Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 06:41 PM EDT

PDB ID	:	2B24
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:

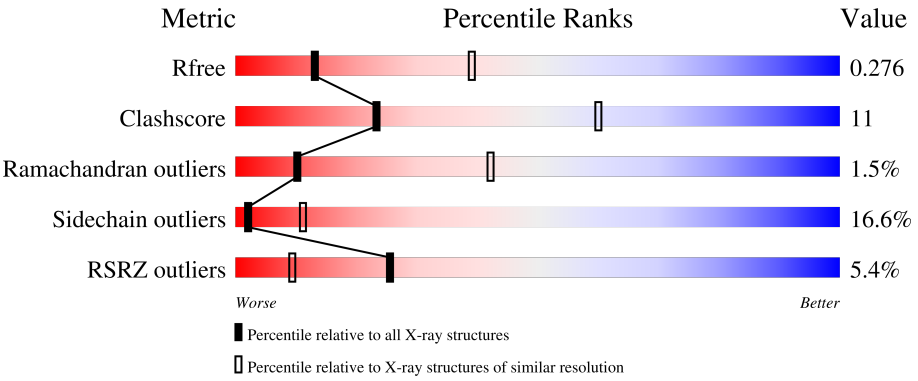
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	6% 62% 27% 5% 6%
1	C	470	6% 61% 26% 5% 6%
1	E	470	6% 61% 27% 5% 6%
2	B	172	3% 55% 32% 9% . .
2	D	172	5% 54% 33% 8% . .

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Mol	Chain	Length	Quality of chain
2	F	172	2% 52% 34% 6%

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	C	503	-	-	-	X

2 Entry composition (i)

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			

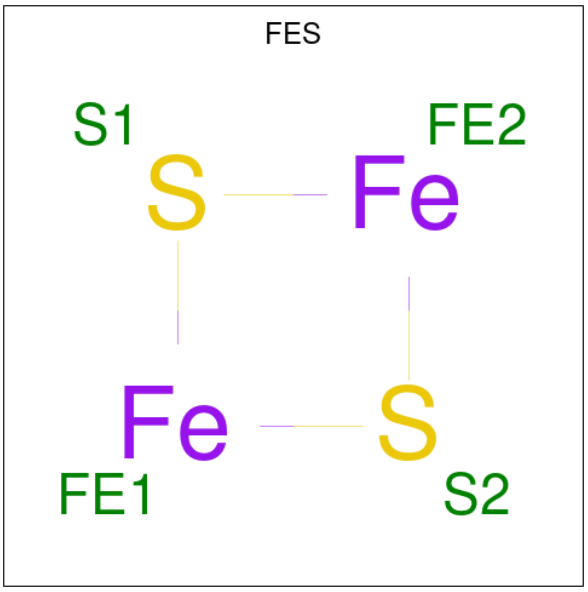
- Molecule 2 is a protein called naphthalene dioxygenase small subunit.

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 (three-letter code: FE) (formula: Fe).

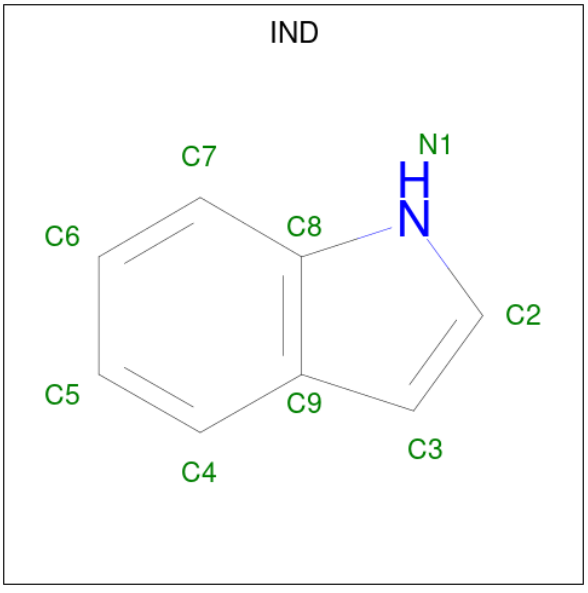
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 5 is INDOLE (three-letter code: IND) (formula: C_8H_7N).



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

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

- Molecule 6 is water.

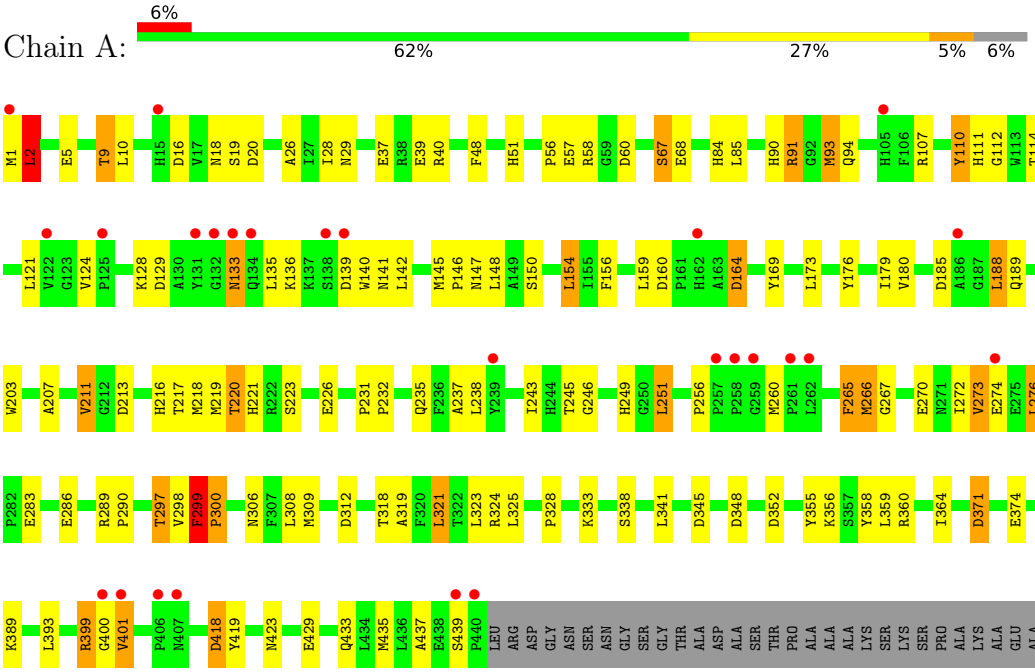
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	66	Total O 66 66	0	0
6	B	35	Total O 35 35	0	0
6	C	64	Total O 64 64	0	0
6	D	29	Total O 29 29	0	0
6	E	82	Total O 82 82	0	0
6	F	36	Total O 36 36	0	0

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.

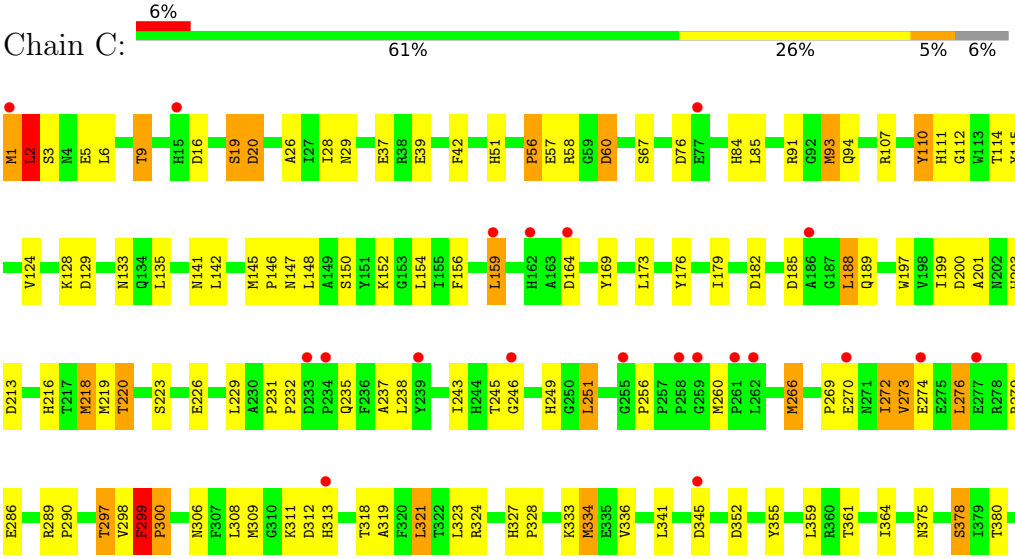
• Molecule 1: naphthalene dioxygenase large subunit

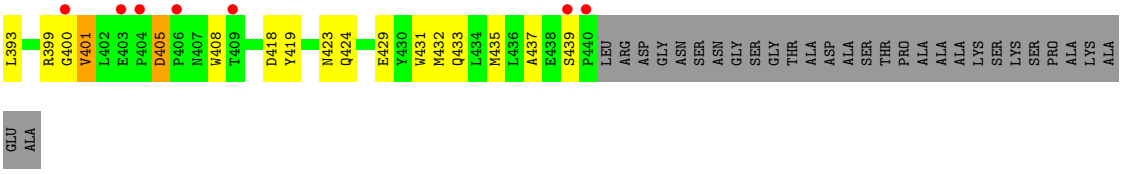
Chain A:



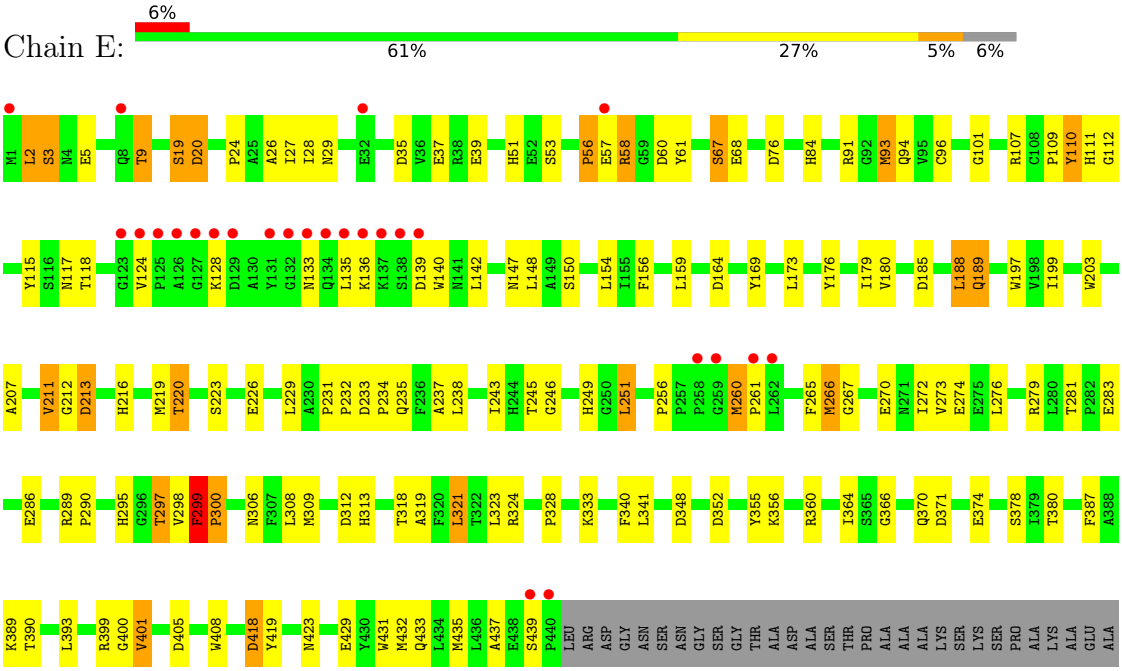
• Molecule 1: naphthalene dioxygenase large subunit

Chain C:

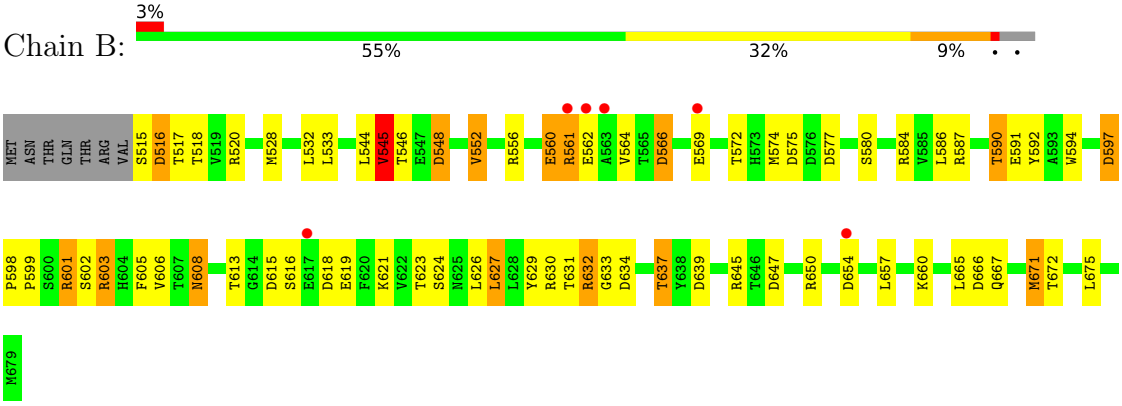




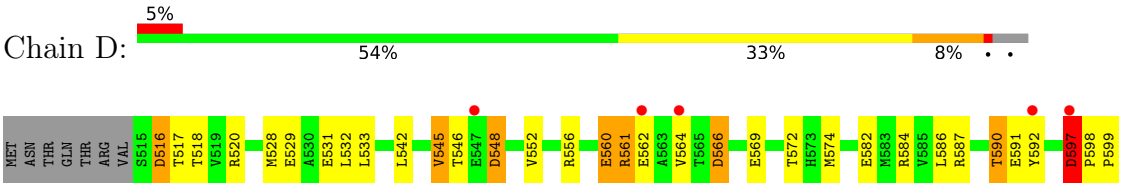
• Molecule 1: naphthalene dioxygenase large subunit

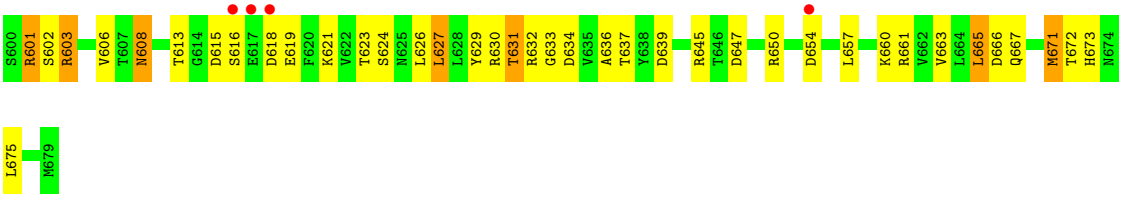


• Molecule 2: naphthalene dioxygenase small subunit



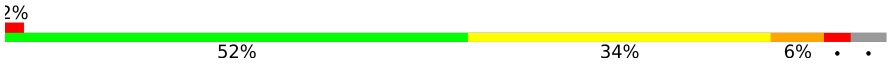
• Molecule 2: naphthalene dioxygenase small subunit

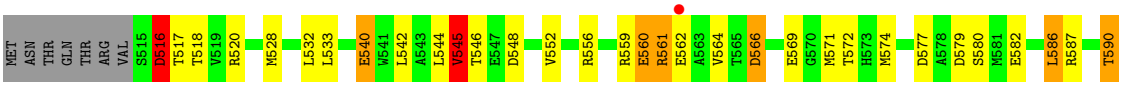


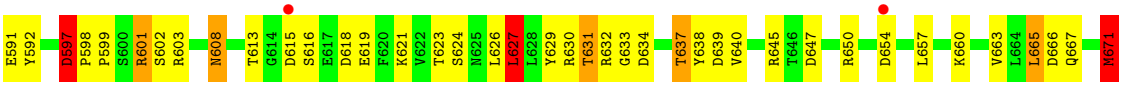


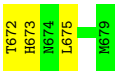
• Molecule 2: naphthalene dioxygenase small subunit

Chain F:









4 Data and refinement statistics (i)

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 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.42-3.00) 99.2 (19.99-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (3.06%)	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)	0.30 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: IND, FE, FES

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	0.47	0/3612	0.80	16/4908 (0.3%)
1	C	0.55	4/3612 (0.1%)	0.95	19/4908 (0.4%)
1	E	0.53	0/3612	0.79	11/4908 (0.2%)
2	B	0.58	0/1350	0.93	10/1831 (0.5%)
2	D	0.51	0/1350	0.93	10/1831 (0.5%)
2	F	0.60	1/1350 (0.1%)	0.96	11/1831 (0.6%)
All	All	0.53	5/14886 (0.0%)	0.87	77/20217 (0.4%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	LEU	C-N	-14.13	1.01	1.34
1	C	2	LEU	CB-CG	7.54	1.74	1.52
1	C	2	LEU	N-CA	7.35	1.61	1.46
1	C	2	LEU	C-O	5.88	1.34	1.23
2	F	671	MET	SD-CE	-5.17	1.48	1.77

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	MET	O-C-N	-30.20	74.38	122.70
1	C	2	LEU	O-C-N	-16.43	96.42	122.70
1	C	2	LEU	C-N-CA	11.78	151.15	121.70
1	C	2	LEU	CA-C-N	10.08	139.38	117.20
1	A	2	LEU	N-CA-C	-9.71	84.79	111.00
1	C	1	MET	C-N-CA	7.38	140.15	121.70
1	A	20	ASP	CB-CG-OD2	7.21	124.79	118.30
2	B	647	ASP	CB-CG-OD2	6.95	124.56	118.30
2	F	647	ASP	CB-CG-OD2	6.92	124.53	118.30
2	F	577	ASP	CB-CG-OD2	6.90	124.51	118.30
2	D	627	LEU	CA-CB-CG	6.82	130.99	115.30
1	C	1	MET	CA-C-N	6.82	132.19	117.20
2	F	597	ASP	CB-CG-OD2	6.47	124.12	118.30
1	C	164	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	312	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	164	ASP	CB-CG-OD2	6.40	124.06	118.30
2	F	627	LEU	CA-CB-CG	6.27	129.72	115.30
2	D	647	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	60	ASP	CB-CG-OD2	6.20	123.88	118.30
1	E	348	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	1	MET	CA-CB-CG	6.09	123.66	113.30
1	C	20	ASP	CB-CG-OD2	6.06	123.75	118.30
2	F	516	ASP	CB-CG-OD2	6.05	123.74	118.30
2	B	654	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	129	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	139	ASP	CB-CG-OD2	5.93	123.64	118.30
1	C	16	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	2	LEU	CB-CA-C	-5.90	98.98	110.20
1	E	213	ASP	CB-CG-OD2	5.89	123.61	118.30
1	C	213	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	348	ASP	CB-CG-OD2	5.84	123.56	118.30
2	D	615	ASP	CB-CG-OD2	5.79	123.51	118.30
2	D	597	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	2	LEU	N-CA-C	-5.70	95.62	111.00
1	C	345	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	312	ASP	CB-CG-OD2	5.67	123.40	118.30
2	B	566	ASP	CB-CG-OD2	5.64	123.37	118.30
2	F	566	ASP	CB-CG-OD2	5.62	123.36	118.30
2	F	579	ASP	CB-CG-OD2	5.62	123.36	118.30
2	F	639	ASP	CB-CG-OD2	5.60	123.34	118.30
2	B	639	ASP	CB-CG-OD2	5.59	123.33	118.30
2	F	654	ASP	CB-CG-OD2	5.57	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	60	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	352	ASP	CB-CG-OD2	5.56	123.30	118.30
1	C	405	ASP	CB-CG-OD2	5.55	123.30	118.30
2	D	566	ASP	CB-CG-OD2	5.54	123.29	118.30
1	E	76	ASP	CB-CG-OD2	5.54	123.28	118.30
2	B	627	LEU	CA-CB-CG	5.54	128.03	115.30
2	D	548	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	160	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	418	ASP	CB-CG-OD2	5.51	123.26	118.30
2	F	615	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	35	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	615	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	213	ASP	CB-CG-OD2	5.42	123.17	118.30
1	E	20	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	352	ASP	CB-CG-OD2	5.40	123.16	118.30
2	B	618	ASP	CB-CG-OD2	5.40	123.16	118.30
2	B	575	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	312	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	139	ASP	CB-CG-OD2	5.34	123.10	118.30
2	B	548	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	200	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	654	ASP	CB-CG-OD2	5.28	123.05	118.30
2	D	666	ASP	CB-CG-OD2	5.26	123.03	118.30
2	D	618	ASP	CB-CG-OD2	5.25	123.03	118.30
1	E	352	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	129	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	164	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	371	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	76	ASP	CB-CG-OD2	5.18	122.96	118.30
2	D	639	ASP	CB-CG-OD2	5.18	122.96	118.30
2	F	618	ASP	CB-CG-OD2	5.14	122.92	118.30
2	B	577	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	345	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	16	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	418	ASP	CB-CG-OD2	5.07	122.86	118.30

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

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3506	0	3333	78	0
1	C	3506	0	3332	82	0
1	E	3506	0	3333	90	0
2	B	1330	0	1303	36	0
2	D	1330	0	1303	33	0
2	F	1330	0	1303	38	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	4	0
6	F	36	0	0	1	0
All	All	14862	0	13928	321	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 (321) 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: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: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:20:ASP:CG	6:E:517:HOH:O	2.37	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:A:300:PRO:C	2.40	0.60
1:C:299:PHE:O	1:C:300:PRO:C	2.40	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
2:F:601:ARG:HH22	2:F:633:GLY:H	1.51	0.58
1:E:299:PHE:O	1:E:300:PRO:C	2.43	0.57
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: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
1:C:270:GLU:CD	1:C:270:GLU:H	2.09	0.56
1:C:107:ARG:HG2	1:E:219:MET:HE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:270:GLU:CD	1:E:270:GLU:H	2.10	0.54
2:F:608:ASN:N	2:F:608:ASN:HD22	2.06	0.54
2:F:546:THR:HG21	2:F:650:ARG:HH21	1.73	0.53
2:D:671:MET:HE2	2:F:638:TYR:HD2	1.73	0.53
1:E:251:LEU:O	1:E:423:ASN:ND2	2.40	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
1:A:270:GLU:H	1:A:270:GLU:CD	2.12	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
1:C:245:THR:HG22	1:C:246:GLY:H	1.75	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:164:ASP:CG	6:A:564:HOH:O	2.50	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: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:A:219:MET:HE2	1:E:107:ARG:HG2	1.94	0.48
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:A:338:SER:OG	1:A:358:TYR:OH	2.30	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
2:D:516:ASP:C	2:D:518:THR:H	2.17	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:E:124:VAL:HG21	1:E:135:LEU:HD21	1.96	0.48
1:A:94:GLN:HB2	1:C:378:SER:HG	1.78	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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:HB3	1:A:68:GLU:H	1.57	0.47
1:E:51:HIS:ND1	1:E:53:SER:OG	2.38	0.47
1:E:124:VAL:HG21	1:E:135:LEU:CD2	2.44	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:C:199:ILE:HG23	2:D:673:HIS:HB2	1.97	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
2:F:516:ASP:C	2:F:518:THR:H	2.19	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
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
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
1:E:216:HIS:HD2	1:E:220:THR:HG21	1.81	0.45
1:E:265:PHE:C	1:E:267:GLY:H	2.20	0.45
2:B:637:THR:N	2:F:671:MET:HE3	2.31	0.45
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:B:516:ASP:C	2:B:518:THR:H	2.20	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:A:323:LEU:HG	1:A:341:LEU:HD13	1.98	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:37:GLU:HA	1:E:435:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:298:VAL:O	1:A:299:PHE:C	2.55	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:107:ARG:HG2	1:C:219:MET:HE2	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
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: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
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
2:B:603:ARG:HG2	2:B:605:PHE:CZ	2.53	0.44
2:D:601:ARG:HH22	2:D:633:GLY:N	2.16	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:19:SER:OG	1:C:20:ASP:N	2.51	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PHE:C	1:A:267:GLY:H	2.21	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: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: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
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:229:LEU:HD11	1:C:313:HIS:HA	2.01	0.42
1:C:145:MET:O	1:C:146:PRO:C	2.58	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
1:E:289:ARG:HB3	1:E:290:PRO:HD3	2.02	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:A:145:MET:O	1:A:146:PRO:C	2.58	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: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
2:D:529:GLU:OE2	2:D:661:ARG:NH1	2.45	0.41
1:C:298:VAL:O	1:C:299:PHE:C	2.58	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
2:B:671:MET:HE3	2:D:636:ALA:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:SER:HA	1:C:141:ASN:CG	2.41	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
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: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: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:D:531:GLU:CD	6:D:293:HOH:O	2.59	0.41
2:B:608:ASN:HD22	2:B:608:ASN:N	2.19	0.41
2:D:671:MET:HE1	2:F:637:THR:N	2.36	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:298:VAL:O	1:E:299:PHE:C	2.60	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%)	8 37
1	C	438/470 (93%)	393 (90%)	39 (9%)	6 (1%)	11 43
1	E	438/470 (93%)	392 (90%)	39 (9%)	7 (2%)	9 40
2	B	163/172 (95%)	147 (90%)	14 (9%)	2 (1%)	13 48
2	D	163/172 (95%)	149 (91%)	12 (7%)	2 (1%)	13 48
2	F	163/172 (95%)	147 (90%)	14 (9%)	2 (1%)	13 48
All	All	1803/1926 (94%)	1623 (90%)	153 (8%)	27 (2%)	10 42

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/389 (95%)	320 (86%)	50 (14%)	4 17
1	C	370/389 (95%)	321 (87%)	49 (13%)	4 18
1	E	370/389 (95%)	325 (88%)	45 (12%)	5 21
2	B	147/154 (96%)	108 (74%)	39 (26%)	0 2
2	D	147/154 (96%)	110 (75%)	37 (25%)	0 3
2	F	147/154 (96%)	109 (74%)	38 (26%)	0 2
All	All	1551/1629 (95%)	1293 (83%)	258 (17%)	2 11

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	9	THR
1	A	19	SER
1	A	39	GLU
1	A	57	GLU
1	A	58	ARG
1	A	67	SER
1	A	91	ARG
1	A	93	MET
1	A	110	TYR
1	A	118	THR

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Mol	Chain	Res	Type
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	189	GLN
1	A	199	ILE
1	A	211	VAL
1	A	218	MET
1	A	220	THR
1	A	223	SER
1	A	226	GLU
1	A	235	GLN
1	A	238	LEU
1	A	251	LEU
1	A	260	MET
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	324	ARG
1	A	333	LYS
1	A	355	TYR
1	A	359	LEU
1	A	378	SER
1	A	399	ARG
1	A	439	SER
2	B	517	THR
2	B	520	ARG
2	B	528	MET

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Mol	Chain	Res	Type
2	B	532	LEU
2	B	533	LEU
2	B	545	VAL
2	B	552	VAL
2	B	556	ARG
2	B	560	GLU
2	B	561	ARG
2	B	564	VAL
2	B	566	ASP
2	B	569	GLU
2	B	580	SER
2	B	584	ARG
2	B	586	LEU
2	B	590	THR
2	B	591	GLU
2	B	601	ARG
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	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
1	C	2	LEU
1	C	9	THR
1	C	19	SER
1	C	39	GLU
1	C	57	GLU
1	C	58	ARG

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Mol	Chain	Res	Type
1	C	67	SER
1	C	91	ARG
1	C	93	MET
1	C	110	TYR
1	C	118	THR
1	C	128	LYS
1	C	133	ASN
1	C	147	ASN
1	C	148	LEU
1	C	150	SER
1	C	159	LEU
1	C	173	LEU
1	C	179	ILE
1	C	188	LEU
1	C	189	GLN
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	251	LEU
1	C	260	MET
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	333	LYS
1	C	334	MET
1	C	355	TYR
1	C	378	SER
1	C	399	ARG
1	C	424	GLN

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Mol	Chain	Res	Type
1	C	439	SER
2	D	517	THR
2	D	520	ARG
2	D	528	MET
2	D	532	LEU
2	D	533	LEU
2	D	545	VAL
2	D	552	VAL
2	D	556	ARG
2	D	560	GLU
2	D	561	ARG
2	D	564	VAL
2	D	566	ASP
2	D	569	GLU
2	D	584	ARG
2	D	586	LEU
2	D	590	THR
2	D	591	GLU
2	D	601	ARG
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	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	9	THR
1	E	19	SER
1	E	39	GLU
1	E	57	GLU

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Mol	Chain	Res	Type
1	E	58	ARG
1	E	67	SER
1	E	91	ARG
1	E	93	MET
1	E	110	TYR
1	E	118	THR
1	E	128	LYS
1	E	133	ASN
1	E	147	ASN
1	E	148	LEU
1	E	150	SER
1	E	159	LEU
1	E	173	LEU
1	E	179	ILE
1	E	180	VAL
1	E	188	LEU
1	E	189	GLN
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	251	LEU
1	E	260	MET
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
1	E	321	LEU
1	E	324	ARG
1	E	333	LYS
1	E	355	TYR
1	E	378	SER
1	E	399	ARG
1	E	439	SER
2	F	517	THR

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Mol	Chain	Res	Type
2	F	520	ARG
2	F	528	MET
2	F	532	LEU
2	F	533	LEU
2	F	540	GLU
2	F	545	VAL
2	F	552	VAL
2	F	556	ARG
2	F	560	GLU
2	F	561	ARG
2	F	564	VAL
2	F	566	ASP
2	F	569	GLU
2	F	580	SER
2	F	586	LEU
2	F	590	THR
2	F	591	GLU
2	F	601	ARG
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
2	F	637	THR
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS

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Mol	Chain	Res	Type
1	A	141	ASN
1	A	244	HIS
1	A	249	HIS
1	A	433	GLN
2	B	608	ASN
1	C	84	HIS
1	C	141	ASN
1	C	244	HIS
1	C	249	HIS
1	C	306	ASN
1	C	375	ASN
1	C	433	GLN
2	D	608	ASN
1	E	84	HIS
1	E	141	ASN
1	E	249	HIS
1	E	433	GLN
2	F	608	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
5	IND	C	503	-	8,10,10	1.57	2 (25%)	9,13,13	1.09	1 (11%)
4	FES	A	501	1	0,4,4	-	-	-		
4	FES	E	501	1	0,4,4	-	-	-		
4	FES	C	501	1	0,4,4	-	-	-		
5	IND	E	503	-	8,10,10	1.42	1 (12%)	9,13,13	1.37	1 (11%)
5	IND	A	503	-	8,10,10	1.21	0	9,13,13	1.29	1 (11%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	IND	C6-C7	2.52	1.42	1.36
5	E	503	IND	C5-C4	2.27	1.41	1.36
5	C	503	IND	C7-C8	2.16	1.45	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	503	IND	C3-C9-C8	2.80	108.59	106.20
5	A	503	IND	C3-C9-C8	2.51	108.35	106.20
5	C	503	IND	C3-C9-C8	2.29	108.16	106.20

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	440/470 (93%)	0.22	26 (5%) 22 7	76, 92, 108, 140	0
1	C	440/470 (93%)	0.36	28 (6%) 19 6	76, 92, 108, 140	0
1	E	440/470 (93%)	0.26	26 (5%) 22 7	76, 92, 108, 140	0
2	B	165/172 (95%)	0.09	6 (3%) 42 17	75, 89, 111, 126	0
2	D	165/172 (95%)	0.17	9 (5%) 25 9	75, 89, 111, 126	0
2	F	165/172 (95%)	0.02	3 (1%) 68 40	75, 89, 111, 126	0
All	All	1815/1926 (94%)	0.23	98 (5%) 25 9	75, 91, 110, 140	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	439	SER	8.3
1	E	440	PRO	7.4
1	E	133	ASN	6.9
1	E	125	PRO	6.8
1	E	132	GLY	6.2
1	A	440	PRO	5.8
1	E	258	PRO	5.7
1	C	440	PRO	5.4
1	E	126	ALA	5.3
1	A	258	PRO	5.2
1	E	137	LYS	4.9
2	F	562	GLU	4.9
1	E	127	GLY	4.6
1	E	134	GLN	4.3
1	C	186	ALA	4.3
1	A	439	SER	4.0
1	C	404	PRO	4.0
1	E	138	SER	4.0
1	A	261	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	138	SER	3.8
1	E	128	LYS	3.8
1	C	259	GLY	3.5
1	E	439	SER	3.5
1	A	259	GLY	3.5
2	B	562	GLU	3.5
1	E	261	PRO	3.4
1	A	400	GLY	3.4
1	C	164	ASP	3.4
1	C	1	MET	3.4
1	E	1	MET	3.4
1	A	134	GLN	3.3
1	C	258	PRO	3.3
1	C	261	PRO	3.3
2	D	547	GLU	3.1
1	A	401	VAL	3.0
1	A	406	PRO	3.0
1	A	139	ASP	3.0
2	B	654	ASP	3.0
2	B	617	GLU	3.0
1	E	135	LEU	3.0
1	A	407	ASN	3.0
2	D	564	VAL	2.9
1	C	233	ASP	2.9
1	A	257	PRO	2.9
1	E	129	ASP	2.9
1	C	400	GLY	2.9
1	C	162	HIS	2.9
2	D	597	ASP	2.9
1	C	409	THR	2.8
1	A	133	ASN	2.8
1	C	345	ASP	2.8
1	A	1	MET	2.8
1	A	274	GLU	2.8
1	C	262	LEU	2.7
1	C	274	GLU	2.7
1	E	57	GLU	2.7
2	B	569	GLU	2.7
1	E	123	GLY	2.6
1	A	132	GLY	2.6
1	E	124	VAL	2.6
2	F	615	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	77	GLU	2.5
1	C	403	GLU	2.5
1	A	131	TYR	2.5
1	A	262	LEU	2.5
2	D	654	ASP	2.5
1	E	8	GLN	2.4
2	D	592	TYR	2.4
1	A	15	HIS	2.4
1	C	406	PRO	2.4
2	D	616	SER	2.4
2	F	654	ASP	2.3
1	E	262	LEU	2.3
1	E	139	ASP	2.3
1	C	313	HIS	2.3
1	C	15	HIS	2.3
1	A	125	PRO	2.2
2	B	563	ALA	2.2
1	C	277	GLU	2.2
2	D	617	GLU	2.2
1	A	162	HIS	2.2
1	C	246	GLY	2.2
1	C	270	GLU	2.2
1	C	255	GLY	2.2
1	C	234	PRO	2.2
1	A	105	HIS	2.1
1	A	239	TYR	2.1
1	E	136	LYS	2.1
2	D	562	GLU	2.1
1	E	259	GLY	2.1
1	A	122	VAL	2.1
2	B	561	ARG	2.1
2	D	618	ASP	2.1
1	C	159	LEU	2.1
1	C	239	TYR	2.1
1	E	32	GLU	2.1
1	A	186	ALA	2.0
1	E	131	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	IND	C	503	9/9	0.72	0.63	71,72,73,73	0
5	IND	E	503	9/9	0.85	0.31	71,72,73,73	0
5	IND	A	503	9/9	0.90	0.42	71,72,73,73	0
3	FE	A	502	1/1	0.94	0.10	66,66,66,66	0
3	FE	C	502	1/1	0.96	0.10	69,69,69,69	0
3	FE	E	502	1/1	0.97	0.08	66,66,66,66	0
4	FES	E	501	4/4	0.98	0.06	58,59,60,62	0
4	FES	A	501	4/4	0.98	0.10	60,60,60,64	0
4	FES	C	501	4/4	0.99	0.05	58,59,59,62	0

6.5 Other polymers (i)

There are no such residues in this entry.