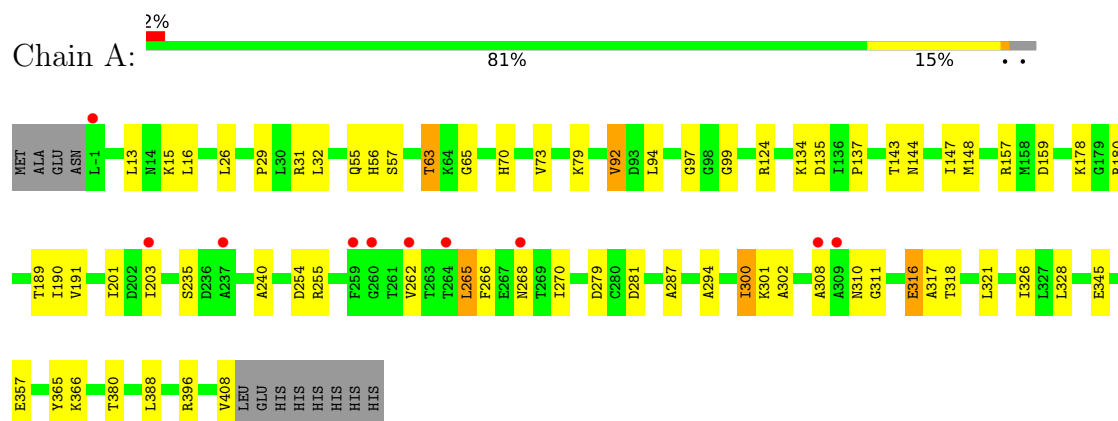
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	56	Total 56	O 56	0	0
3	D	47	Total 47	O 47	0	0
3	F	97	Total 97	O 97	0	0
3	E	84	Total 84	O 84	0	0

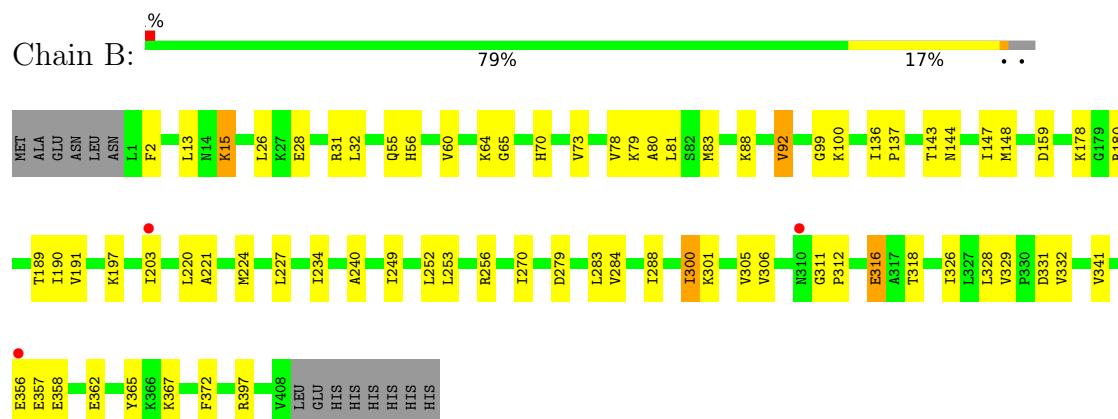
3 Residue-property plots [i](#)

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.

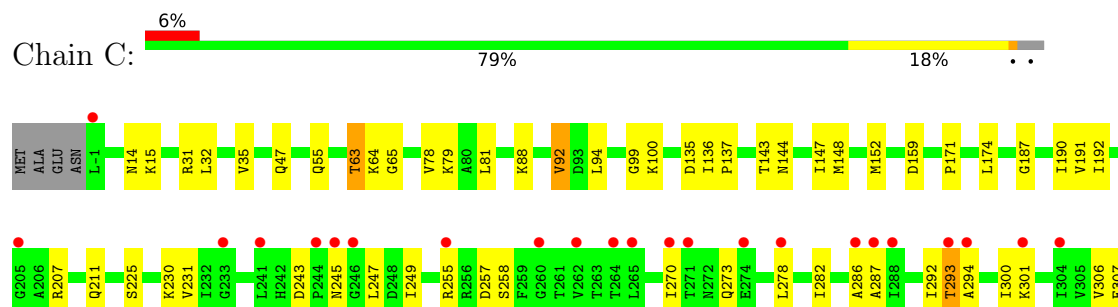
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.13Å 126.67Å 223.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.62 48.22 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.22-2.62) 99.1 (48.22-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.198 , 0.250 (Not available) , 0.215	Depositor DCC
R_{free} test set	4029 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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

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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3230	0.28	0/4369
1	B	0.11	0/3214	0.28	0/4347
1	C	0.11	0/3230	0.30	0/4369
1	D	0.11	0/2558	0.28	0/3447
1	E	0.11	0/3252	0.30	1/4399 (0.0%)
1	F	0.12	0/3269	0.31	0/4422
All	All	0.11	0/18753	0.29	1/25353 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	287	ALA	CB-CA-C	-5.36	108.71	116.54

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	3173	0	3167	40	0
1	B	3157	0	3150	41	0
1	C	3173	0	3167	42	0
1	D	2511	0	2520	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3195	0	3184	35	0
1	F	3212	0	3201	35	0
2	F	4	0	6	0	0
3	A	68	0	0	1	0
3	B	84	0	0	2	0
3	C	56	0	0	2	0
3	D	47	0	0	1	0
3	E	84	0	0	2	0
3	F	97	0	0	2	0
All	All	18861	0	18395	217	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 (217) 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: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: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:D:192:ILE:HG21	1:D:224:MET:HE1	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:366:LYS:NZ	1:F:356:GLU:OE2	2.24	0.61
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:336:ALA:HB3	1:D:368:MET:HE1	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:VAL:HG22	1:C:396:ARG:HH22	1.74	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
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:E:356:GLU:CD	1:E:356:GLU:H	2.17	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:D:147:ILE:HG22	1:D:148:MET:HE2	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:B:356:GLU:CD	1:B:356:GLU:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:E:140:ASP:H	1:E:143:THR:HG1	1.62	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: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:D:327:LEU:HD11	1:D:386:MET:HE3	1.98	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:C:152:MET:HE2	1:C:174:LEU:HB3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASP:OD1	1:D:331:ASP:N	2.49	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:211:GLN:C	1:C:286:ALA:HB2	2.45	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: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 ⓘ

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	408/422 (97%)	394 (97%)	12 (3%)	2 (0%)	24	44
1	B	406/422 (96%)	396 (98%)	10 (2%)	0	100	100
1	C	408/422 (97%)	393 (96%)	14 (3%)	1 (0%)	43	64
1	D	318/422 (75%)	312 (98%)	6 (2%)	0	100	100
1	E	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%)	48	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	310	ASN
1	A	262	VAL
1	A	311	GLY

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	337/348 (97%)	326 (97%)	11 (3%)	33	59
1	B	335/348 (96%)	323 (96%)	12 (4%)	31	56
1	C	337/348 (97%)	324 (96%)	13 (4%)	28	53
1	D	265/348 (76%)	252 (95%)	13 (5%)	22	44
1	E	339/348 (97%)	330 (97%)	9 (3%)	39	65
1	F	341/348 (98%)	333 (98%)	8 (2%)	44	69
All	All	1954/2088 (94%)	1888 (97%)	66 (3%)	32	58

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	92	VAL

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Mol	Chain	Res	Type
1	A	159	ASP
1	A	189	THR
1	A	191	VAL
1	A	203	ILE
1	A	265	LEU
1	A	300	ILE
1	A	316	GLU
1	A	380	THR
1	A	408	VAL
1	B	15	LYS
1	B	60	VAL
1	B	78	VAL
1	B	92	VAL
1	B	159	ASP
1	B	189	THR
1	B	197	LYS
1	B	203	ILE
1	B	234	ILE
1	B	288	ILE
1	B	300	ILE
1	B	316	GLU
1	C	14	ASN
1	C	35	VAL
1	C	47	GLN
1	C	63	THR
1	C	78	VAL
1	C	88	LYS
1	C	92	VAL
1	C	159	ASP
1	C	245	ASN
1	C	255	ARG
1	C	270	ILE
1	C	293	THR
1	C	300	ILE
1	D	7	GLU
1	D	35	VAL
1	D	159	ASP
1	D	181	ASP
1	D	190	ILE
1	D	191	VAL
1	D	203	ILE
1	D	329	VAL

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Mol	Chain	Res	Type
1	D	368	MET
1	D	386	MET
1	D	395	VAL
1	D	403	ARG
1	D	408	VAL
1	F	4	SER
1	F	35	VAL
1	F	63	THR
1	F	78	VAL
1	F	191	VAL
1	F	209	VAL
1	F	234	ILE
1	F	300	ILE
1	E	35	VAL
1	E	159	ASP
1	E	191	VAL
1	E	209	VAL
1	E	234	ILE
1	E	241	LEU
1	E	242	HIS
1	E	313	THR
1	E	366	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	242	HIS
1	A	290	ASN
1	A	298	HIS
1	B	146	GLN
1	C	298	HIS
1	E	298	HIS

5.3.3 RNA ⓘ

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](#)

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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	F	501	-	3,3,3	0.44	0	2,2,2	0.40	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

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	410/422 (97%)	0.02	10 (2%) 59 54	25, 41, 87, 124	0
1	B	408/422 (96%)	-0.18	3 (0%) 84 82	27, 43, 66, 87	0
1	C	410/422 (97%)	0.30	26 (6%) 26 21	26, 50, 113, 141	0
1	D	322/422 (76%)	0.33	38 (11%) 9 7	29, 47, 113, 154	0
1	E	413/422 (97%)	-0.19	4 (0%) 79 76	26, 40, 64, 91	0
1	F	415/422 (98%)	-0.30	2 (0%) 87 85	23, 37, 55, 87	0
All	All	2378/2532 (93%)	-0.02	83 (3%) 47 41	23, 42, 97, 154	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	LEU	4.4
1	C	260	GLY	3.9
1	D	213	PHE	3.9
1	D	327	LEU	3.8
1	A	260	GLY	3.7
1	C	287	ALA	3.6
1	D	196	ALA	3.5
1	D	212	GLY	3.4
1	F	-4	ALA	3.2
1	D	322	THR	3.1
1	C	270	ILE	3.0
1	D	329	VAL	3.0
1	C	286	ALA	3.0
1	C	205	GLY	2.9
1	A	262	VAL	2.9
1	D	195	ALA	2.9
1	C	-1	LEU	2.9
1	D	214	GLY	2.9
1	D	203	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	265	LEU	2.8
1	D	215	ASN	2.8
1	D	321	LEU	2.8
1	D	191	VAL	2.8
1	D	318	THR	2.8
1	E	294	ALA	2.8
1	D	315	SER	2.7
1	C	308	ALA	2.7
1	E	271	THR	2.7
1	C	271	THR	2.7
1	C	262	VAL	2.6
1	E	-4	ALA	2.6
1	D	210	ILE	2.6
1	F	409	LEU	2.6
1	A	308	ALA	2.6
1	D	201	ILE	2.6
1	B	310	ASN	2.6
1	C	278	LEU	2.5
1	A	259	PHE	2.5
1	D	380	THR	2.5
1	D	319	LYS	2.5
1	D	218	SER	2.5
1	D	211	GLN	2.5
1	A	203	ILE	2.4
1	C	274	GLU	2.4
1	C	264	THR	2.4
1	D	316	GLU	2.4
1	D	206	ALA	2.4
1	C	244	PRO	2.4
1	C	246	GLY	2.4
1	A	264	THR	2.3
1	C	301	LYS	2.3
1	D	207	ARG	2.3
1	D	216	ALA	2.3
1	B	356	GLU	2.3
1	A	268	ASN	2.3
1	A	309	ALA	2.2
1	D	331	ASP	2.2
1	C	255	ARG	2.2
1	D	205	GLY	2.2
1	A	237	ALA	2.2
1	C	304	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	190	ILE	2.2
1	C	294	ALA	2.2
1	C	245	ASN	2.2
1	D	224	MET	2.2
1	B	203	ILE	2.2
1	D	204	LYS	2.1
1	D	391	TYR	2.1
1	C	293	THR	2.1
1	D	223	PHE	2.1
1	C	233	GLY	2.1
1	D	326	ILE	2.1
1	E	270	ILE	2.1
1	D	385	ASP	2.1
1	C	309	ALA	2.1
1	D	225	SER	2.1
1	D	197	LYS	2.1
1	D	200	ASN	2.1
1	C	288	ILE	2.1
1	D	369	TYR	2.1
1	D	209	VAL	2.0
1	C	241	LEU	2.0
1	C	408	VAL	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](#)

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	EDO	F	501	4/4	0.88	0.17	27,28,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.