



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:56 PM UTC

PDB ID : 2B24 / pdb_00002b24
Title : Crystal structure of naphthalene 1,2-dioxygenase from Rhodococcus sp. bound to indole
Authors : Gakhar, L.; Malik, Z.A.; Allen, C.C.; Lipscomb, D.A.; Larkin, M.J.; Ramaswamy, S.
Deposited on : 2005-09-16
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
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

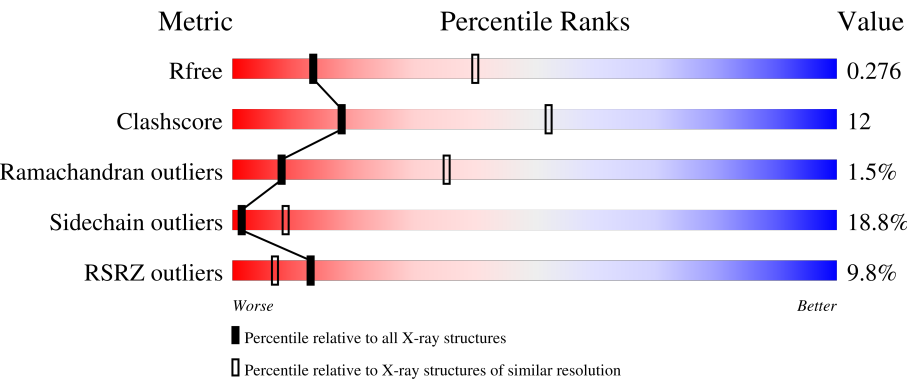
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	470	8% 62%27%6%
1	C	470	8% 59%29%6%
1	E	470	9% 59%29%6%
2	B	172	13% 55%31%8%
2	D	172	12% 54%33%8%

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Mol	Chain	Length	Quality of chain
2	F	172	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FES	A	501	-	-	X	-
5	IND	A	503	-	X	-	-
5	IND	C	503	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14862 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 naphthalene dioxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3506	2232	605	649	20			
1	C	440	Total	C	N	O	S	0	0	0
			3506	2232	605	649	20			
1	E	440	Total	C	N	O	S	0	0	0
			3506	2232	605	649	20			

- Molecule 2 is a protein called naphthalene dioxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1330	827	229	266	8			
2	D	165	Total	C	N	O	S	0	0	0
			1330	827	229	266	8			
2	F	165	Total	C	N	O	S	0	0	0
			1330	827	229	266	8			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

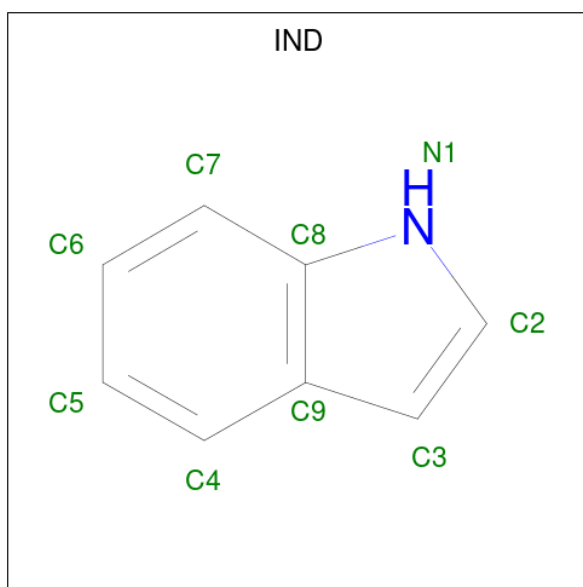
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is INDOLE (CCD ID: IND) (formula: C₈H₇N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			9	8	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			9	8	1		
5	E	1	Total	C	N	0	0
			9	8	1		

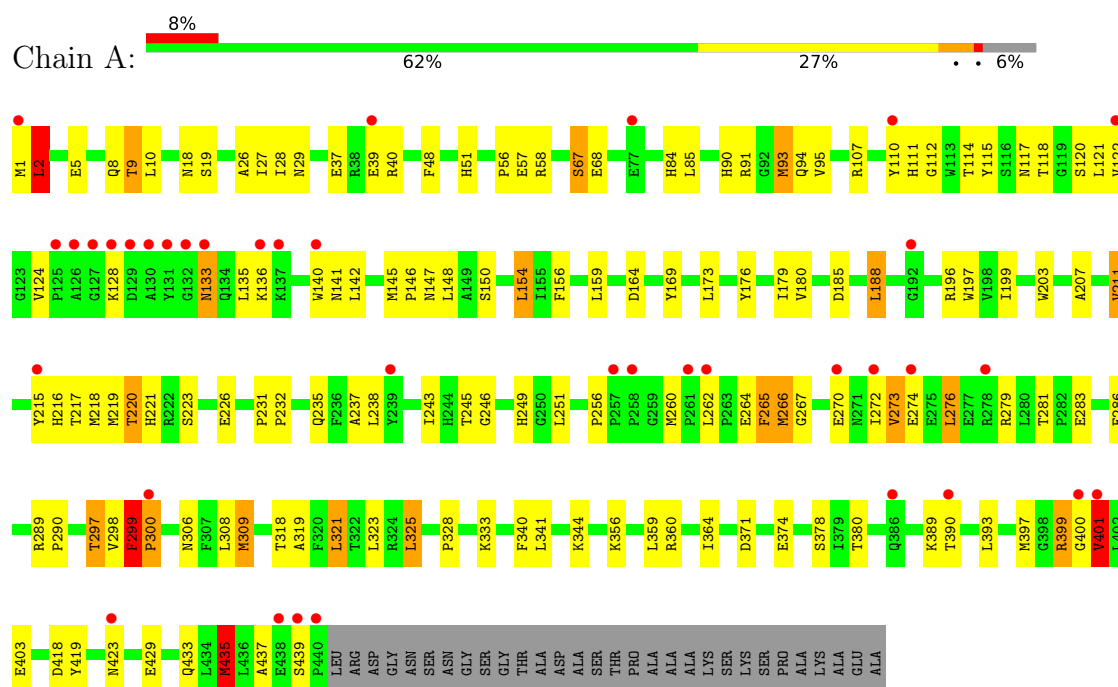
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		
6	B	35	Total	O	0	0
			35	35		
6	C	64	Total	O	0	0
			64	64		
6	D	29	Total	O	0	0
			29	29		
6	E	82	Total	O	0	0
			82	82		
6	F	36	Total	O	0	0
			36	36		

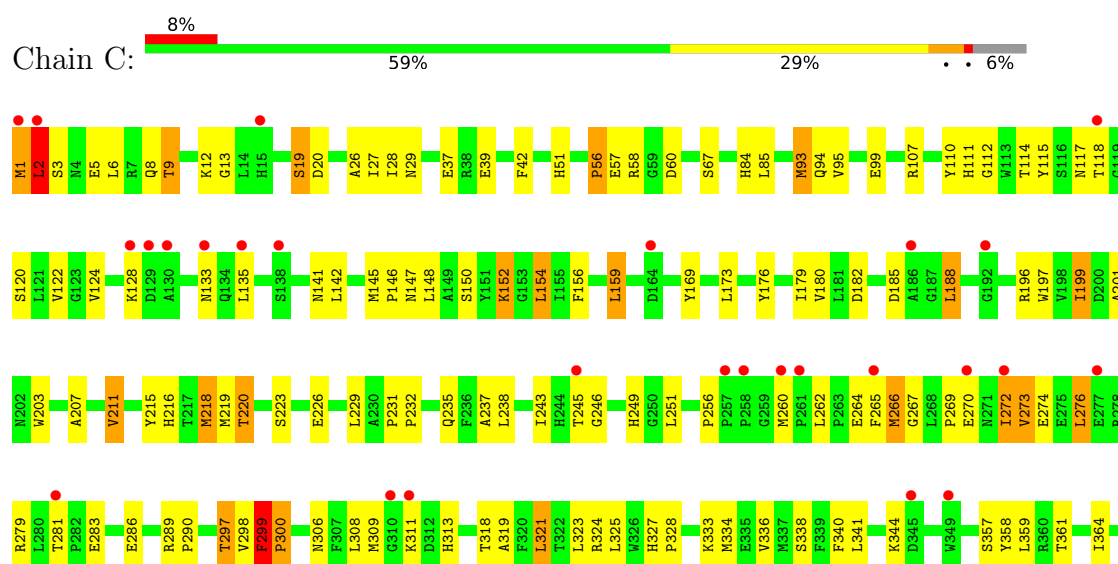
3 Residue-property plots

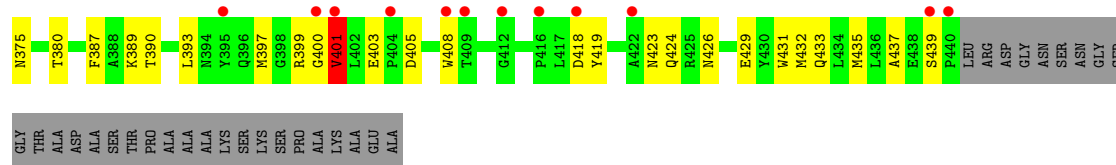
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: naphthalene dioxygenase large subunit

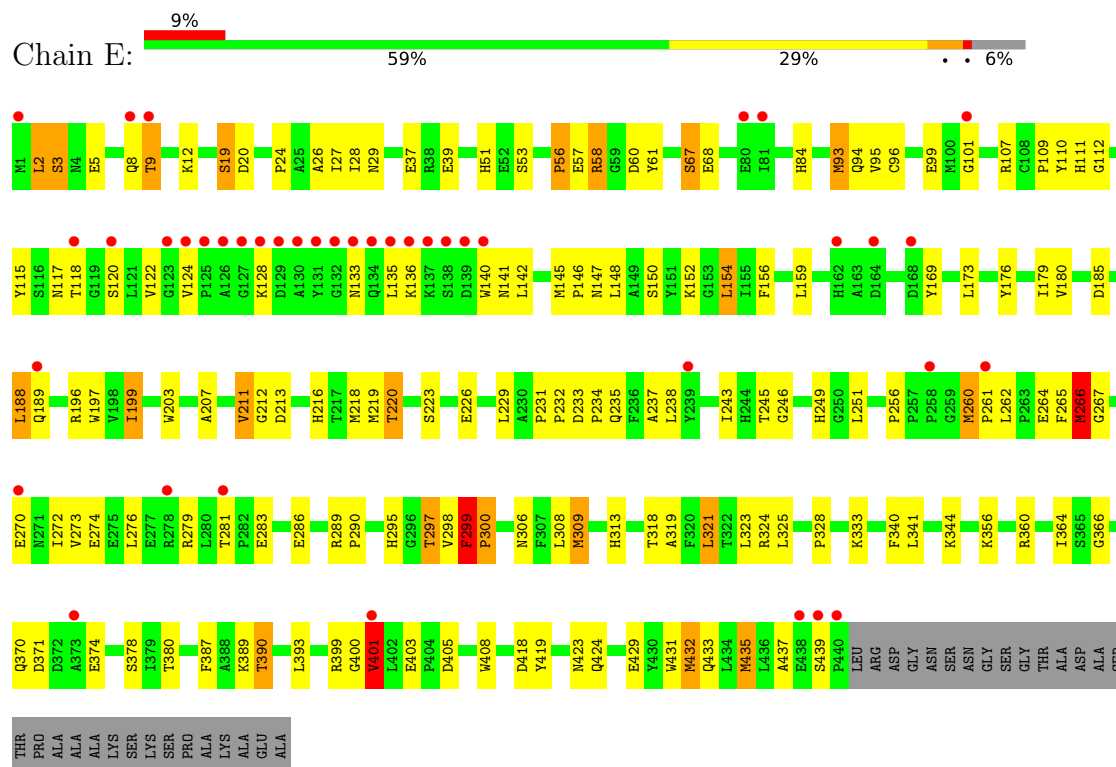


- Molecule 1: naphthalene dioxygenase large subunit

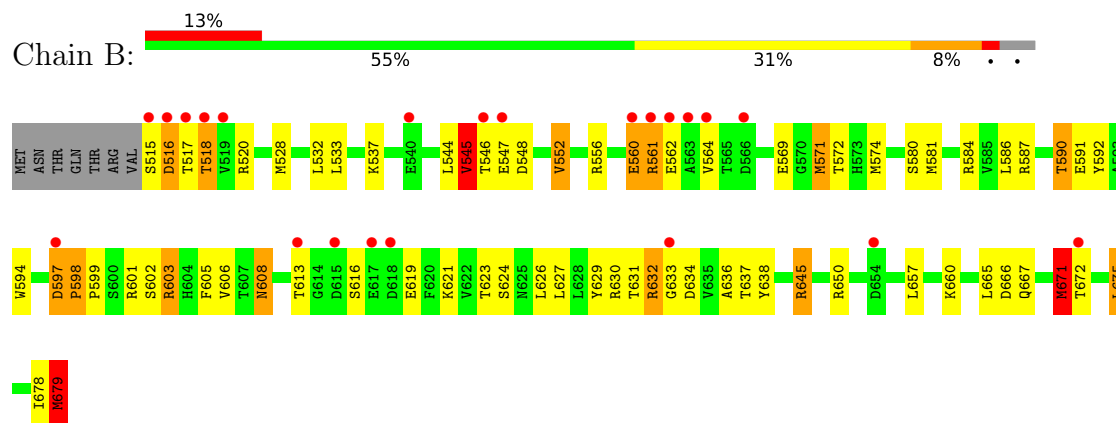




• Molecule 1: naphthalene dioxygenase large subunit



• Molecule 2: naphthalene dioxygenase small subunit



• Molecule 2: naphthalene dioxygenase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.36Å 179.36Å 245.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.42 – 3.00 20.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.42-3.00) 98.9 (20.42-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, R_{free}	0.287 , 0.300 0.265 , 0.276	Depositor DCC
R_{free} test set	2441 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	14862	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, IND, FE

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	0.66	2/3612 (0.1%)	0.97	2/4908 (0.0%)
1	C	0.77	4/3612 (0.1%)	1.13	7/4908 (0.1%)
1	E	0.74	5/3612 (0.1%)	0.95	1/4908 (0.0%)
2	B	0.86	3/1350 (0.2%)	1.03	2/1831 (0.1%)
2	D	0.72	1/1350 (0.1%)	1.03	1/1831 (0.1%)
2	F	0.90	3/1350 (0.2%)	1.06	2/1831 (0.1%)
All	All	0.75	18/14886 (0.1%)	1.02	15/20217 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	4
1	E	0	1
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	9

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	LEU	C-N	-22.95	1.01	1.33
1	C	2	LEU	N-CA	12.85	1.61	1.46
2	F	671	MET	SD-CE	-12.27	1.48	1.79
1	C	2	LEU	CB-CG	10.48	1.74	1.53
2	B	671	MET	SD-CE	-10.44	1.53	1.79
2	F	571	MET	SD-CE	-9.87	1.54	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	571	MET	SD-CE	-8.73	1.57	1.79
2	D	671	MET	SD-CE	-8.15	1.59	1.79
1	C	2	LEU	C-O	8.00	1.34	1.24
2	B	679	MET	SD-CE	-6.86	1.62	1.79
1	E	218	MET	SD-CE	-6.52	1.63	1.79
1	E	309	MET	SD-CE	-6.03	1.64	1.79
1	A	435	MET	SD-CE	-5.86	1.64	1.79
1	A	309	MET	SD-CE	-5.73	1.65	1.79
1	E	435	MET	SD-CE	-5.69	1.65	1.79
1	E	266	MET	SD-CE	-5.38	1.66	1.79
2	F	581	MET	SD-CE	-5.17	1.66	1.79
1	E	432	MET	SD-CE	-5.12	1.66	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	MET	O-C-N	-30.39	74.38	123.00
1	C	2	LEU	O-C-N	-21.01	96.42	122.26
1	A	2	LEU	N-CA-C	-15.76	84.79	110.17
1	C	2	LEU	CA-C-N	15.50	151.15	121.54
1	C	2	LEU	C-N-CA	15.50	151.15	121.54
1	C	1	MET	CA-C-N	10.99	140.15	122.67
1	C	1	MET	C-N-CA	10.99	140.15	122.67
2	D	598	PRO	N-CA-C	-7.58	101.46	110.70
1	C	2	LEU	CB-CA-C	-7.48	98.98	111.02
2	B	598	PRO	N-CA-C	-7.43	101.63	110.70
2	F	598	PRO	N-CA-C	-6.95	102.22	110.70
1	E	2	LEU	N-CA-C	-6.00	95.62	107.69
1	A	2	LEU	N-CA-CB	5.78	120.05	110.63
2	B	518	THR	N-CA-C	-5.49	105.71	112.90
2	F	572	THR	OG1-CB-CG2	-5.20	98.90	109.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	PHE	Peptide
2	B	597	ASP	Peptide
1	C	1	MET	Mainchain
1	C	2	LEU	Mainchain,Peptide
1	C	299	PHE	Peptide
2	D	597	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	E	299	PHE	Peptide
2	F	597	ASP	Peptide

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	3506	0	3333	81	0
1	C	3506	0	3332	90	0
1	E	3506	0	3333	96	0
2	B	1330	0	1303	41	0
2	D	1330	0	1303	36	0
2	F	1330	0	1303	42	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	4	0	0	3	0
4	C	4	0	0	1	0
4	E	4	0	0	1	0
5	A	9	0	7	0	0
5	C	9	0	7	0	0
5	E	9	0	7	0	0
6	A	66	0	0	2	0
6	B	35	0	0	2	0
6	C	64	0	0	2	0
6	D	29	0	0	1	0
6	E	82	0	0	5	0
6	F	36	0	0	1	0
All	All	14862	0	13928	347	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 12.

All (347) 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:C:5:GLU:O	1:C:9:THR:HG22	1.85	0.77
1:A:112:GLY:HA2	1:C:219:MET:HG2	1.68	0.75
1:E:286:GLU:OE2	1:E:289:ARG:NH1	2.20	0.75
1:A:5:GLU:O	1:A:9:THR:HG22	1.86	0.74
1:E:5:GLU:O	1:E:9:THR:HG22	1.87	0.74
2:F:598:PRO:O	2:F:632:ARG:NH2	2.21	0.74
1:C:249:HIS:HD2	1:C:299:PHE:H	1.35	0.73
1:C:111:HIS:HB2	4:C:501:FES:S1	2.30	0.71
1:C:286:GLU:OE2	1:C:289:ARG:NH1	2.23	0.71
1:E:249:HIS:HD2	1:E:299:PHE:H	1.38	0.71
2:D:598:PRO:O	2:D:632:ARG:NH2	2.24	0.70
2:B:598:PRO:O	2:B:632:ARG:NH2	2.25	0.69
1:E:270:GLU:HB3	6:E:550:HOH:O	1.91	0.69
1:E:20:ASP:CG	6:E:517:HOH:O	2.37	0.68
1:A:110:TYR:O	1:C:220:THR:HG22	1.94	0.68
1:C:93:MET:HG3	1:C:94:GLN:N	2.09	0.68
2:F:590:THR:HG23	2:F:592:TYR:H	1.58	0.68
1:A:249:HIS:HD2	1:A:299:PHE:H	1.40	0.67
2:D:590:THR:HG23	2:D:592:TYR:H	1.57	0.67
2:D:572:THR:HG22	2:D:574:MET:H	1.59	0.67
2:B:572:THR:HG22	2:B:574:MET:H	1.60	0.67
1:A:111:HIS:HB2	4:A:501:FES:S1	2.34	0.67
2:B:626:LEU:HB2	2:B:645:ARG:HD2	1.77	0.67
1:A:219:MET:HG2	1:E:112:GLY:HA2	1.78	0.66
1:C:266:MET:HB3	1:C:319:ALA:HB2	1.77	0.66
2:F:601:ARG:NH2	2:F:633:GLY:H	1.94	0.65
2:B:590:THR:HG23	2:B:592:TYR:H	1.60	0.65
1:A:299:PHE:O	1:A:300:PRO:C	2.40	0.65
1:C:299:PHE:O	1:C:300:PRO:C	2.40	0.65
1:A:286:GLU:OE2	1:A:289:ARG:NH1	2.30	0.65
1:E:249:HIS:HD2	1:E:299:PHE:N	1.94	0.65
2:B:601:ARG:NH2	2:B:633:GLY:H	1.95	0.64
1:A:93:MET:HG3	1:A:94:GLN:N	2.13	0.64
1:E:93:MET:HG3	1:E:94:GLN:N	2.12	0.64
2:D:597:ASP:OD1	2:D:597:ASP:O	2.15	0.64
2:B:548:ASP:OD2	2:B:650:ARG:NH2	2.30	0.64
1:E:299:PHE:HB3	1:E:300:PRO:HD3	1.79	0.63
1:C:299:PHE:HB3	1:C:300:PRO:HD3	1.79	0.63
2:B:597:ASP:OD1	2:B:597:ASP:O	2.17	0.63
1:E:340:PHE:HB3	2:F:571:MET:HE3	1.79	0.63
1:C:249:HIS:HD2	1:C:299:PHE:N	1.97	0.63
2:F:572:THR:HG22	2:F:574:MET:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:HIS:HB2	4:E:501:FES:S1	2.39	0.62
1:A:266:MET:HB3	1:A:319:ALA:HB2	1.80	0.62
1:E:245:THR:HG22	1:E:246:GLY:H	1.63	0.62
1:E:299:PHE:O	1:E:300:PRO:C	2.43	0.62
2:F:626:LEU:HB2	2:F:645:ARG:HD2	1.81	0.62
1:C:188:LEU:HD21	1:C:321:LEU:HD12	1.82	0.61
1:C:311:LYS:HA	6:C:544:HOH:O	1.99	0.61
2:D:601:ARG:NH2	2:D:633:GLY:H	1.99	0.61
1:A:249:HIS:HD2	1:A:299:PHE:N	1.98	0.61
1:C:270:GLU:CD	1:C:270:GLU:H	2.09	0.61
2:F:560:GLU:OE2	2:F:562:GLU:HB3	1.99	0.61
2:D:560:GLU:OE2	2:D:562:GLU:HB3	2.01	0.61
2:D:626:LEU:HB2	2:D:645:ARG:HD2	1.82	0.60
1:E:245:THR:HG22	1:E:246:GLY:N	2.16	0.60
1:E:266:MET:HB3	1:E:319:ALA:HB2	1.82	0.60
1:A:299:PHE:HB3	1:A:300:PRO:HD3	1.83	0.60
1:C:110:TYR:O	1:E:220:THR:HG22	2.02	0.59
2:F:597:ASP:OD1	2:F:597:ASP:O	2.21	0.59
1:C:112:GLY:HA2	1:E:219:MET:HG2	1.84	0.59
2:D:548:ASP:OD2	2:D:650:ARG:NH2	2.35	0.59
1:A:245:THR:HG22	1:A:246:GLY:N	2.18	0.59
2:B:560:GLU:OE2	2:B:562:GLU:HB3	2.02	0.59
2:B:599:PRO:HG3	2:F:561:ARG:HG3	1.85	0.58
2:B:666:ASP:OD1	2:D:603:ARG:NH1	2.36	0.58
1:E:270:GLU:CD	1:E:270:GLU:H	2.10	0.58
2:F:601:ARG:HH22	2:F:633:GLY:H	1.51	0.58
2:B:561:ARG:HG3	2:D:599:PRO:HG3	1.86	0.57
1:C:361:THR:HG23	6:C:544:HOH:O	2.03	0.57
1:A:281:THR:HG22	1:A:283:GLU:H	1.70	0.57
2:D:561:ARG:HG3	2:F:599:PRO:HG3	1.86	0.57
1:A:270:GLU:H	1:A:270:GLU:CD	2.12	0.57
1:E:101:GLY:HA2	2:F:559:ARG:NH2	2.20	0.57
1:C:251:LEU:O	1:C:423:ASN:ND2	2.36	0.57
2:F:548:ASP:OD2	2:F:650:ARG:NH2	2.38	0.56
2:B:581:MET:HE2	2:B:678:ILE:HD11	1.87	0.56
2:D:581:MET:HE2	2:D:678:ILE:HD11	1.88	0.56
1:A:245:THR:HG22	1:A:246:GLY:H	1.71	0.56
1:E:207:ALA:O	1:E:297:THR:HG21	2.06	0.56
1:A:207:ALA:O	1:A:297:THR:HG21	2.06	0.55
1:A:220:THR:HG22	1:E:110:TYR:O	2.06	0.55
2:B:671:MET:HE2	2:D:638:TYR:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:THR:HG22	1:C:246:GLY:N	2.20	0.55
1:E:203:TRP:CD1	1:E:328:PRO:HB3	2.41	0.55
1:A:112:GLY:CA	1:C:219:MET:HG2	2.37	0.55
1:A:188:LEU:HD21	1:A:321:LEU:HD12	1.89	0.54
1:A:84:HIS:HE1	1:A:117:ASN:O	1.90	0.54
1:C:203:TRP:CD1	1:C:328:PRO:HB3	2.41	0.54
1:E:340:PHE:HB3	2:F:571:MET:CE	2.38	0.54
1:A:237:ALA:HB3	1:A:419:TYR:CE2	2.43	0.54
1:A:90:HIS:HB3	4:A:501:FES:S2	2.48	0.54
1:A:107:ARG:HG3	1:A:114:THR:OG1	2.07	0.54
2:B:601:ARG:HH22	2:B:633:GLY:H	1.55	0.54
1:C:29:ASN:ND2	1:C:380:THR:HG22	2.23	0.54
2:B:546:THR:HG21	2:B:650:ARG:HH21	1.73	0.54
2:F:608:ASN:N	2:F:608:ASN:HD22	2.06	0.54
1:E:51:HIS:ND1	1:E:53:SER:OG	2.38	0.53
2:F:546:THR:HG21	2:F:650:ARG:HH21	1.73	0.53
1:A:164:ASP:CG	6:A:564:HOH:O	2.50	0.53
1:A:340:PHE:HB3	2:B:571:MET:HE3	1.89	0.53
1:E:251:LEU:O	1:E:423:ASN:ND2	2.40	0.53
2:D:516:ASP:C	2:D:518:THR:H	2.17	0.53
1:C:203:TRP:HZ3	1:C:300:PRO:O	1.92	0.53
1:E:281:THR:HG22	1:E:283:GLU:H	1.72	0.53
1:E:429:GLU:HG2	1:E:433:GLN:HE21	1.74	0.53
1:C:188:LEU:HD21	1:C:321:LEU:CD1	2.39	0.52
2:D:671:MET:HE3	2:F:636:ALA:C	2.34	0.52
1:C:281:THR:HG22	1:C:283:GLU:H	1.75	0.52
1:E:211:VAL:HG13	1:E:297:THR:HG23	1.91	0.52
2:B:561:ARG:NH1	6:B:259:HOH:O	2.41	0.52
2:B:619:GLU:OE2	2:B:650:ARG:NH1	2.43	0.52
1:C:154:LEU:HB3	1:C:156:PHE:CE1	2.44	0.52
1:A:188:LEU:HD21	1:A:321:LEU:CD1	2.40	0.52
1:A:203:TRP:CD1	1:A:328:PRO:HB3	2.44	0.52
1:C:26:ALA:HA	1:C:389:LYS:HG2	1.91	0.51
1:E:207:ALA:O	1:E:211:VAL:HG22	2.11	0.51
1:A:399:ARG:HB3	6:A:506:HOH:O	2.10	0.51
1:C:124:VAL:HG21	1:C:135:LEU:HD21	1.92	0.51
1:A:237:ALA:HB1	1:A:418:ASP:HB3	1.92	0.51
2:B:561:ARG:HB3	6:B:255:HOH:O	2.09	0.51
2:D:601:ARG:HH22	2:D:633:GLY:H	1.58	0.51
2:F:619:GLU:OE2	2:F:650:ARG:NH1	2.44	0.51
2:F:516:ASP:C	2:F:518:THR:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:THR:HG22	1:C:246:GLY:H	1.75	0.50
2:F:581:MET:HE2	2:F:678:ILE:HD11	1.93	0.50
1:A:211:VAL:HG13	1:A:297:THR:HG23	1.93	0.50
1:C:84:HIS:HE1	1:C:117:ASN:O	1.94	0.50
1:E:265:PHE:C	1:E:267:GLY:H	2.20	0.50
2:B:516:ASP:C	2:B:518:THR:H	2.20	0.50
1:C:207:ALA:O	1:C:297:THR:HG21	2.11	0.50
1:C:237:ALA:HB1	1:C:418:ASP:HB3	1.93	0.50
1:E:136:LYS:O	1:E:140:TRP:CD1	2.65	0.49
2:F:581:MET:HE1	2:F:584:ARG:HD2	1.94	0.49
1:A:2:LEU:HD12	1:A:40:ARG:NH1	2.28	0.49
2:F:601:ARG:HB2	2:F:631:THR:HG22	1.94	0.49
2:D:608:ASN:N	2:D:608:ASN:HD22	2.10	0.49
1:E:115:TYR:CD2	1:E:142:LEU:HG	2.47	0.49
1:E:188:LEU:HD21	1:E:321:LEU:HD12	1.94	0.49
1:E:323:LEU:HG	1:E:341:LEU:HD13	1.94	0.49
1:A:207:ALA:O	1:A:211:VAL:HG22	2.11	0.49
2:B:603:ARG:NH1	2:F:666:ASP:OD1	2.46	0.49
1:C:273:VAL:HA	1:C:276:LEU:HD23	1.94	0.49
1:E:58:ARG:HD3	6:E:521:HOH:O	2.11	0.49
1:A:298:VAL:O	1:A:299:PHE:C	2.55	0.49
1:C:357:SER:O	1:C:361:THR:OG1	2.27	0.49
1:E:203:TRP:HZ3	1:E:300:PRO:O	1.96	0.49
1:C:185:ASP:HA	1:C:279:ARG:NH1	2.28	0.49
1:C:197:TRP:HB3	1:C:364:ILE:HD12	1.94	0.49
1:C:124:VAL:HG21	1:C:135:LEU:CD2	2.43	0.48
1:A:2:LEU:HD21	1:A:10:LEU:HD12	1.95	0.48
2:D:619:GLU:OE2	2:D:650:ARG:NH1	2.45	0.48
1:C:169:TYR:O	1:C:249:HIS:HE1	1.95	0.48
1:E:28:ILE:HD11	1:E:393:LEU:HD11	1.94	0.48
1:E:37:GLU:HA	1:E:435:MET:CE	2.44	0.48
1:A:29:ASN:ND2	1:A:380:THR:HG22	2.28	0.48
2:B:602:SER:HA	2:B:629:TYR:O	2.14	0.48
1:C:107:ARG:HG2	1:E:219:MET:HE2	1.95	0.48
1:E:124:VAL:HG21	1:E:135:LEU:HD21	1.96	0.48
1:A:251:LEU:O	1:A:423:ASN:ND2	2.46	0.48
2:B:546:THR:HG22	2:B:548:ASP:H	1.78	0.48
2:B:638:TYR:HD2	2:F:671:MET:HE2	1.79	0.48
1:A:400:GLY:O	1:A:401:VAL:HG23	2.14	0.48
1:A:85:LEU:HD13	1:C:387:PHE:HD2	1.79	0.47
1:A:265:PHE:C	1:A:267:GLY:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:601:ARG:HB2	2:D:631:THR:HG22	1.95	0.47
1:E:26:ALA:HA	1:E:389:LYS:HG2	1.95	0.47
2:F:546:THR:HG22	2:F:548:ASP:H	1.79	0.47
1:C:340:PHE:HB3	2:D:571:MET:HE3	1.96	0.47
1:A:84:HIS:CE1	1:A:117:ASN:O	2.68	0.47
1:A:115:TYR:CD2	1:A:142:LEU:HG	2.49	0.47
1:A:203:TRP:HZ3	1:A:300:PRO:O	1.97	0.47
1:A:429:GLU:HG2	1:A:433:GLN:HE21	1.79	0.47
1:C:42:PHE:CZ	1:C:328:PRO:HG3	2.49	0.47
1:C:338:SER:OG	1:C:358:TYR:OH	2.21	0.47
1:A:356:LYS:O	1:A:360:ARG:HD3	2.14	0.47
1:E:2:LEU:O	1:E:3:SER:O	2.32	0.47
1:E:188:LEU:HD21	1:E:321:LEU:CD1	2.43	0.47
1:A:18:ASN:ND2	1:A:429:GLU:OE2	2.27	0.47
1:A:67:SER:HB3	1:A:68:GLU:H	1.57	0.47
1:E:124:VAL:HG21	1:E:135:LEU:CD2	2.44	0.47
1:A:1:MET:HE2	1:C:5:GLU:OE1	2.15	0.47
1:E:199:ILE:HG23	2:F:673:HIS:HB2	1.97	0.47
1:E:212:GLY:HA2	1:E:295:HIS:HE1	1.79	0.47
1:A:145:MET:O	1:A:146:PRO:C	2.58	0.47
1:C:145:MET:O	1:C:146:PRO:C	2.58	0.47
1:C:199:ILE:HG23	2:D:673:HIS:HB2	1.97	0.47
1:E:136:LYS:NZ	6:E:575:HOH:O	2.48	0.47
1:E:371:ASP:OD2	2:F:587:ARG:NH1	2.39	0.47
2:D:546:THR:HG21	2:D:650:ARG:HH21	1.78	0.47
1:C:37:GLU:HA	1:C:435:MET:CE	2.45	0.46
1:C:400:GLY:O	1:C:401:VAL:HG23	2.15	0.46
1:E:387:PHE:O	1:E:390:THR:HB	2.15	0.46
1:A:124:VAL:HG21	1:A:135:LEU:HD21	1.97	0.46
1:E:356:LYS:O	1:E:360:ARG:HD3	2.15	0.46
1:C:120:SER:HA	1:C:141:ASN:CG	2.41	0.46
2:D:602:SER:HA	2:D:629:TYR:O	2.16	0.46
2:B:606:VAL:H	2:F:608:ASN:HD21	1.64	0.46
1:C:298:VAL:O	1:C:299:PHE:C	2.58	0.46
2:D:542:LEU:HD21	2:D:582:GLU:HA	1.98	0.46
1:A:26:ALA:HA	1:A:389:LYS:HG2	1.97	0.46
1:A:256:PRO:HD3	1:A:290:PRO:O	2.16	0.46
1:E:176:TYR:CZ	1:E:243:ILE:HG21	2.51	0.46
1:A:185:ASP:HA	1:A:279:ARG:NH1	2.31	0.45
2:D:531:GLU:CD	6:D:293:HOH:O	2.59	0.45
1:E:216:HIS:HD2	1:E:220:THR:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:HIS:HE1	1:E:117:ASN:O	1.98	0.45
1:E:237:ALA:HB1	1:E:418:ASP:HB3	1.97	0.45
2:F:601:ARG:HH22	2:F:633:GLY:N	2.12	0.45
1:A:51:HIS:HD2	1:A:154:LEU:HD12	1.81	0.45
1:E:298:VAL:O	1:E:299:PHE:C	2.60	0.45
1:A:323:LEU:HG	1:A:341:LEU:HD13	1.98	0.45
1:C:265:PHE:C	1:C:267:GLY:H	2.25	0.45
1:A:37:GLU:HA	1:A:435:MET:CE	2.47	0.45
1:A:249:HIS:CD2	1:A:299:PHE:H	2.29	0.45
1:E:265:PHE:O	1:E:267:GLY:N	2.50	0.45
2:B:587:ARG:O	2:B:590:THR:HG22	2.17	0.45
2:D:587:ARG:O	2:D:590:THR:HG22	2.17	0.45
1:C:28:ILE:HD11	1:C:393:LEU:HD11	1.99	0.45
1:E:154:LEU:HB3	1:E:156:PHE:CE1	2.51	0.45
2:B:552:VAL:HA	2:B:574:MET:O	2.17	0.45
1:C:237:ALA:HB3	1:C:419:TYR:CE2	2.52	0.45
1:A:28:ILE:HD11	1:A:393:LEU:HD11	1.98	0.44
2:B:666:ASP:OD2	2:D:603:ARG:HD2	2.16	0.44
1:E:29:ASN:ND2	1:E:380:THR:HG22	2.32	0.44
1:E:58:ARG:NH1	6:E:522:HOH:O	2.48	0.44
2:F:602:SER:HA	2:F:629:TYR:O	2.16	0.44
1:A:48:PHE:HB3	1:A:325:LEU:HD11	1.99	0.44
1:C:107:ARG:HG3	1:C:114:THR:OG1	2.16	0.44
1:C:207:ALA:O	1:C:211:VAL:HG22	2.17	0.44
1:C:51:HIS:HD2	1:C:154:LEU:HD12	1.82	0.44
1:C:323:LEU:HG	1:C:341:LEU:HD13	1.99	0.44
1:A:216:HIS:HD2	1:A:220:THR:HG21	1.83	0.44
1:C:429:GLU:HG2	1:C:433:GLN:HE21	1.81	0.44
2:D:663:VAL:HG12	2:D:665:LEU:HD13	1.99	0.44
1:E:169:TYR:O	1:E:249:HIS:HE1	2.00	0.44
2:B:636:ALA:C	2:F:671:MET:HE3	2.42	0.44
1:C:115:TYR:CD2	1:C:142:LEU:HG	2.53	0.44
1:C:176:TYR:CZ	1:C:243:ILE:HG21	2.53	0.44
1:C:197:TRP:CH2	1:C:336:VAL:HG11	2.52	0.44
1:C:201:ALA:O	1:C:334:MET:HG2	2.17	0.44
1:A:169:TYR:O	1:A:249:HIS:HE1	2.00	0.44
1:C:188:LEU:HG	1:C:341:LEU:HB3	1.99	0.44
1:E:264:GLU:C	1:E:265:PHE:O	2.60	0.44
1:A:91:ARG:N	4:A:501:FES:S2	2.87	0.44
1:E:229:LEU:HD11	1:E:313:HIS:HA	2.00	0.44
2:F:540:GLU:OE2	6:F:247:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:544:LEU:O	2:F:545:VAL:HG22	2.18	0.44
1:A:371:ASP:OD2	2:B:587:ARG:NH1	2.42	0.44
1:C:215:TYR:CD2	1:C:397:MET:HE1	2.53	0.44
2:B:603:ARG:HG2	2:B:605:PHE:CZ	2.53	0.44
2:B:675:LEU:HG	2:B:679:MET:HE1	2.00	0.44
2:D:601:ARG:HH22	2:D:633:GLY:N	2.16	0.44
2:D:675:LEU:HG	2:D:679:MET:HE1	2.00	0.44
1:E:197:TRP:HB3	1:E:364:ILE:HD12	1.99	0.44
1:A:136:LYS:O	1:A:140:TRP:CD1	2.71	0.43
1:C:13:GLY:HA3	1:C:432:MET:HE1	2.00	0.43
1:E:51:HIS:HD2	1:E:154:LEU:HD12	1.82	0.43
2:F:542:LEU:HD21	2:F:582:GLU:HA	2.00	0.43
1:A:219:MET:HG2	1:E:112:GLY:CA	2.47	0.43
1:C:264:GLU:C	1:C:265:PHE:O	2.61	0.43
1:C:387:PHE:O	1:C:390:THR:HB	2.18	0.43
1:E:61:TYR:CE1	1:E:96:CYS:SG	3.11	0.43
1:E:145:MET:O	1:E:146:PRO:C	2.61	0.43
1:E:19:SER:OG	1:E:20:ASP:N	2.52	0.43
1:E:374:GLU:OE2	2:F:632:ARG:NH1	2.52	0.43
1:A:120:SER:HA	1:A:141:ASN:CG	2.43	0.43
1:C:203:TRP:CZ3	1:C:300:PRO:O	2.71	0.43
1:E:56:PRO:HD2	1:E:60:ASP:OD2	2.19	0.43
1:C:146:PRO:HG2	1:C:159:LEU:HA	2.00	0.43
1:C:154:LEU:HB3	1:C:156:PHE:HE1	1.84	0.43
1:C:84:HIS:CE1	1:C:117:ASN:O	2.71	0.43
1:E:366:GLY:O	1:E:370:GLN:NE2	2.51	0.43
1:A:215:TYR:CD2	1:A:397:MET:HE1	2.54	0.43
1:C:218:MET:H	1:C:218:MET:HG2	1.70	0.43
1:A:197:TRP:HB3	1:A:364:ILE:HD12	2.01	0.42
1:A:264:GLU:C	1:A:265:PHE:O	2.61	0.42
1:E:136:LYS:O	1:E:140:TRP:HD1	2.01	0.42
1:E:185:ASP:HA	1:E:279:ARG:NH1	2.34	0.42
2:F:675:LEU:HG	2:F:679:MET:HE1	2.01	0.42
1:A:154:LEU:HB3	1:A:156:PHE:CE1	2.54	0.42
1:A:273:VAL:HA	1:A:276:LEU:HD23	2.00	0.42
2:B:515:SER:O	2:B:516:ASP:O	2.37	0.42
1:C:19:SER:OG	1:C:20:ASP:N	2.51	0.42
1:C:229:LEU:HD11	1:C:313:HIS:HA	2.01	0.42
1:C:211:VAL:HG13	1:C:297:THR:HG23	2.00	0.42
1:C:220:THR:HB	1:C:375:ASN:HD21	1.85	0.42
1:C:231:PRO:HA	1:C:232:PRO:HD3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:ARG:HB3	1:E:290:PRO:HD3	2.02	0.42
1:E:37:GLU:HA	1:E:435:MET:HE1	2.02	0.42
1:E:37:GLU:N	1:E:435:MET:HE1	2.34	0.42
1:E:237:ALA:HB3	1:E:419:TYR:CE2	2.54	0.42
1:A:374:GLU:OE2	2:B:632:ARG:NH1	2.53	0.42
1:C:56:PRO:HD2	1:C:60:ASP:OD2	2.20	0.42
2:B:603:ARG:HB2	2:F:666:ASP:OD2	2.20	0.42
1:C:2:LEU:O	1:C:6:LEU:HB3	2.19	0.42
1:C:85:LEU:HD13	1:E:387:PHE:HD2	1.85	0.42
1:E:67:SER:HB3	1:E:68:GLU:H	1.63	0.42
1:A:176:TYR:CZ	1:A:243:ILE:HG21	2.55	0.42
1:E:24:PRO:O	1:E:27:ILE:HG12	2.20	0.42
1:A:107:ARG:HG2	1:C:219:MET:HE2	2.02	0.42
1:A:265:PHE:O	1:A:267:GLY:N	2.52	0.42
1:E:249:HIS:CD2	1:E:299:PHE:H	2.27	0.42
1:E:431:TRP:HE3	1:E:432:MET:HG3	1.84	0.42
2:B:608:ASN:HD21	2:D:606:VAL:H	1.67	0.41
1:C:405:ASP:HB3	1:C:408:TRP:HB2	2.01	0.41
1:A:203:TRP:CZ3	1:A:300:PRO:O	2.73	0.41
1:A:219:MET:HE2	1:E:107:ARG:HG2	2.02	0.41
2:D:529:GLU:OE2	2:D:661:ARG:NH1	2.45	0.41
1:E:120:SER:HA	1:E:141:ASN:CG	2.44	0.41
2:D:560:GLU:H	2:D:560:GLU:HG3	1.42	0.41
2:D:601:ARG:HH21	2:D:631:THR:HG23	1.84	0.41
1:E:203:TRP:CZ3	1:E:300:PRO:O	2.73	0.41
1:A:188:LEU:HG	1:A:341:LEU:HB3	2.02	0.41
2:F:582:GLU:O	2:F:586:LEU:HB2	2.20	0.41
1:C:216:HIS:HD2	1:C:220:THR:HG21	1.85	0.41
1:C:359:LEU:HD23	1:C:359:LEU:HA	1.93	0.41
1:C:152:LYS:HE2	1:C:182:ASP:OD2	2.21	0.41
2:D:581:MET:HE2	2:D:678:ILE:CD1	2.50	0.41
1:E:231:PRO:HA	1:E:232:PRO:HD3	1.78	0.41
1:E:256:PRO:HD3	1:E:290:PRO:O	2.21	0.41
1:E:400:GLY:O	1:E:401:VAL:HG23	2.20	0.41
2:F:587:ARG:O	2:F:590:THR:HG22	2.20	0.41
2:F:627:LEU:HD13	2:F:640:VAL:HG13	2.03	0.41
2:F:663:VAL:HG12	2:F:665:LEU:HD13	2.01	0.41
1:E:405:ASP:HB3	1:E:408:TRP:HB2	2.03	0.41
1:A:121:LEU:H	1:A:141:ASN:ND2	2.19	0.41
1:A:231:PRO:HA	1:A:232:PRO:HD3	1.76	0.41
2:B:581:MET:HE2	2:B:678:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:TRP:CD2	1:E:109:PRO:HB3	2.56	0.41
2:B:601:ARG:HH22	2:B:633:GLY:N	2.16	0.41
1:C:37:GLU:N	1:C:435:MET:HE1	2.35	0.41
1:C:269:PRO:HB2	1:C:272:ILE:HG23	2.03	0.41
1:C:431:TRP:HE3	1:C:432:MET:HG3	1.85	0.41
2:B:608:ASN:HD22	2:B:608:ASN:N	2.19	0.41
1:E:189:GLN:O	1:E:341:LEU:HA	2.21	0.41
1:E:260:MET:HA	1:E:261:PRO:HD3	1.83	0.40
1:A:217:THR:O	1:A:221:HIS:HB2	2.21	0.40
2:B:544:LEU:O	2:B:545:VAL:HG22	2.21	0.40
1:C:327:HIS:HA	1:C:328:PRO:HD3	1.98	0.40
1:E:188:LEU:HG	1:E:341:LEU:HB3	2.03	0.40
1:E:213:ASP:OD1	1:E:216:HIS:HB3	2.21	0.40
1:E:233:ASP:HA	1:E:234:PRO:HD3	1.94	0.40
1:C:256:PRO:HD3	1:C:290:PRO:O	2.21	0.40
2:D:546:THR:HG22	2:D:548:ASP:H	1.86	0.40
2:F:546:THR:CG2	2:F:548:ASP:OD2	2.70	0.40
1:E:84:HIS:CE1	1:E:117:ASN:O	2.75	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	438/470 (93%)	395 (90%)	35 (8%)	8 (2%)	6	31
1	C	438/470 (93%)	393 (90%)	39 (9%)	6 (1%)	9	36
1	E	438/470 (93%)	392 (90%)	39 (9%)	7 (2%)	7	34
2	B	163/172 (95%)	147 (90%)	14 (9%)	2 (1%)	10	40
2	D	163/172 (95%)	149 (91%)	12 (7%)	2 (1%)	10	40
2	F	163/172 (95%)	147 (90%)	14 (9%)	2 (1%)	10	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1803/1926 (94%)	1623 (90%)	153 (8%)	27 (2%)	8	35

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	PHE
2	B	516	ASP
2	B	545	VAL
1	C	3	SER
1	C	299	PHE
2	D	516	ASP
2	D	545	VAL
1	E	3	SER
1	E	299	PHE
2	F	516	ASP
2	F	545	VAL
1	A	437	ALA
1	C	437	ALA
1	E	437	ALA
1	A	266	MET
1	E	266	MET
1	E	300	PRO
1	A	300	PRO
1	C	300	PRO
1	A	133	ASN
1	A	401	VAL
1	C	401	VAL
1	A	265	PHE
1	A	56	PRO
1	C	56	PRO
1	E	401	VAL
1	E	56	PRO

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	370/389 (95%)	314 (85%)	56 (15%)	3	14
1	C	370/389 (95%)	311 (84%)	59 (16%)	2	13
1	E	370/389 (95%)	314 (85%)	56 (15%)	3	14
2	B	147/154 (96%)	106 (72%)	41 (28%)	0	2
2	D	147/154 (96%)	107 (73%)	40 (27%)	0	2
2	F	147/154 (96%)	108 (74%)	39 (26%)	0	3
All	All	1551/1629 (95%)	1260 (81%)	291 (19%)	1	9

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	8	GLN
1	A	9	THR
1	A	19	SER
1	A	27	ILE
1	A	39	GLU
1	A	57	GLU
1	A	58	ARG
1	A	67	SER
1	A	93	MET
1	A	95	VAL
1	A	118	THR
1	A	122	VAL
1	A	128	LYS
1	A	133	ASN
1	A	147	ASN
1	A	148	LEU
1	A	150	SER
1	A	154	LEU
1	A	159	LEU
1	A	173	LEU
1	A	179	ILE
1	A	180	VAL
1	A	188	LEU
1	A	196	ARG
1	A	199	ILE
1	A	211	VAL
1	A	218	MET
1	A	220	THR
1	A	223	SER

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Mol	Chain	Res	Type
1	A	226	GLU
1	A	235	GLN
1	A	238	LEU
1	A	260	MET
1	A	262	LEU
1	A	272	ILE
1	A	273	VAL
1	A	274	GLU
1	A	276	LEU
1	A	297	THR
1	A	306	ASN
1	A	308	LEU
1	A	309	MET
1	A	318	THR
1	A	321	LEU
1	A	325	LEU
1	A	333	LYS
1	A	344	LYS
1	A	359	LEU
1	A	378	SER
1	A	390	THR
1	A	399	ARG
1	A	401	VAL
1	A	403	GLU
1	A	435	MET
1	A	439	SER
2	B	517	THR
2	B	520	ARG
2	B	528	MET
2	B	532	LEU
2	B	533	LEU
2	B	537	LYS
2	B	545	VAL
2	B	547	GLU
2	B	552	VAL
2	B	556	ARG
2	B	560	GLU
2	B	561	ARG
2	B	564	VAL
2	B	569	GLU
2	B	580	SER
2	B	584	ARG

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Mol	Chain	Res	Type
2	B	586	LEU
2	B	590	THR
2	B	591	GLU
2	B	603	ARG
2	B	608	ASN
2	B	613	THR
2	B	616	SER
2	B	621	LYS
2	B	623	THR
2	B	624	SER
2	B	627	LEU
2	B	630	ARG
2	B	631	THR
2	B	632	ARG
2	B	634	ASP
2	B	637	THR
2	B	645	ARG
2	B	657	LEU
2	B	660	LYS
2	B	665	LEU
2	B	667	GLN
2	B	671	MET
2	B	672	THR
2	B	675	LEU
2	B	679	MET
1	C	2	LEU
1	C	8	GLN
1	C	9	THR
1	C	12	LYS
1	C	19	SER
1	C	27	ILE
1	C	39	GLU
1	C	57	GLU
1	C	58	ARG
1	C	67	SER
1	C	93	MET
1	C	95	VAL
1	C	99	GLU
1	C	118	THR
1	C	122	VAL
1	C	128	LYS
1	C	133	ASN

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Mol	Chain	Res	Type
1	C	147	ASN
1	C	148	LEU
1	C	150	SER
1	C	152	LYS
1	C	154	LEU
1	C	159	LEU
1	C	173	LEU
1	C	179	ILE
1	C	180	VAL
1	C	188	LEU
1	C	196	ARG
1	C	199	ILE
1	C	211	VAL
1	C	218	MET
1	C	220	THR
1	C	223	SER
1	C	226	GLU
1	C	235	GLN
1	C	238	LEU
1	C	260	MET
1	C	262	LEU
1	C	266	MET
1	C	272	ILE
1	C	273	VAL
1	C	274	GLU
1	C	276	LEU
1	C	297	THR
1	C	306	ASN
1	C	308	LEU
1	C	309	MET
1	C	318	THR
1	C	321	LEU
1	C	324	ARG
1	C	325	LEU
1	C	333	LYS
1	C	344	LYS
1	C	399	ARG
1	C	401	VAL
1	C	403	GLU
1	C	424	GLN
1	C	426	ASN
1	C	439	SER

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Mol	Chain	Res	Type
2	D	517	THR
2	D	520	ARG
2	D	528	MET
2	D	532	LEU
2	D	533	LEU
2	D	537	LYS
2	D	545	VAL
2	D	547	GLU
2	D	552	VAL
2	D	556	ARG
2	D	560	GLU
2	D	561	ARG
2	D	564	VAL
2	D	569	GLU
2	D	571	MET
2	D	584	ARG
2	D	586	LEU
2	D	590	THR
2	D	591	GLU
2	D	603	ARG
2	D	608	ASN
2	D	613	THR
2	D	616	SER
2	D	621	LYS
2	D	623	THR
2	D	624	SER
2	D	627	LEU
2	D	630	ARG
2	D	631	THR
2	D	634	ASP
2	D	637	THR
2	D	645	ARG
2	D	651	ARG
2	D	657	LEU
2	D	660	LYS
2	D	665	LEU
2	D	667	GLN
2	D	671	MET
2	D	672	THR
2	D	675	LEU
1	E	8	GLN
1	E	9	THR

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Mol	Chain	Res	Type
1	E	12	LYS
1	E	19	SER
1	E	39	GLU
1	E	57	GLU
1	E	58	ARG
1	E	67	SER
1	E	93	MET
1	E	95	VAL
1	E	99	GLU
1	E	118	THR
1	E	122	VAL
1	E	128	LYS
1	E	133	ASN
1	E	147	ASN
1	E	148	LEU
1	E	150	SER
1	E	152	LYS
1	E	154	LEU
1	E	159	LEU
1	E	173	LEU
1	E	179	ILE
1	E	180	VAL
1	E	188	LEU
1	E	196	ARG
1	E	199	ILE
1	E	211	VAL
1	E	220	THR
1	E	223	SER
1	E	226	GLU
1	E	235	GLN
1	E	238	LEU
1	E	260	MET
1	E	262	LEU
1	E	272	ILE
1	E	273	VAL
1	E	274	GLU
1	E	276	LEU
1	E	297	THR
1	E	306	ASN
1	E	308	LEU
1	E	309	MET
1	E	318	THR

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Mol	Chain	Res	Type
1	E	321	LEU
1	E	324	ARG
1	E	325	LEU
1	E	333	LYS
1	E	344	LYS
1	E	378	SER
1	E	390	THR
1	E	399	ARG
1	E	401	VAL
1	E	403	GLU
1	E	424	GLN
1	E	439	SER
2	F	517	THR
2	F	520	ARG
2	F	528	MET
2	F	532	LEU
2	F	533	LEU
2	F	537	LYS
2	F	545	VAL
2	F	547	GLU
2	F	552	VAL
2	F	556	ARG
2	F	560	GLU
2	F	561	ARG
2	F	564	VAL
2	F	569	GLU
2	F	571	MET
2	F	580	SER
2	F	586	LEU
2	F	590	THR
2	F	591	GLU
2	F	603	ARG
2	F	608	ASN
2	F	613	THR
2	F	616	SER
2	F	621	LYS
2	F	623	THR
2	F	624	SER
2	F	627	LEU
2	F	630	ARG
2	F	631	THR
2	F	634	ASP

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Mol	Chain	Res	Type
2	F	637	THR
2	F	645	ARG
2	F	657	LEU
2	F	660	LYS
2	F	665	LEU
2	F	667	GLN
2	F	671	MET
2	F	672	THR
2	F	675	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	84	HIS
1	A	141	ASN
1	A	209	ASN
1	A	244	HIS
1	A	249	HIS
1	A	271	ASN
1	A	306	ASN
1	A	375	ASN
1	A	424	GLN
1	A	433	GLN
2	B	608	ASN
1	C	15	HIS
1	C	29	ASN
1	C	34	HIS
1	C	84	HIS
1	C	141	ASN
1	C	249	HIS
1	C	271	ASN
1	C	306	ASN
1	C	375	ASN
1	C	424	GLN
1	C	433	GLN
2	D	608	ASN
1	E	15	HIS
1	E	84	HIS
1	E	141	ASN
1	E	209	ASN
1	E	249	HIS

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Mol	Chain	Res	Type
1	E	271	ASN
1	E	375	ASN
1	E	424	GLN
1	E	433	GLN
2	F	608	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
4	FES	A	501	1	0,4,4	-	-	-		
5	IND	C	503	-	10,10,10	2.17	5 (50%)	13,13,13	2.15	6 (46%)
5	IND	E	503	-	10,10,10	2.04	4 (40%)	13,13,13	1.69	3 (23%)
4	FES	E	501	1	0,4,4	-	-	-		
4	FES	C	501	1	0,4,4	-	-	-		
5	IND	A	503	-	10,10,10	1.81	4 (40%)	13,13,13	2.39	6 (46%)

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
4	FES	A	501	1	-	-	0/1/1/1
5	IND	C	503	-	-	-	0/2/2/2
5	IND	E	503	-	-	-	0/2/2/2
4	FES	E	501	1	-	-	0/1/1/1
4	FES	C	501	1	-	-	0/1/1/1
5	IND	A	503	-	-	-	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	IND	C7-C8	3.64	1.45	1.39
5	E	503	IND	C7-C8	3.41	1.45	1.39
5	C	503	IND	C2-C3	3.04	1.41	1.36
5	A	503	IND	C2-C3	2.92	1.41	1.36
5	E	503	IND	C2-C3	2.75	1.41	1.36
5	A	503	IND	C8-N1	-2.71	1.33	1.37
5	E	503	IND	C9-C8	2.67	1.45	1.41
5	C	503	IND	C9-C8	2.57	1.45	1.41
5	E	503	IND	C4-C9	2.35	1.45	1.41
5	C	503	IND	C4-C9	2.17	1.44	1.41
5	A	503	IND	C7-C8	2.12	1.43	1.39
5	C	503	IND	C6-C7	2.07	1.42	1.38
5	A	503	IND	C9-C3	-2.03	1.37	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	IND	C8-N1-C2	-4.88	105.35	108.91
5	C	503	IND	C8-N1-C2	-4.58	105.57	108.91
5	A	503	IND	C9-C8-N1	3.27	110.16	107.53
5	C	503	IND	C7-C8-C9	-3.19	119.24	122.13
5	E	503	IND	C8-C9-C3	3.17	108.59	106.59
5	A	503	IND	C9-C3-C2	-3.01	103.38	107.05
5	A	503	IND	C7-C8-C9	-2.90	119.50	122.13
5	A	503	IND	C8-C9-C3	2.78	108.35	106.59
5	E	503	IND	C8-N1-C2	-2.52	107.08	108.91
5	C	503	IND	C9-C3-C2	-2.49	104.02	107.05
5	C	503	IND	C8-C9-C3	2.48	108.16	106.59
5	C	503	IND	C9-C8-N1	2.47	109.51	107.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	503	IND	C9-C3-C2	-2.32	104.22	107.05
5	A	503	IND	C3-C2-N1	2.17	112.75	110.25
5	C	503	IND	C3-C2-N1	2.15	112.73	110.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	FES	3	0
4	E	501	FES	1	0
4	C	501	FES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2:LEU	C	3:SER	N	1.01

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	440/470 (93%)	0.78	37 (8%) 17 9	76, 92, 108, 140	0
1	C	440/470 (93%)	0.93	39 (8%) 15 8	76, 92, 108, 140	0
1	E	440/470 (93%)	0.98	41 (9%) 14 7	76, 92, 108, 140	0
2	B	165/172 (95%)	0.88	22 (13%) 7 4	75, 89, 111, 126	0
2	D	165/172 (95%)	0.81	20 (12%) 8 5	75, 89, 111, 126	0
2	F	165/172 (95%)	0.94	18 (10%) 10 6	75, 89, 111, 126	0
All	All	1815/1926 (94%)	0.89	177 (9%) 13 7	75, 91, 110, 140	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	137	LYS	9.7
1	E	133	ASN	9.5
1	E	135	LEU	9.1
1	C	440	PRO	8.6
1	E	132	GLY	7.9
2	F	562	GLU	7.4
1	E	126	ALA	7.3
1	E	125	PRO	7.2
1	E	127	GLY	7.0
1	E	440	PRO	6.7
1	E	136	LYS	6.3
2	D	515	SER	6.2
1	A	440	PRO	6.0
1	E	123	GLY	5.5
2	F	515	SER	5.4
2	B	515	SER	5.3
1	A	257	PRO	5.3
2	F	597	ASP	5.2
2	F	560	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	597	ASP	4.7
1	E	138	SER	4.7
1	E	164	ASP	4.6
1	E	140	TRP	4.6
2	F	561	ARG	4.4
2	B	562	GLU	4.4
1	E	134	GLN	4.4
1	E	124	VAL	4.3
1	E	129	ASP	4.3
1	E	131	TYR	4.2
1	A	258	PRO	4.2
1	E	1	MET	4.2
1	E	128	LYS	4.1
2	F	563	ALA	4.1
1	E	118	THR	3.8
1	A	215	TYR	3.7
1	C	401	VAL	3.7
2	D	654	ASP	3.6
1	E	258	PRO	3.5
2	B	540	GLU	3.5
2	B	516	ASP	3.5
2	D	566	ASP	3.5
1	C	257	PRO	3.5
2	D	561	ARG	3.4
2	B	563	ALA	3.4
2	F	654	ASP	3.3
2	B	517	THR	3.3
2	B	518	THR	3.3
1	A	131	TYR	3.2
1	A	125	PRO	3.2
1	A	439	SER	3.2
1	A	127	GLY	3.2
1	E	270	GLU	3.2
2	B	560	GLU	3.2
2	D	597	ASP	3.2
1	C	439	SER	3.1
1	C	133	ASN	3.1
1	E	261	PRO	3.1
1	A	130	ALA	3.1
1	C	118	THR	3.1
1	C	192	GLY	3.1
2	B	546	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	400	GLY	3.1
2	B	617	GLU	3.0
2	F	616	SER	3.0
2	B	615	ASP	3.0
1	E	373	ALA	3.0
1	A	400	GLY	3.0
1	A	128	LYS	3.0
1	C	270	GLU	3.0
1	E	139	ASP	3.0
1	C	277	GLU	3.0
1	C	345	ASP	3.0
1	C	1	MET	3.0
2	D	616	SER	2.9
1	A	122	VAL	2.9
1	E	168	ASP	2.9
1	E	438	GLU	2.9
1	A	110	TYR	2.9
1	C	310	GLY	2.9
2	B	564	VAL	2.9
1	C	138	SER	2.8
1	C	418	ASP	2.8
1	A	126	ALA	2.8
1	A	270	GLU	2.8
2	D	618	ASP	2.8
2	F	633	GLY	2.8
1	A	137	LYS	2.8
1	E	120	SER	2.8
2	B	633	GLY	2.8
1	C	261	PRO	2.8
1	C	311	LYS	2.7
1	E	130	ALA	2.7
1	A	39	GLU	2.7
2	D	560	GLU	2.7
2	F	516	ASP	2.7
1	A	133	ASN	2.7
1	E	439	SER	2.7
2	F	518	THR	2.7
1	E	401	VAL	2.7
1	A	300	PRO	2.7
1	C	404	PRO	2.7
2	D	517	THR	2.7
1	C	128	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	562	GLU	2.6
2	B	561	ARG	2.6
1	C	258	PRO	2.6
1	A	278	ARG	2.6
2	D	653	GLY	2.5
1	A	261	PRO	2.5
1	C	245	THR	2.5
2	B	618	ASP	2.5
2	D	592	TYR	2.5
1	C	186	ALA	2.4
1	A	129	ASP	2.4
2	D	631	THR	2.4
1	A	401	VAL	2.4
1	E	281	THR	2.4
1	C	260	MET	2.4
1	C	416	PRO	2.4
2	D	647	ASP	2.3
1	A	386	GLN	2.3
2	D	651	ARG	2.3
1	C	135	LEU	2.3
1	A	274	GLU	2.3
2	B	547	GLU	2.3
2	F	564	VAL	2.3
2	D	563	ALA	2.3
2	B	654	ASP	2.3
2	D	516	ASP	2.3
2	D	617	GLU	2.3
2	B	672	THR	2.3
1	E	101	GLY	2.3
2	F	517	THR	2.3
1	A	239	TYR	2.3
1	E	80	GLU	2.2
2	F	547	GLU	2.2
2	F	659	ALA	2.2
2	B	566	ASP	2.2
2	F	521	GLU	2.2
2	F	566	ASP	2.2
1	C	412	GLY	2.2
1	C	422	ALA	2.2
1	C	281	THR	2.2
1	C	272	ILE	2.2
1	A	192	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	130	ALA	2.2
1	A	140	TRP	2.2
2	F	620	PHE	2.2
2	B	519	VAL	2.2
1	A	1	MET	2.2
1	C	408	TRP	2.2
1	C	409	THR	2.2
1	E	239	TYR	2.2
1	C	395	TYR	2.1
1	E	8	GLN	2.1
1	A	132	GLY	2.1
1	A	423	ASN	2.1
1	C	15	HIS	2.1
2	B	613	THR	2.1
1	C	129	ASP	2.1
1	A	438	GLU	2.1
1	C	349	TRP	2.1
2	D	547	GLU	2.1
1	E	278	ARG	2.1
2	D	590	THR	2.1
1	A	272	ILE	2.0
1	C	2	LEU	2.0
1	E	162	HIS	2.0
1	A	390	THR	2.0
1	C	164	ASP	2.0
1	E	9	THR	2.0
1	E	189	GLN	2.0
1	A	136	LYS	2.0
1	E	81	ILE	2.0
1	C	265	PHE	2.0
1	A	77	GLU	2.0
1	A	262	LEU	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($\text{\AA}^2$)	Q<0.9
5	IND	C	503	9/9	0.88	0.28	71,72,73,73	0
5	IND	E	503	9/9	0.88	0.19	71,72,73,73	0
5	IND	A	503	9/9	0.93	0.22	71,72,73,73	0
3	FE	C	502	1/1	0.96	0.07	69,69,69,69	0
3	FE	E	502	1/1	0.97	0.07	66,66,66,66	0
4	FES	A	501	4/4	0.98	0.11	60,60,60,64	0
3	FE	A	502	1/1	0.98	0.07	66,66,66,66	0
4	FES	E	501	4/4	0.99	0.05	58,59,60,62	0
4	FES	C	501	4/4	0.99	0.06	58,59,59,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.