



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:48 am BST

PDB ID : 5OAT
Title : PINK1 structure
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Deposited on : 2017-06-23
Resolution : 2.78 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 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 : 2.11
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) : 2.11

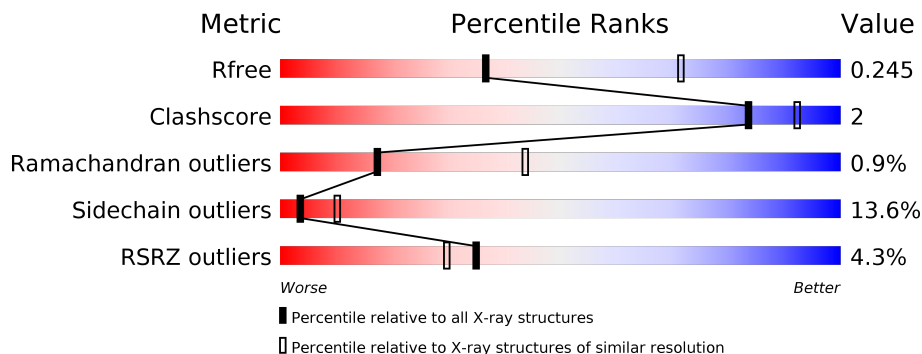
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 on 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	411	 3% 73% 13% • 12%
1	B	411	 5% 73% 13% • 12%
1	C	411	 4% 71% 15% • 12%
1	D	411	 5% 71% 14% • 12%
1	E	411	 3% 73% 14% • 12%
1	F	411	 3% 72% 14% • 12%

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
2	MG	A	601	-	-	-	X
2	MG	C	602	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16758 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 Serine/threonine-protein kinase PINK1, mitochondrial-like Protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	360	2787	1793	464	512	1	17	0	0	0
1	B	360	2787	1793	464	512	1	17	0	0	0
1	C	360	2787	1793	464	512	1	17	0	0	0
1	D	360	2787	1793	464	512	1	17	0	0	0
1	E	360	2787	1793	464	512	1	17	0	0	0
1	F	360	2787	1793	464	512	1	17	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	GLU	SER	conflict	UNP D6WMX4
A	?	-	ILE	deletion	UNP D6WMX4
A	?	-	GLN	deletion	UNP D6WMX4
A	?	-	GLU	deletion	UNP D6WMX4
A	?	-	LEU	deletion	UNP D6WMX4
A	?	-	GLU	deletion	UNP D6WMX4
A	?	-	GLY	deletion	UNP D6WMX4
A	?	-	SER	deletion	UNP D6WMX4
A	?	-	LYS	deletion	UNP D6WMX4
A	?	-	ASP	deletion	UNP D6WMX4
A	?	-	LEU	deletion	UNP D6WMX4
A	527	ALA	GLU	conflict	UNP D6WMX4
A	528	ALA	LYS	conflict	UNP D6WMX4
B	205	GLU	SER	conflict	UNP D6WMX4
B	?	-	ILE	deletion	UNP D6WMX4
B	?	-	GLN	deletion	UNP D6WMX4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP D6WMX4
B	?	-	LEU	deletion	UNP D6WMX4
B	?	-	GLU	deletion	UNP D6WMX4
B	?	-	GLY	deletion	UNP D6WMX4
B	?	-	SER	deletion	UNP D6WMX4
B	?	-	LYS	deletion	UNP D6WMX4
B	?	-	ASP	deletion	UNP D6WMX4
B	?	-	LEU	deletion	UNP D6WMX4
B	527	ALA	GLU	conflict	UNP D6WMX4
B	528	ALA	LYS	conflict	UNP D6WMX4
C	205	GLU	SER	conflict	UNP D6WMX4
C	?	-	ILE	deletion	UNP D6WMX4
C	?	-	GLN	deletion	UNP D6WMX4
C	?	-	GLU	deletion	UNP D6WMX4
C	?	-	LEU	deletion	UNP D6WMX4
C	?	-	GLU	deletion	UNP D6WMX4
C	?	-	GLY	deletion	UNP D6WMX4
C	?	-	SER	deletion	UNP D6WMX4
C	?	-	LYS	deletion	UNP D6WMX4
C	?	-	ASP	deletion	UNP D6WMX4
C	?	-	LEU	deletion	UNP D6WMX4
C	527	ALA	GLU	conflict	UNP D6WMX4
C	528	ALA	LYS	conflict	UNP D6WMX4
D	205	GLU	SER	conflict	UNP D6WMX4
D	?	-	ILE	deletion	UNP D6WMX4
D	?	-	GLN	deletion	UNP D6WMX4
D	?	-	GLU	deletion	UNP D6WMX4
D	?	-	LEU	deletion	UNP D6WMX4
D	?	-	GLU	deletion	UNP D6WMX4
D	?	-	GLY	deletion	UNP D6WMX4
D	?	-	SER	deletion	UNP D6WMX4
D	?	-	LYS	deletion	UNP D6WMX4
D	?	-	ASP	deletion	UNP D6WMX4
D	?	-	LEU	deletion	UNP D6WMX4
D	527	ALA	GLU	conflict	UNP D6WMX4
D	528	ALA	LYS	conflict	UNP D6WMX4
E	205	GLU	SER	conflict	UNP D6WMX4
E	?	-	ILE	deletion	UNP D6WMX4
E	?	-	GLN	deletion	UNP D6WMX4
E	?	-	GLU	deletion	UNP D6WMX4
E	?	-	LEU	deletion	UNP D6WMX4
E	?	-	GLU	deletion	UNP D6WMX4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLY	deletion	UNP D6WMX4
E	?	-	SER	deletion	UNP D6WMX4
E	?	-	LYS	deletion	UNP D6WMX4
E	?	-	ASP	deletion	UNP D6WMX4
E	?	-	LEU	deletion	UNP D6WMX4
E	527	ALA	GLU	conflict	UNP D6WMX4
E	528	ALA	LYS	conflict	UNP D6WMX4
F	205	GLU	SER	conflict	UNP D6WMX4
F	?	-	ILE	deletion	UNP D6WMX4
F	?	-	GLN	deletion	UNP D6WMX4
F	?	-	GLU	deletion	UNP D6WMX4
F	?	-	LEU	deletion	UNP D6WMX4
F	?	-	GLU	deletion	UNP D6WMX4
F	?	-	GLY	deletion	UNP D6WMX4
F	?	-	SER	deletion	UNP D6WMX4
F	?	-	LYS	deletion	UNP D6WMX4
F	?	-	ASP	deletion	UNP D6WMX4
F	?	-	LEU	deletion	UNP D6WMX4
F	527	ALA	GLU	conflict	UNP D6WMX4
F	528	ALA	LYS	conflict	UNP D6WMX4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	C	2	Total Mg 2 2	0	0
2	F	1	Total Mg 1 1	0	0
2	E	2	Total Mg 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	9	Total O 9 9	0	0
3	C	3	Total O 3 3	0	0

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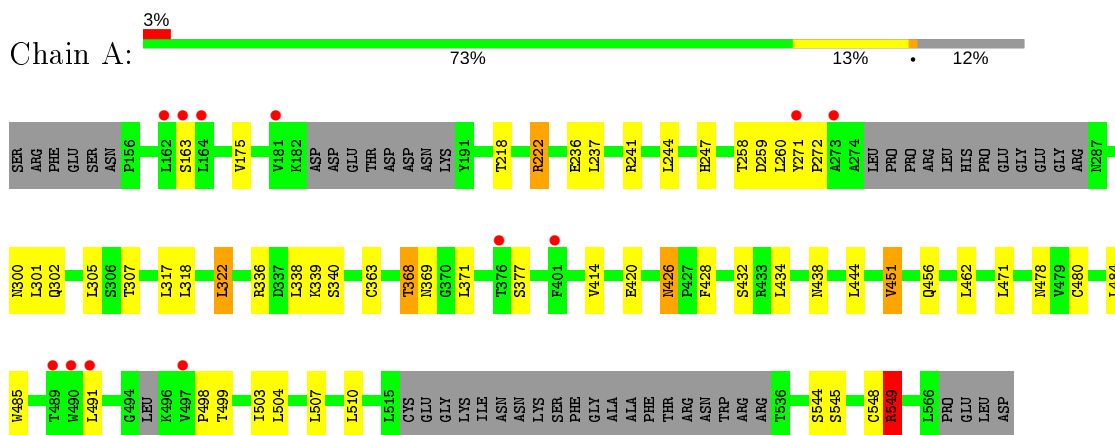
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	6	Total O 6 6	0	0
3	E	1	Total O 1 1	0	0
3	F	5	Total O 5 5	0	0

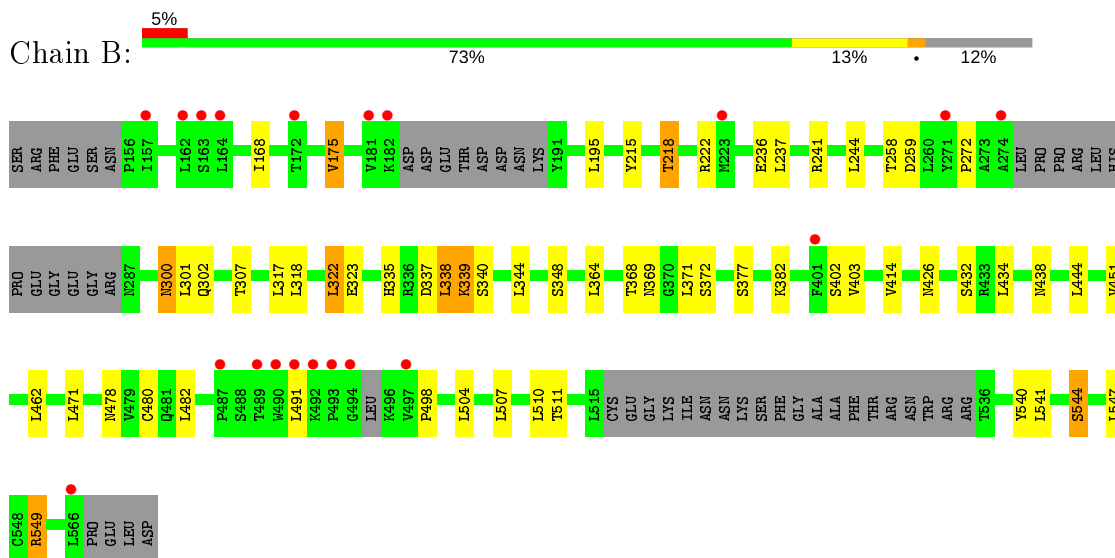
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Serine/threonine-protein kinase PINK1, mitochondrial-like Protein

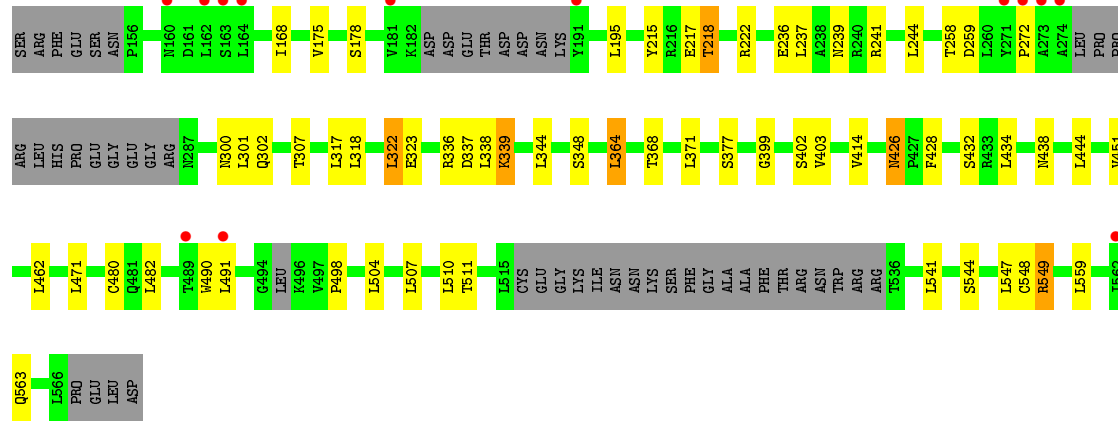
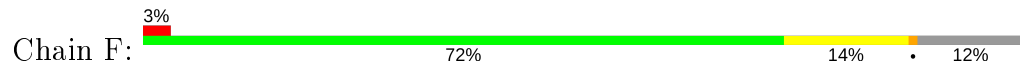


- Molecule 1: Serine/threonine-protein kinase PINK1, mitochondrial-like Protein



- Molecule 1: Serine/threonine-protein kinase PINK1, mitochondrial-like Protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.92Å 116.74Å 179.34Å 90.00° 94.29° 90.00°	Depositor
Resolution (Å)	178.84 – 2.78 47.11 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (178.84-2.78) 99.8 (47.11-2.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.77Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.205 , 0.246 0.206 , 0.245	Depositor DCC
R_{free} test set	4195 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtrriage
Anisotropy	0.192	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16758	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7648e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, SEP

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	0/2842	0.87	3/3876 (0.1%)
1	B	0.72	0/2842	0.89	2/3876 (0.1%)
1	C	0.68	0/2842	0.87	1/3876 (0.0%)
1	D	0.70	0/2842	0.88	5/3876 (0.1%)
1	E	0.66	0/2842	0.83	4/3876 (0.1%)
1	F	0.69	1/2842 (0.0%)	0.89	2/3876 (0.1%)
All	All	0.69	1/17052 (0.0%)	0.87	17/23256 (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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	399	GLY	C-O	-5.09	1.15	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	549	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	D	222	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	438	ASN	CB-CA-C	-6.42	97.56	110.40
1	E	549	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	E	222	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	D	175	VAL	CB-CA-C	-6.17	99.67	111.40
1	E	438	ASN	CB-CA-C	-5.85	98.71	110.40
1	B	438	ASN	CB-CA-C	-5.83	98.74	110.40
1	D	438	ASN	CB-CA-C	-5.77	98.86	110.40
1	F	438	ASN	CB-CA-C	-5.70	99.00	110.40
1	B	175	VAL	CB-CA-C	-5.67	100.64	111.40
1	D	549	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	C	549	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	F	549	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	222	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	E	175	VAL	CB-CA-C	-5.16	101.61	111.40
1	D	222	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	432	SER	Peptide
1	B	432	SER	Peptide
1	C	432	SER	Peptide
1	D	432	SER	Peptide
1	E	432	SER	Peptide
1	F	432	SER	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	2787	0	2740	12	0
1	B	2787	0	2740	12	0
1	C	2787	0	2740	16	0
1	D	2787	0	2741	20	0
1	E	2787	0	2740	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2787	0	2740	12	0
2	A	1	0	0	0	0
2	C	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	0	0	0
3	B	9	0	0	0	0
3	C	3	0	0	0	0
3	D	6	0	0	2	0
3	E	1	0	0	0	0
3	F	5	0	0	0	0
All	All	16758	0	16441	78	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 2.

All (78) 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:A:322:LEU:HD13	1:A:414:VAL:HG11	1.80	0.64
1:B:168:ILE:O	1:C:239:ASN:ND2	2.31	0.64
1:F:322:LEU:HD13	1:F:414:VAL:HG11	1.81	0.63
1:E:322:LEU:HD13	1:E:414:VAL:HG11	1.82	0.61
1:A:260:LEU:C	1:A:271:TYR:N	2.55	0.60
1:B:215:TYR:O	1:B:218:THR:HB	2.01	0.60
1:C:322:LEU:HD13	1:C:414:VAL:HG11	1.84	0.59
1:A:478:ASN:OD1	1:A:549:ARG:NH2	2.35	0.58
1:A:426:ASN:HD22	1:A:428:PHE:H	1.53	0.56
1:C:511:THR:HG22	1:C:547:LEU:HD13	1.88	0.56
1:F:168:ILE:HD11	1:F:178:SER:HB3	1.89	0.55
1:B:511:THR:HG22	1:B:547:LEU:HD13	1.89	0.54
1:D:215:TYR:O	1:D:218:THR:HB	2.08	0.54
1:A:305:LEU:HD13	1:A:420:GLU:O	2.10	0.52
1:C:168:ILE:HD11	1:C:178:SER:HB3	1.91	0.52
1:C:215:TYR:O	1:C:218:THR:HB	2.09	0.52
1:C:300:ASN:C	1:C:300:ASN:HD22	2.13	0.52
1:D:498:PRO:HA	3:D:603:HOH:O	2.09	0.52
1:F:323:GLU:OE2	1:F:549:ARG:HD3	2.10	0.52
1:D:540:TYR:O	1:D:544:SER:OG	2.28	0.51
1:E:323:GLU:OE2	1:E:549:ARG:NH1	2.40	0.51
1:E:511:THR:HG22	1:E:547:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:511:THR:HG22	1:F:547:LEU:HD13	1.92	0.51
1:D:322:LEU:HD13	1:D:414:VAL:HG11	1.92	0.51
1:B:322:LEU:HD13	1:B:414:VAL:HG11	1.94	0.49
1:C:540:TYR:O	1:C:544:SER:OG	2.29	0.49
1:D:168:ILE:O	1:F:239:ASN:ND2	2.46	0.48
1:D:168:ILE:HD11	1:D:178:SER:HB3	1.95	0.48
1:D:478:ASN:OD1	1:D:549:ARG:NH2	2.45	0.48
1:C:337:ASP:OD1	1:C:339:LYS:HE3	2.12	0.48
1:A:499:THR:O	1:A:503:ILE:HG12	2.14	0.47
1:E:323:GLU:OE2	1:E:549:ARG:HD3	2.14	0.47
1:D:207:SEP:O3P	1:E:425:HIS:CE1	2.67	0.47
1:D:319:ALA:HB3	1:D:542:LEU:HD21	1.97	0.47
1:F:426:ASN:HD22	1:F:428:PHE:H	1.63	0.47
1:B:337:ASP:OD1	1:B:339:LYS:HE3	2.15	0.46
1:D:511:THR:HG22	1:D:547:LEU:HD13	1.96	0.46
1:D:472:ASP:HB3	3:D:604:HOH:O	2.14	0.46
1:C:369:ASN:HB3	1:C:372:SER:O	2.15	0.46
1:D:236:GLU:OE1	1:E:303:SER:OG	2.20	0.45
1:F:337:ASP:OD1	1:F:339:LYS:HE3	2.17	0.45
1:C:260:LEU:C	1:C:271:TYR:HA	2.38	0.45
1:D:300:ASN:HD22	1:D:300:ASN:C	2.19	0.45
1:D:169:ALA:HA	1:F:239:ASN:HD21	1.81	0.44
1:D:305:LEU:HD13	1:D:420:GLU:O	2.18	0.44
1:D:335:HIS:CG	1:D:338:LEU:HD13	2.52	0.44
1:B:478:ASN:OD1	1:B:549:ARG:NH2	2.51	0.44
1:E:168:ILE:HD11	1:E:178:SER:HB3	1.99	0.44
1:B:300:ASN:C	1:B:300:ASN:HD22	2.22	0.43
1:C:426:ASN:HD22	1:C:428:PHE:H	1.65	0.43
1:A:451:VAL:HG23	1:A:456:GLN:HG2	2.00	0.43
1:C:323:GLU:OE2	1:C:549:ARG:NH1	2.47	0.43
1:E:478:ASN:OD1	1:E:549:ARG:NH2	2.52	0.43
1:B:369:ASN:HB3	1:B:372:SER:O	2.19	0.43
1:E:215:TYR:O	1:E:218:THR:HB	2.19	0.42
1:E:319:ALA:HB3	1:E:542:LEU:HD21	2.00	0.42
1:E:499:THR:O	1:E:503:ILE:HG12	2.19	0.42
1:A:336:ARG:HH11	1:A:363:CYS:C	2.23	0.42
1:A:247:HIS:HE2	1:A:545:SER:HG	1.65	0.42
1:B:323:GLU:OE2	1:B:549:ARG:NH1	2.42	0.42
1:C:197:MET:HG2	1:C:291:PHE:CD2	2.54	0.42
1:D:207:SEP:O3P	1:E:425:HIS:NE2	2.52	0.42
1:D:426:ASN:HD22	1:D:428:PHE:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:ARG:HD2	1:F:364:LEU:HB2	2.02	0.42
1:C:490:TRP:HB3	1:C:559:LEU:HD21	2.02	0.41
1:D:229:ASP:OD1	1:E:173:ASN:HB2	2.20	0.41
1:F:490:TRP:HB3	1:F:559:LEU:HD21	2.02	0.41
1:F:215:TYR:O	1:F:218:THR:HB	2.21	0.41
1:A:368:THR:HB	1:A:369:ASN:OD1	2.21	0.41
1:C:471:LEU:HD11	1:C:561:TRP:CD1	2.56	0.41
1:A:484:LEU:HB3	1:A:485:TRP:CD2	2.56	0.41
1:C:197:MET:HG2	1:C:291:PHE:CE2	2.57	0.40
1:F:490:TRP:O	1:F:563:GLN:NE2	2.54	0.40
1:D:337:ASP:OD1	1:D:339:LYS:HE3	2.21	0.40
1:A:484:LEU:HB3	1:A:485:TRP:CE2	2.57	0.40
1:B:323:GLU:OE2	1:B:549:ARG:HD3	2.22	0.40
1:B:335:HIS:CG	1:B:338:LEU:HD13	2.56	0.40
1:B:540:TYR:O	1:B:544:SER:OG	2.39	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	347/411 (84%)	325 (94%)	20 (6%)	2 (1%)	25	54
1	B	347/411 (84%)	326 (94%)	18 (5%)	3 (1%)	17	44
1	C	347/411 (84%)	328 (94%)	15 (4%)	4 (1%)	13	36
1	D	347/411 (84%)	323 (93%)	20 (6%)	4 (1%)	13	36
1	E	347/411 (84%)	327 (94%)	17 (5%)	3 (1%)	17	44
1	F	347/411 (84%)	325 (94%)	19 (6%)	3 (1%)	17	44
All	All	2082/2466 (84%)	1954 (94%)	109 (5%)	19 (1%)	17	44

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	PRO
1	B	272	PRO
1	E	272	PRO
1	F	272	PRO
1	B	402	SER
1	C	402	SER
1	D	272	PRO
1	F	402	SER
1	A	498	PRO
1	C	498	PRO
1	D	498	PRO
1	E	498	PRO
1	D	385	ASN
1	D	402	SER
1	E	402	SER
1	F	498	PRO
1	B	498	PRO
1	C	272	PRO
1	C	452	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	300/360 (83%)	263 (88%)	37 (12%)	4	13
1	B	300/360 (83%)	257 (86%)	43 (14%)	3	9
1	C	300/360 (83%)	258 (86%)	42 (14%)	3	9
1	D	300/360 (83%)	259 (86%)	41 (14%)	3	10
1	E	300/360 (83%)	260 (87%)	40 (13%)	4	11
1	F	300/360 (83%)	258 (86%)	42 (14%)	3	9
All	All	1800/2160 (83%)	1555 (86%)	245 (14%)	3	10

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	SER
1	A	175	VAL
1	A	218	THR
1	A	222	ARG
1	A	236	GLU
1	A	237	LEU
1	A	241	ARG
1	A	244	LEU
1	A	258	THR
1	A	259	ASP
1	A	300	ASN
1	A	301	LEU
1	A	302	GLN
1	A	307	THR
1	A	317	LEU
1	A	318	LEU
1	A	322	LEU
1	A	338	LEU
1	A	339	LYS
1	A	340	SER
1	A	368	THR
1	A	371	LEU
1	A	377	SER
1	A	426	ASN
1	A	434	LEU
1	A	444	LEU
1	A	451	VAL
1	A	462	LEU
1	A	471	LEU
1	A	480	CYS
1	A	491	LEU
1	A	504	LEU
1	A	507	LEU
1	A	510	LEU
1	A	544	SER
1	A	548	CYS
1	A	549	ARG
1	B	175	VAL
1	B	195	LEU
1	B	218	THR
1	B	222	ARG
1	B	236	GLU
1	B	237	LEU

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Mol	Chain	Res	Type
1	B	241	ARG
1	B	244	LEU
1	B	258	THR
1	B	259	ASP
1	B	300	ASN
1	B	301	LEU
1	B	302	GLN
1	B	307	THR
1	B	317	LEU
1	B	318	LEU
1	B	322	LEU
1	B	338	LEU
1	B	339	LYS
1	B	340	SER
1	B	344	LEU
1	B	348	SER
1	B	364	LEU
1	B	368	THR
1	B	371	LEU
1	B	377	SER
1	B	382	LYS
1	B	403	VAL
1	B	426	ASN
1	B	434	LEU
1	B	444	LEU
1	B	451	VAL
1	B	462	LEU
1	B	471	LEU
1	B	480	CYS
1	B	482	LEU
1	B	491	LEU
1	B	504	LEU
1	B	507	LEU
1	B	510	LEU
1	B	541	LEU
1	B	544	SER
1	B	549	ARG
1	C	175	VAL
1	C	195	LEU
1	C	217	GLU
1	C	218	THR
1	C	222	ARG

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Mol	Chain	Res	Type
1	C	236	GLU
1	C	237	LEU
1	C	241	ARG
1	C	244	LEU
1	C	258	THR
1	C	259	ASP
1	C	300	ASN
1	C	301	LEU
1	C	302	GLN
1	C	307	THR
1	C	317	LEU
1	C	318	LEU
1	C	322	LEU
1	C	338	LEU
1	C	339	LYS
1	C	340	SER
1	C	344	LEU
1	C	348	SER
1	C	364	LEU
1	C	368	THR
1	C	371	LEU
1	C	377	SER
1	C	382	LYS
1	C	403	VAL
1	C	426	ASN
1	C	444	LEU
1	C	451	VAL
1	C	462	LEU
1	C	471	LEU
1	C	480	CYS
1	C	482	LEU
1	C	491	LEU
1	C	504	LEU
1	C	507	LEU
1	C	510	LEU
1	C	541	LEU
1	C	544	SER
1	D	217	GLU
1	D	218	THR
1	D	222	ARG
1	D	236	GLU
1	D	237	LEU

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Mol	Chain	Res	Type
1	D	241	ARG
1	D	244	LEU
1	D	258	THR
1	D	259	ASP
1	D	300	ASN
1	D	301	LEU
1	D	302	GLN
1	D	307	THR
1	D	317	LEU
1	D	318	LEU
1	D	322	LEU
1	D	338	LEU
1	D	339	LYS
1	D	340	SER
1	D	344	LEU
1	D	348	SER
1	D	364	LEU
1	D	368	THR
1	D	371	LEU
1	D	377	SER
1	D	403	VAL
1	D	426	ASN
1	D	434	LEU
1	D	444	LEU
1	D	451	VAL
1	D	462	LEU
1	D	471	LEU
1	D	480	CYS
1	D	482	LEU
1	D	491	LEU
1	D	504	LEU
1	D	507	LEU
1	D	510	LEU
1	D	541	LEU
1	D	544	SER
1	D	549	ARG
1	E	195	LEU
1	E	218	THR
1	E	222	ARG
1	E	236	GLU
1	E	237	LEU
1	E	241	ARG

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Mol	Chain	Res	Type
1	E	244	LEU
1	E	258	THR
1	E	300	ASN
1	E	301	LEU
1	E	302	GLN
1	E	307	THR
1	E	317	LEU
1	E	318	LEU
1	E	322	LEU
1	E	338	LEU
1	E	339	LYS
1	E	340	SER
1	E	344	LEU
1	E	348	SER
1	E	364	LEU
1	E	368	THR
1	E	371	LEU
1	E	377	SER
1	E	382	LYS
1	E	403	VAL
1	E	426	ASN
1	E	434	LEU
1	E	444	LEU
1	E	451	VAL
1	E	462	LEU
1	E	471	LEU
1	E	480	CYS
1	E	482	LEU
1	E	491	LEU
1	E	504	LEU
1	E	507	LEU
1	E	510	LEU
1	E	541	LEU
1	E	544	SER
1	F	175	VAL
1	F	195	LEU
1	F	217	GLU
1	F	218	THR
1	F	222	ARG
1	F	236	GLU
1	F	237	LEU
1	F	241	ARG

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Mol	Chain	Res	Type
1	F	244	LEU
1	F	258	THR
1	F	259	ASP
1	F	300	ASN
1	F	301	LEU
1	F	302	GLN
1	F	307	THR
1	F	317	LEU
1	F	318	LEU
1	F	322	LEU
1	F	338	LEU
1	F	339	LYS
1	F	344	LEU
1	F	348	SER
1	F	364	LEU
1	F	368	THR
1	F	371	LEU
1	F	377	SER
1	F	403	VAL
1	F	426	ASN
1	F	434	LEU
1	F	444	LEU
1	F	451	VAL
1	F	462	LEU
1	F	471	LEU
1	F	480	CYS
1	F	482	LEU
1	F	491	LEU
1	F	504	LEU
1	F	507	LEU
1	F	510	LEU
1	F	541	LEU
1	F	544	SER
1	F	548	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	249	ASN
1	A	300	ASN
1	A	302	GLN

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Mol	Chain	Res	Type
1	A	327	HIS
1	A	426	ASN
1	A	565	ASN
1	B	227	ASN
1	B	232	ASN
1	B	243	HIS
1	B	249	ASN
1	B	300	ASN
1	B	302	GLN
1	B	327	HIS
1	B	426	ASN
1	B	565	ASN
1	C	232	ASN
1	C	239	ASN
1	C	243	HIS
1	C	249	ASN
1	C	300	ASN
1	C	302	GLN
1	C	327	HIS
1	C	426	ASN
1	C	565	ASN
1	D	227	ASN
1	D	232	ASN
1	D	249	ASN
1	D	300	ASN
1	D	302	GLN
1	D	327	HIS
1	D	426	ASN
1	E	232	ASN
1	E	243	HIS
1	E	249	ASN
1	E	300	ASN
1	E	327	HIS
1	E	426	ASN
1	E	565	ASN
1	F	232	ASN
1	F	239	ASN
1	F	243	HIS
1	F	249	ASN
1	F	300	ASN
1	F	302	GLN
1	F	327	HIS

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Mol	Chain	Res	Type
1	F	426	ASN
1	F	563	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	F	207	1	8,9,10	0.76	0	8,12,14	2.40	1 (12%)
1	SEP	D	207	1	8,9,10	0.86	0	8,12,14	2.26	1 (12%)
1	SEP	E	207	1	8,9,10	0.70	0	8,12,14	2.30	3 (37%)
1	SEP	B	207	1	8,9,10	0.82	0	8,12,14	2.52	3 (37%)
1	SEP	C	207	1	8,9,10	0.81	0	8,12,14	2.56	1 (12%)
1	SEP	A	207	1	8,9,10	0.73	0	8,12,14	2.66	1 (12%)

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
1	SEP	F	207	1	-	2/5/8/10	-
1	SEP	D	207	1	-	1/5/8/10	-
1	SEP	E	207	1	-	3/5/8/10	-
1	SEP	B	207	1	-	4/5/8/10	-
1	SEP	C	207	1	-	2/5/8/10	-
1	SEP	A	207	1	-	1/5/8/10	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	207	SEP	OG-CB-CA	6.83	114.79	108.14
1	C	207	SEP	OG-CB-CA	6.70	114.66	108.14
1	F	207	SEP	OG-CB-CA	6.05	114.04	108.14
1	B	207	SEP	OG-CB-CA	5.98	113.96	108.14
1	D	207	SEP	OG-CB-CA	5.52	113.52	108.14
1	E	207	SEP	OG-CB-CA	5.08	113.09	108.14
1	E	207	SEP	O2P-P-OG	-2.35	100.47	106.73
1	E	207	SEP	O3P-P-O2P	2.30	116.42	107.64
1	B	207	SEP	OG-P-O1P	-2.25	100.16	106.47
1	B	207	SEP	O2P-P-O1P	2.21	119.33	110.68

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	207	SEP	N-CA-CB-OG
1	D	207	SEP	N-CA-CB-OG
1	E	207	SEP	N-CA-CB-OG
1	B	207	SEP	N-CA-CB-OG
1	B	207	SEP	CB-OG-P-O1P
1	B	207	SEP	CB-OG-P-O2P
1	C	207	SEP	N-CA-CB-OG
1	A	207	SEP	N-CA-CB-OG
1	E	207	SEP	CB-OG-P-O1P
1	F	207	SEP	CB-OG-P-O2P
1	E	207	SEP	CB-OG-P-O2P
1	B	207	SEP	CB-OG-P-O3P
1	C	207	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	207	SEP	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	E	1
1	B	1
1	C	1
1	A	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	260:LEU	C	271:TYR	N	3.02
1	C	260:LEU	C	271:TYR	N	3.00
1	E	260:LEU	C	271:TYR	N	2.93
1	F	260:LEU	C	271:TYR	N	2.86
1	D	260:LEU	C	271:TYR	N	2.82
1	A	260:LEU	C	271:TYR	N	2.55

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	359/411 (87%)	-0.00	12 (3%) 46 41	44, 76, 124, 157	0
1	B	359/411 (87%)	0.10	20 (5%) 24 19	43, 72, 119, 174	0
1	C	359/411 (87%)	0.11	17 (4%) 31 25	47, 81, 133, 189	0
1	D	359/411 (87%)	0.13	19 (5%) 26 21	42, 74, 124, 178	0
1	E	359/411 (87%)	0.05	11 (3%) 49 44	45, 80, 136, 166	0
1	F	359/411 (87%)	0.03	13 (3%) 42 37	44, 75, 123, 194	0
All	All	2154/2466 (87%)	0.07	92 (4%) 35 30	42, 76, 128, 194	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	274	ALA	7.8
1	B	497	VAL	7.1
1	D	401	PHE	5.6
1	E	497	VAL	5.4
1	C	273	ALA	5.3
1	F	274	ALA	5.2
1	C	181	VAL	4.6
1	A	497	VAL	4.5
1	B	157	ILE	4.5
1	B	401	PHE	4.4
1	D	491	LEU	4.4
1	C	271	TYR	4.2
1	F	272	PRO	4.2
1	D	489	THR	4.1
1	B	491	LEU	4.0
1	E	401	PHE	3.9
1	B	493	PRO	3.8
1	C	182	LYS	3.7
1	B	490	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	160	ASN	3.6
1	D	378	TYR	3.5
1	C	162	LEU	3.4
1	C	483	PHE	3.4
1	F	181	VAL	3.3
1	D	497	VAL	3.3
1	E	491	LEU	3.3
1	F	164	LEU	3.3
1	A	401	PHE	3.2
1	C	489	THR	3.1
1	D	157	ILE	3.1
1	C	566	LEU	3.1
1	F	160	ASN	3.1
1	D	163	SER	3.1
1	A	490	TRP	3.1
1	A	376	THR	3.0
1	D	490	TRP	3.0
1	D	162	LEU	3.0
1	E	494	GLY	3.0
1	A	491	LEU	3.0
1	F	491	LEU	2.9
1	B	163	SER	2.9
1	F	562	ILE	2.9
1	C	562	ILE	2.9
1	D	181	VAL	2.9
1	F	271	TYR	2.9
1	B	182	LYS	2.8
1	A	489	THR	2.8
1	F	162	LEU	2.8
1	C	272	PRO	2.8
1	A	164	LEU	2.7
1	E	191	TYR	2.7
1	B	181	VAL	2.7
1	D	271	TYR	2.6
1	C	164	LEU	2.6
1	D	493	PRO	2.6
1	D	164	LEU	2.6
1	B	489	THR	2.5
1	A	162	LEU	2.5
1	C	490	TRP	2.5
1	D	274	ALA	2.5
1	B	223	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	172	THR	2.4
1	B	271	TYR	2.4
1	B	162	LEU	2.4
1	A	181	VAL	2.4
1	A	271	TYR	2.4
1	E	181	VAL	2.3
1	F	163	SER	2.3
1	D	380	MET	2.3
1	C	351	GLU	2.3
1	B	494	GLY	2.3
1	B	172	THR	2.3
1	F	273	ALA	2.3
1	B	164	LEU	2.3
1	F	489	THR	2.3
1	A	163	SER	2.2
1	B	274	ALA	2.2
1	B	492	LYS	2.2
1	C	491	LEU	2.2
1	D	562	ILE	2.2
1	C	563	GLN	2.2
1	B	487	PRO	2.2
1	E	376	THR	2.2
1	E	163	SER	2.2
1	A	273	ALA	2.2
1	B	566	LEU	2.2
1	F	191	TYR	2.1
1	D	566	LEU	2.1
1	E	274	ALA	2.1
1	E	490	TRP	2.1
1	D	381	ASP	2.1
1	E	225	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	F	207	10/11	0.92	0.14	71,90,141,160	0
1	SEP	C	207	10/11	0.93	0.15	69,88,143,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	B	207	10/11	0.94	0.14	57,78,116,121	0
1	SEP	D	207	10/11	0.95	0.14	64,80,123,130	0
1	SEP	A	207	10/11	0.95	0.16	63,86,131,135	0
1	SEP	E	207	10/11	0.96	0.12	72,88,120,121	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	MG	C	602	1/1	0.79	0.91	92,92,92,92	0
2	MG	A	601	1/1	0.80	0.70	73,73,73,73	0
2	MG	E	602	1/1	0.83	0.99	98,98,98,98	0
2	MG	E	601	1/1	0.90	0.58	81,81,81,81	0
2	MG	F	601	1/1	0.95	0.29	74,74,74,74	0
2	MG	C	601	1/1	0.96	0.46	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.