



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:50 AM UTC

PDB ID : 6PBR / pdb_00006pbr
Title : Catalytic domain of E.coli dihydrolipoamide succinyltransferase in I4 space group
Authors : Andi, B.; Soares, A.S.; Shi, W.; Fuchs, M.R.; McSweeney, S.; Liu, Q.
Deposited on : 2019-06-14
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

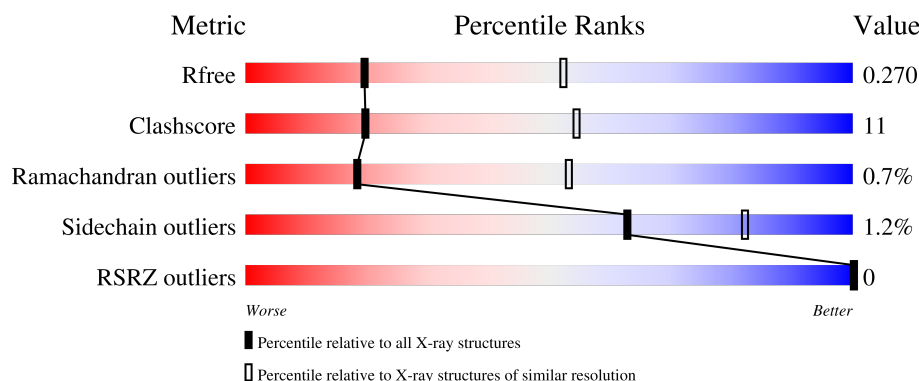
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	233	 72% 27% .
1	B	233	 76% 24%
1	C	233	 80% 20%
1	D	233	 73% 26% .
1	E	233	 73% 25% .

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Mol	Chain	Length	Quality of chain
1	F	233	 76%23%•

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10974 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 Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1827	1158	319	338	12			
1	B	233	Total	C	N	O	S	0	0	0
			1827	1158	319	338	12			
1	C	233	Total	C	N	O	S	0	0	0
			1827	1158	319	338	12			
1	D	233	Total	C	N	O	S	0	0	0
			1827	1158	319	338	12			
1	E	233	Total	C	N	O	S	0	0	0
			1827	1158	319	338	12			
1	F	233	Total	C	N	O	S	0	0	0
			1827	1158	319	338	12			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

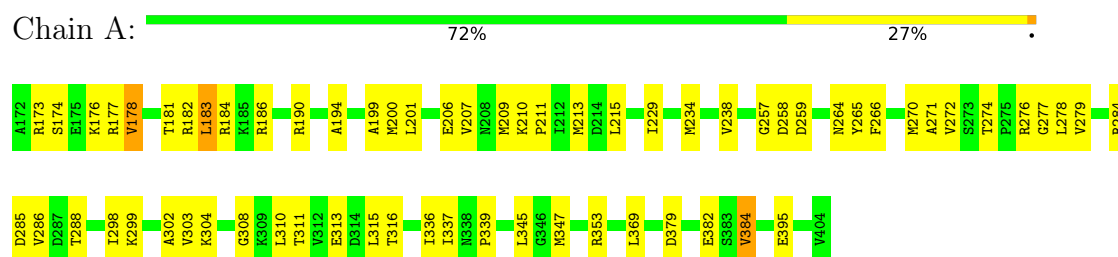
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	2	Total 2	O 2	0	0
3	C	1	Total 1	O 1	0	0
3	D	2	Total 2	O 2	0	0

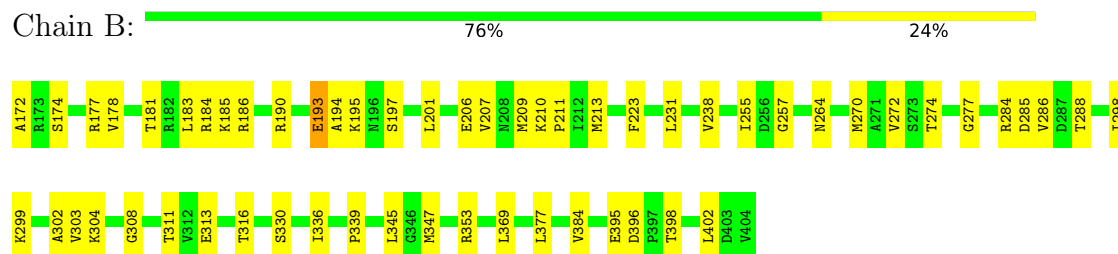
3 Residue-property plots

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.

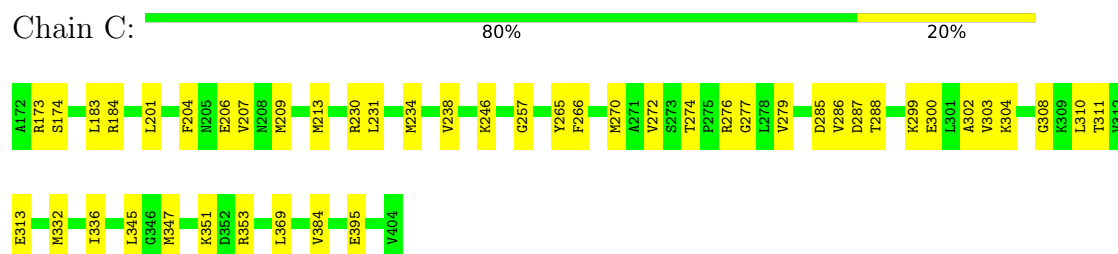
- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex



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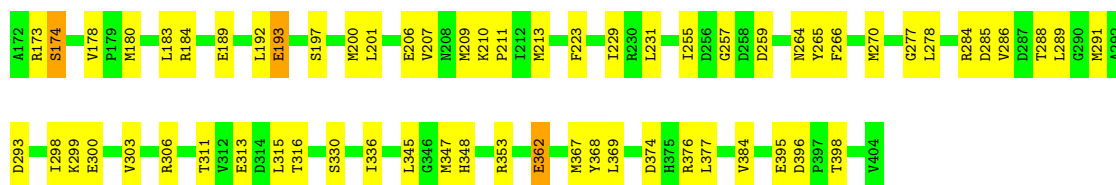


- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex



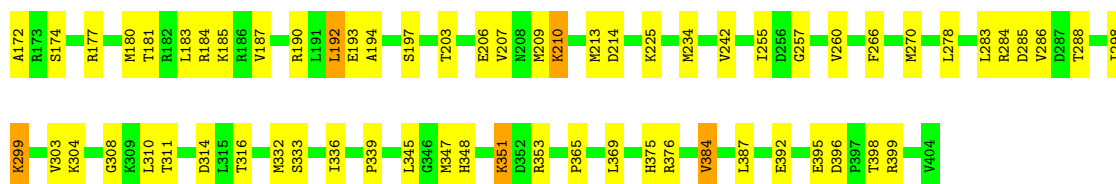
- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex





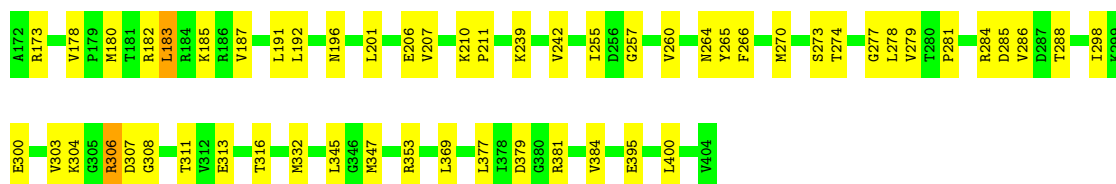
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Chain E: 73% 25% .



- Molecule 1: Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex

Chain F: 76% 23% .



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	128.60Å 128.60Å 249.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.36 – 3.00 47.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	82.8 (47.36-3.00) 82.8 (47.36-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.230 , 0.272 0.229 , 0.270	Depositor DCC
R_{free} test set	1641 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10974	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: NA

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	1.08	1/1856 (0.1%)	1.59	2/2502 (0.1%)
1	B	1.09	1/1856 (0.1%)	1.57	2/2502 (0.1%)
1	C	1.07	0/1856	1.59	2/2502 (0.1%)
1	D	1.09	1/1856 (0.1%)	1.54	2/2502 (0.1%)
1	E	1.08	0/1856	1.56	2/2502 (0.1%)
1	F	1.10	1/1856 (0.1%)	1.57	1/2502 (0.0%)
All	All	1.08	4/11136 (0.0%)	1.57	11/15012 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	VAL	N-CA	5.19	1.49	1.45
1	F	178	VAL	N-CA	5.19	1.49	1.45
1	B	178	VAL	N-CA	5.17	1.49	1.45
1	D	178	VAL	N-CA	5.15	1.49	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	384	VAL	CA-C-N	5.53	126.12	119.98
1	D	384	VAL	C-N-CA	5.53	126.12	119.98
1	F	185	LYS	CA-C-O	-5.47	115.26	121.00
1	E	384	VAL	CA-C-N	5.37	125.94	119.98
1	E	384	VAL	C-N-CA	5.37	125.94	119.98
1	A	384	VAL	CA-C-N	5.35	125.92	119.98
1	A	384	VAL	C-N-CA	5.35	125.92	119.98
1	B	384	VAL	CA-C-N	5.19	125.74	119.98
1	B	384	VAL	C-N-CA	5.19	125.74	119.98
1	C	384	VAL	CA-C-N	5.13	125.67	119.98
1	C	384	VAL	C-N-CA	5.13	125.67	119.98

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	1827	0	1886	58	0
1	B	1827	0	1886	46	0
1	C	1827	0	1886	33	0
1	D	1827	0	1886	61	0
1	E	1827	0	1886	59	0
1	F	1827	0	1886	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
All	All	10974	0	11316	256	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 11.

All (256) 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:E:270:MET:HE1	1:E:298:ILE:HG12	1.33	1.06
1:A:183:LEU:HD12	1:A:184:ARG:N	1.69	1.06
1:A:183:LEU:HD12	1:A:184:ARG:H	1.11	1.06
1:C:183:LEU:HD12	1:C:184:ARG:N	1.79	0.97
1:B:396:ASP:OD1	1:B:398:THR:HG22	1.64	0.96
1:D:396:ASP:OD1	1:D:398:THR:HG22	1.65	0.95
1:B:264:ASN:HD21	1:C:174:SER:HB2	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:HB1	1:A:278:LEU:HD21	1.53	0.89
1:D:189:GLU:O	1:D:193:GLU:HG2	1.75	0.86
1:E:310:LEU:HD12	1:E:310:LEU:O	1.75	0.85
1:A:265:TYR:CD2	1:B:172:ALA:HA	2.13	0.82
1:B:238:VAL:CG1	1:B:286:VAL:HG11	2.08	0.82
1:A:259:ASP:OD2	1:B:177:ARG:HD3	1.82	0.80
1:A:379:ASP:OD1	1:A:382:GLU:HG2	1.81	0.80
1:D:345:LEU:HG	1:D:347:MET:HE3	1.64	0.79
1:E:270:MET:HE1	1:E:298:ILE:CG1	2.13	0.77
1:B:181:THR:HB	1:B:183:LEU:HB3	1.66	0.76
1:B:264:ASN:ND2	1:C:174:SER:HB2	1.99	0.76
1:B:345:LEU:HG	1:B:347:MET:HE3	1.69	0.75
1:C:345:LEU:HG	1:C:347:MET:HE3	1.67	0.75
1:A:258:ASP:OD1	1:B:185:LYS:HE2	1.86	0.75
1:F:345:LEU:HG	1:F:347:MET:HE3	1.68	0.74
1:A:345:LEU:HG	1:A:347:MET:HE3	1.69	0.74
1:A:186:ARG:O	1:A:190:ARG:HG2	1.88	0.74
1:B:186:ARG:O	1:B:190:ARG:HG3	1.89	0.72
1:A:200:MET:HE2	1:A:337:ILE:H	1.54	0.72
1:A:183:LEU:CD1	1:A:184:ARG:H	1.98	0.72
1:A:258:ASP:OD1	1:B:185:LYS:CE	2.37	0.71
1:E:345:LEU:HG	1:E:347:MET:HE3	1.71	0.71
1:A:200:MET:HE1	1:A:336:ILE:HG13	1.70	0.71
1:D:174:SER:HB2	1:F:264:ASN:HD21	1.56	0.71
1:C:183:LEU:HD12	1:C:184:ARG:H	1.57	0.70
1:D:201:LEU:HD21	1:E:336:ILE:HB	1.73	0.70
1:D:289:LEU:HD22	1:D:293:ASP:HB3	1.76	0.68
1:A:181:THR:HB	1:A:183:LEU:HG	1.76	0.67
1:D:173:ARG:HB3	1:F:265:TYR:HB3	1.77	0.67
1:D:180:MET:HE3	1:F:260:VAL:HB	1.76	0.66
1:B:402:LEU:HD23	1:D:291:MET:HE2	1.75	0.66
1:B:402:LEU:CD2	1:D:291:MET:HE2	2.25	0.66
1:B:206:GLU:OE2	1:C:351:LYS:NZ	2.26	0.65
1:A:173:ARG:NH1	1:C:287:ASP:OD2	2.30	0.64
1:A:274:THR:HG21	1:A:279:VAL:HG23	1.81	0.63
1:C:204:PHE:CD1	1:C:332:MET:HE2	2.34	0.63
1:D:336:ILE:HB	1:F:201:LEU:HD11	1.81	0.62
1:E:311:THR:CG2	1:E:314:ASP:CG	2.74	0.61
1:D:376:ARG:HD2	1:E:192:LEU:CD1	2.31	0.60
1:E:396:ASP:OD1	1:E:398:THR:HG22	2.01	0.60
1:A:284:ARG:NH2	1:A:316:THR:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:TYR:CG	1:E:172:ALA:HA	2.37	0.59
1:B:284:ARG:NH2	1:B:316:THR:O	2.34	0.59
1:A:336:ILE:HB	1:C:201:LEU:HD11	1.83	0.59
1:E:284:ARG:NH2	1:E:316:THR:O	2.34	0.59
1:A:183:LEU:CD1	1:A:184:ARG:N	2.57	0.59
1:A:272:VAL:HG11	1:A:302:ALA:HA	1.84	0.59
1:E:375:HIS:CD2	1:F:191:LEU:HD13	2.38	0.59
1:F:284:ARG:NH2	1:F:316:THR:O	2.32	0.59
1:F:311:THR:HG22	1:F:313:GLU:H	1.68	0.59
1:B:347:MET:HE1	1:B:369:LEU:HD22	1.84	0.59
1:C:230:ARG:NH1	1:C:231:LEU:O	2.36	0.58
1:A:199:ALA:HA	1:B:195:LYS:HD2	1.85	0.58
1:D:206:GLU:OE2	1:E:351:LYS:NZ	2.30	0.58
1:D:180:MET:SD	1:F:260:VAL:HG23	2.44	0.58
1:E:183:LEU:HD12	1:E:183:LEU:O	2.04	0.58
1:F:274:THR:HB	1:F:277:GLY:O	2.04	0.58
1:F:182:ARG:O	1:F:183:LEU:CB	2.51	0.58
1:D:180:MET:HE2	1:D:180:MET:HA	1.85	0.58
1:E:270:MET:CE	1:E:298:ILE:HG12	2.22	0.58
1:D:348:HIS:H	1:D:367:MET:HE2	1.68	0.57
1:D:284:ARG:NH2	1:D:316:THR:O	2.37	0.57
1:E:206:GLU:OE1	1:E:353:ARG:NH2	2.38	0.57
1:F:206:GLU:OE1	1:F:353:ARG:NH2	2.38	0.57
1:C:207:VAL:HG23	1:C:395:GLU:HG3	1.87	0.56
1:B:396:ASP:OD1	1:B:398:THR:CG2	2.46	0.56
1:C:206:GLU:OE1	1:C:353:ARG:NH2	2.38	0.56
1:A:347:MET:HE1	1:A:369:LEU:HD22	1.88	0.56
1:A:199:ALA:HA	1:B:195:LYS:CD	2.36	0.56
1:E:392:GLU:HB3	1:E:399:ARG:NH2	2.21	0.55
1:A:206:GLU:OE1	1:A:353:ARG:NH2	2.40	0.55
1:D:396:ASP:OD1	1:D:398:THR:CG2	2.48	0.55
1:B:270:MET:HE1	1:B:298:ILE:HG23	1.87	0.55
1:A:311:THR:HG22	1:A:313:GLU:H	1.71	0.55
1:D:207:VAL:HG23	1:D:395:GLU:HG3	1.88	0.55
1:A:279:VAL:HG11	1:A:310:LEU:HD23	1.89	0.55
1:D:265:TYR:CD2	1:E:172:ALA:HA	2.42	0.55
1:E:210:LYS:NZ	1:E:214:ASP:OD1	2.39	0.55
1:B:206:GLU:OE1	1:B:353:ARG:NH2	2.39	0.55
1:F:239:LYS:HB3	1:F:400:LEU:HD21	1.89	0.55
1:C:347:MET:HE1	1:C:369:LEU:HD22	1.88	0.55
1:D:278:LEU:HD13	1:F:379:ASP:OD2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:347:MET:HE1	1:F:369:LEU:HD22	1.89	0.54
1:A:207:VAL:HG23	1:A:395:GLU:HG3	1.90	0.54
1:D:180:MET:SD	1:F:260:VAL:CG2	2.95	0.54
1:E:180:MET:HE3	1:E:185:LYS:HE3	1.90	0.54
1:B:311:THR:HG22	1:B:313:GLU:H	1.73	0.54
1:D:311:THR:HG22	1:D:313:GLU:H	1.73	0.54
1:F:207:VAL:HG23	1:F:395:GLU:HG3	1.88	0.53
1:E:270:MET:CE	1:E:283:LEU:HD11	2.38	0.53
1:E:311:THR:HG22	1:E:314:ASP:OD2	2.09	0.53
1:A:299:LYS:O	1:A:303:VAL:HG23	2.09	0.53
1:E:347:MET:HE1	1:E:369:LEU:HD22	1.89	0.53
1:D:330:SER:HB3	1:F:384:VAL:CG1	2.39	0.53
1:D:347:MET:HE1	1:D:369:LEU:HD22	1.89	0.53
1:F:311:THR:CG2	1:F:313:GLU:OE1	2.56	0.53
1:B:207:VAL:HG23	1:B:395:GLU:HG3	1.89	0.53
1:A:258:ASP:OD1	1:B:185:LYS:HE3	2.08	0.53
1:F:192:LEU:O	1:F:196:ASN:ND2	2.39	0.53
1:C:279:VAL:HG21	1:C:310:LEU:CD1	2.39	0.52
1:D:330:SER:HB3	1:F:384:VAL:HG13	1.91	0.52
1:E:311:THR:HG22	1:E:314:ASP:CG	2.35	0.52
1:A:201:LEU:HD11	1:B:336:ILE:HB	1.91	0.52
1:B:238:VAL:HG11	1:B:286:VAL:HG11	1.90	0.52
1:A:200:MET:HE1	1:A:336:ILE:CG1	2.40	0.51
1:E:255:ILE:O	1:E:255:ILE:HG23	2.08	0.51
1:D:206:GLU:OE1	1:D:353:ARG:NH2	2.42	0.51
1:A:173:ARG:HB2	1:C:265:TYR:HB3	1.93	0.51
1:C:311:THR:HG22	1:C:313:GLU:H	1.76	0.51
1:D:200:MET:C	1:D:201:LEU:HD12	2.36	0.51
1:B:299:LYS:O	1:B:303:VAL:HG23	2.11	0.51
1:E:396:ASP:CG	1:E:398:THR:HG22	2.36	0.51
1:E:207:VAL:HG23	1:E:395:GLU:HG3	1.93	0.50
1:E:299:LYS:O	1:E:303:VAL:HG23	2.12	0.50
1:B:345:LEU:CG	1:B:347:MET:HE3	2.41	0.50
1:D:174:SER:HB2	1:F:264:ASN:ND2	2.22	0.50
1:C:345:LEU:HG	1:C:347:MET:CE	2.40	0.49
1:D:192:LEU:CD2	1:D:193:GLU:OE2	2.60	0.49
1:E:203:THR:HG21	1:E:384:VAL:HG22	1.94	0.49
1:E:332:MET:HE1	1:F:332:MET:HE1	1.94	0.49
1:D:210:LYS:HB3	1:D:211:PRO:HD3	1.95	0.49
1:D:184:ARG:HG3	1:D:184:ARG:O	2.14	0.48
1:D:223:PHE:CD2	1:D:231:LEU:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ASP:OD2	1:E:177:ARG:HD3	2.13	0.48
1:B:223:PHE:CD2	1:B:231:LEU:HB2	2.48	0.48
1:D:362:GLU:HA	1:D:362:GLU:OE1	2.14	0.48
1:C:204:PHE:CG	1:C:332:MET:HE2	2.48	0.48
1:E:213:MET:HE2	1:E:365:PRO:HG3	1.94	0.48
1:F:311:THR:HG22	1:F:313:GLU:OE1	2.13	0.47
1:D:345:LEU:HG	1:D:347:MET:CE	2.41	0.47
1:B:238:VAL:HG12	1:B:286:VAL:HG11	1.93	0.47
1:A:194:ALA:HB1	1:A:339:PRO:HG2	1.96	0.47
1:B:210:LYS:HB3	1:B:211:PRO:HD3	1.96	0.47
1:E:333:SER:OG	1:E:348:HIS:CE1	2.68	0.47
1:D:197:SER:O	1:E:192:LEU:HD11	2.15	0.47
1:C:300:GLU:O	1:C:303:VAL:HG22	2.14	0.46
1:D:255:ILE:HD11	1:D:377:LEU:HB2	1.97	0.46
1:D:277:GLY:O	1:D:278:LEU:HD12	2.16	0.46
1:A:176:LYS:HE3	1:A:178:VAL:CG1	2.45	0.46
1:B:285:ASP:O	1:B:288:THR:OG1	2.34	0.46
1:E:255:ILE:HG21	1:E:376:ARG:NH2	2.30	0.46
1:D:229:ILE:CD1	1:D:299:LYS:HD2	2.45	0.46
1:E:197:SER:O	1:E:376:ARG:NH1	2.49	0.45
1:F:239:LYS:HB3	1:F:400:LEU:CD2	2.46	0.45
1:A:271:ALA:CB	1:A:278:LEU:HD21	2.37	0.45
1:D:353:ARG:NH1	1:D:368:TYR:OH	2.49	0.45
1:F:345:LEU:CG	1:F:347:MET:HE3	2.44	0.45
1:F:345:LEU:HG	1:F:347:MET:CE	2.41	0.45
1:A:210:LYS:HB3	1:A:211:PRO:HD3	1.98	0.45
1:E:194:ALA:CB	1:E:339:PRO:HG2	2.47	0.45
1:C:274:THR:O	1:C:277:GLY:O	2.34	0.45
1:C:345:LEU:CG	1:C:347:MET:HE3	2.43	0.45
1:A:176:LYS:HE3	1:A:178:VAL:HG11	1.99	0.44
1:D:374:ASP:OD1	1:D:376:ARG:HD3	2.17	0.44
1:E:181:THR:HB	1:E:183:LEU:HG	1.98	0.44
1:F:273:SER:HA	1:F:278:LEU:HG	1.99	0.44
1:D:311:THR:O	1:D:315:LEU:HD13	2.18	0.44
1:A:183:LEU:CD1	1:A:184:ARG:HG3	2.48	0.44
1:E:181:THR:O	1:E:185:LYS:HB2	2.18	0.44
1:F:300:GLU:O	1:F:303:VAL:HG22	2.17	0.44
1:F:187:VAL:O	1:F:191:LEU:HG	2.17	0.44
1:A:211:PRO:O	1:A:215:LEU:HD13	2.18	0.44
1:E:311:THR:HG23	1:E:314:ASP:CG	2.43	0.44
1:D:209:MET:O	1:D:213:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:MET:CE	1:E:365:PRO:HG3	2.48	0.44
1:F:210:LYS:HB3	1:F:211:PRO:HD3	1.99	0.44
1:C:266:PHE:O	1:C:286:VAL:HG22	2.18	0.44
1:D:300:GLU:O	1:D:303:VAL:HG22	2.18	0.44
1:F:270:MET:HE1	1:F:298:ILE:HG23	1.98	0.44
1:D:348:HIS:O	1:D:367:MET:HE2	2.18	0.43
1:F:266:PHE:O	1:F:286:VAL:HG22	2.18	0.43
1:C:272:VAL:HG21	1:C:302:ALA:HA	1.99	0.43
1:A:304:LYS:O	1:A:308:GLY:N	2.51	0.43
1:D:193:GLU:O	1:D:197:SER:HB3	2.18	0.43
1:D:285:ASP:O	1:D:288:THR:OG1	2.35	0.43
1:E:183:LEU:O	1:E:184:ARG:HB3	2.19	0.43
1:F:255:ILE:HD11	1:F:377:LEU:HB2	1.98	0.43
1:D:201:LEU:HD11	1:E:336:ILE:HD12	2.01	0.43
1:A:229:ILE:HD11	1:A:299:LYS:HD2	2.01	0.43
1:A:384:VAL:HG13	1:B:330:SER:HB2	2.00	0.43
1:A:345:LEU:CG	1:A:347:MET:HE3	2.44	0.43
1:B:345:LEU:HG	1:B:347:MET:CE	2.44	0.43
1:A:234:MET:HE2	1:A:270:MET:SD	2.59	0.43
1:B:304:LYS:O	1:B:308:GLY:N	2.51	0.43
1:B:201:LEU:HD11	1:C:336:ILE:HB	2.00	0.43
1:E:266:PHE:O	1:E:286:VAL:HG22	2.19	0.43
1:A:285:ASP:O	1:A:288:THR:OG1	2.35	0.42
1:D:348:HIS:O	1:D:367:MET:CE	2.67	0.42
1:A:264:ASN:ND2	1:B:174:SER:OG	2.42	0.42
1:C:234:MET:HE2	1:C:270:MET:SD	2.59	0.42
1:D:183:LEU:O	1:D:184:ARG:HB3	2.19	0.42
1:A:266:PHE:O	1:A:286:VAL:HG22	2.19	0.42
1:D:192:LEU:HD22	1:D:193:GLU:OE2	2.18	0.42
1:D:270:MET:HE1	1:D:298:ILE:HG23	2.01	0.42
1:B:272:VAL:HG11	1:B:302:ALA:HA	2.00	0.42
1:F:306:ARG:HG3	1:F:307:ASP:OD1	2.19	0.42
1:E:255:ILE:O	1:E:255:ILE:CG2	2.68	0.42
1:E:285:ASP:O	1:E:288:THR:OG1	2.35	0.42
1:A:183:LEU:HD12	1:A:184:ARG:CA	2.47	0.42
1:E:184:ARG:HA	1:E:187:VAL:CG1	2.50	0.42
1:E:304:LYS:O	1:E:308:GLY:N	2.50	0.42
1:B:255:ILE:HD11	1:B:377:LEU:HB2	2.02	0.42
1:C:304:LYS:O	1:C:308:GLY:N	2.51	0.42
1:D:266:PHE:O	1:D:286:VAL:HG22	2.19	0.42
1:D:353:ARG:NH1	1:D:368:TYR:CZ	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:ARG:HD3	1:E:190:ARG:HA	1.91	0.42
1:A:270:MET:HE1	1:A:298:ILE:HG23	2.02	0.42
1:D:278:LEU:HD11	1:F:381:ARG:NH1	2.33	0.42
1:E:234:MET:HE2	1:E:270:MET:SD	2.60	0.42
1:A:209:MET:O	1:A:213:MET:HG3	2.20	0.41
1:A:274:THR:O	1:A:277:GLY:O	2.38	0.41
1:F:304:LYS:O	1:F:308:GLY:N	2.51	0.41
1:B:193:GLU:O	1:B:197:SER:HB3	2.20	0.41
1:E:242:VAL:HG21	1:E:286:VAL:HG23	2.03	0.41
1:C:285:ASP:O	1:C:288:THR:OG1	2.35	0.41
1:C:299:LYS:O	1:C:303:VAL:HG13	2.20	0.41
1:D:174:SER:O	1:F:265:TYR:CD1	2.73	0.41
1:D:264:ASN:ND2	1:E:174:SER:OG	2.44	0.41
1:C:209:MET:O	1:C:213:MET:HG3	2.20	0.41
1:E:278:LEU:O	1:E:278:LEU:HD12	2.20	0.41
1:F:182:ARG:O	1:F:183:LEU:HB2	2.19	0.41
1:A:234:MET:O	1:A:238:VAL:HG23	2.21	0.41
1:B:274:THR:O	1:B:277:GLY:O	2.39	0.41
1:E:184:ARG:HA	1:E:187:VAL:HG12	2.00	0.41
1:E:345:LEU:HG	1:E:347:MET:CE	2.44	0.41
1:A:265:TYR:CE2	1:B:172:ALA:HA	2.52	0.41
1:A:279:VAL:CG1	1:A:315:LEU:HD21	2.50	0.41
1:B:209:MET:O	1:B:213:MET:HG3	2.20	0.41
1:D:192:LEU:HD23	1:D:193:GLU:OE2	2.20	0.41
1:C:183:LEU:CD1	1:C:184:ARG:N	2.68	0.41
1:E:209:MET:O	1:E:213:MET:HG3	2.20	0.41
1:E:260:VAL:HG23	1:F:180:MET:HG2	2.02	0.41
1:C:183:LEU:HD12	1:C:184:ARG:CA	2.49	0.41
1:B:183:LEU:O	1:B:184:ARG:HB2	2.21	0.41
1:C:246:LYS:HG2	1:C:266:PHE:CZ	2.56	0.41
1:F:285:ASP:O	1:F:288:THR:OG1	2.36	0.41
1:D:345:LEU:CG	1:D:347:MET:HE3	2.41	0.41
1:F:242:VAL:CG2	1:F:286:VAL:HG23	2.51	0.41
1:A:181:THR:HG22	1:A:182:ARG:N	2.36	0.40
1:A:345:LEU:HG	1:A:347:MET:CE	2.43	0.40
1:A:379:ASP:OD1	1:A:382:GLU:CG	2.60	0.40
1:A:384:VAL:CG1	1:B:330:SER:HB2	2.51	0.40
1:E:194:ALA:HB1	1:E:339:PRO:HG2	2.02	0.40
1:E:369:LEU:HB3	1:E:387:LEU:HD11	2.04	0.40
1:F:279:VAL:HG13	1:F:281:PRO:HD3	2.02	0.40
1:B:194:ALA:HB2	1:B:339:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:MET:O	1:C:238:VAL:HG23	2.22	0.40
1:E:193:GLU:O	1:E:197:SER:HB3	2.21	0.40
1:F:182:ARG:O	1:F:183:LEU:HB3	2.20	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	Percentiles	
1	A	231/233 (99%)	223 (96%)	6 (3%)	2 (1%)	14	48
1	B	231/233 (99%)	224 (97%)	6 (3%)	1 (0%)	30	65
1	C	231/233 (99%)	223 (96%)	6 (3%)	2 (1%)	14	48
1	D	231/233 (99%)	223 (96%)	7 (3%)	1 (0%)	30	65
1	E	231/233 (99%)	223 (96%)	7 (3%)	1 (0%)	30	65
1	F	231/233 (99%)	224 (97%)	4 (2%)	3 (1%)	9	38
All	All	1386/1398 (99%)	1340 (97%)	36 (3%)	10 (1%)	18	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	183	LEU
1	F	173	ARG
1	A	183	LEU
1	F	257	GLY
1	E	257	GLY
1	C	173	ARG
1	A	257	GLY
1	C	257	GLY
1	D	257	GLY
1	B	257	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	201/201 (100%)	198 (98%)	3 (2%)	57	80
1	B	201/201 (100%)	200 (100%)	1 (0%)	81	89
1	C	201/201 (100%)	200 (100%)	1 (0%)	81	89
1	D	201/201 (100%)	197 (98%)	4 (2%)	48	76
1	E	201/201 (100%)	196 (98%)	5 (2%)	42	72
1	F	201/201 (100%)	200 (100%)	1 (0%)	81	89
All	All	1206/1206 (100%)	1191 (99%)	15 (1%)	63	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	SER
1	A	177	ARG
1	A	276	ARG
1	B	193	GLU
1	C	276	ARG
1	D	174	SER
1	D	193	GLU
1	D	306	ARG
1	D	362	GLU
1	E	192	LEU
1	E	210	LYS
1	E	225	LYS
1	E	299	LYS
1	E	351	LYS
1	F	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	360	GLN

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Mol	Chain	Res	Type
1	A	375	HIS
1	B	264	ASN
1	B	358	ASN
1	C	208	ASN
1	C	263	HIS
1	C	264	ASN
1	C	358	ASN
1	D	358	ASN
1	E	263	HIS
1	E	348	HIS
1	E	358	ASN
1	E	375	HIS
1	F	196	ASN
1	F	358	ASN
1	F	360	GLN
1	F	375	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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, 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	233/233 (100%)	-0.32	0 100 100	42, 69, 123, 164	0
1	B	233/233 (100%)	-0.35	0 100 100	42, 65, 113, 155	0
1	C	233/233 (100%)	-0.24	0 100 100	42, 71, 113, 137	0
1	D	233/233 (100%)	-0.19	0 100 100	53, 81, 136, 223	0
1	E	233/233 (100%)	-0.23	0 100 100	59, 87, 130, 177	0
1	F	233/233 (100%)	-0.15	0 100 100	54, 86, 129, 185	0
All	All	1398/1398 (100%)	-0.25	0 100 100	42, 78, 127, 223	0

There are no RSRZ outliers to report.

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	NA	D	501	1/1	0.84	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	B	501	1/1	0.91	0.06	41,41,41,41	0
2	NA	F	501	1/1	0.92	0.04	55,55,55,55	0
2	NA	E	501	1/1	0.93	0.11	41,41,41,41	0
2	NA	C	501	1/1	0.95	0.09	29,29,29,29	0
2	NA	A	501	1/1	0.95	0.06	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.