WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2017 – 03:21 PM EDT

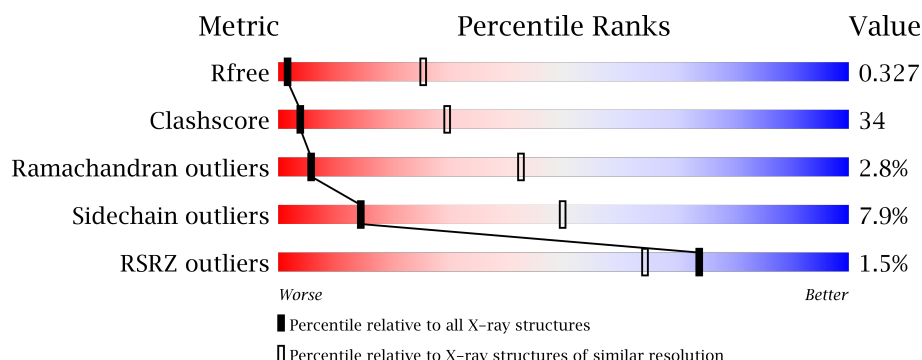|		
PDB ID	:	5DO7
Title	:	Crystal Structure of the Human Sterol Transporter ABCG5/ABCG8
Authors	:	Lee, J.-Y.; Kinch, L.N.; Borek, D.M.; Urbatsch, I.L.; Xie, X.-S.; Grishin, N.V.; Cohen, J.C.; Otwinowski, Z.; Hobbs, H.H.; Rosenbaum, D.M.
Deposited on	:	unknown
Resolution	:	3.93 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.93 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	Percentile Ranks	Value
Rfree		0.327
Clashscore		34
Ramachandran outliers		2.8%
Sidechain outliers		7.9%
RSRZ outliers		1.5%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1021 (4.28-3.60)
Clashscore	112137	1117 (4.28-3.60)
Ramachandran outliers	110173	1076 (4.28-3.60)
Sidechain outliers	110143	1067 (4.28-3.60)
RSRZ outliers	101464	1034 (4.28-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	666	.% 39% 44% 5% · 12%
1	C	666	.% 42% 41% · 13%
2	B	685	2% 40% 36% 5% · 18%
2	D	685	.% 38% 39% 6% · 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18150 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 ATP-binding cassette sub-family G member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total 4606	C 2982	N 780	O 816	S 28	0	0	0
1	C	579	Total 4551	C 2945	N 770	O 807	S 29	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	GLY	engineered mutation	UNP Q9H222
A	652	GLY	-	expression tag	UNP Q9H222
A	653	SER	-	expression tag	UNP Q9H222
A	654	HIS	-	expression tag	UNP Q9H222
A	655	HIS	-	expression tag	UNP Q9H222
A	656	HIS	-	expression tag	UNP Q9H222
A	657	HIS	-	expression tag	UNP Q9H222
A	658	HIS	-	expression tag	UNP Q9H222
A	659	HIS	-	expression tag	UNP Q9H222
A	660	GLY	-	expression tag	UNP Q9H222
A	661	HIS	-	expression tag	UNP Q9H222
A	662	HIS	-	expression tag	UNP Q9H222
A	663	HIS	-	expression tag	UNP Q9H222
A	664	HIS	-	expression tag	UNP Q9H222
A	665	HIS	-	expression tag	UNP Q9H222
A	666	HIS	-	expression tag	UNP Q9H222
C	2	GLU	GLY	engineered mutation	UNP Q9H222
C	652	GLY	-	expression tag	UNP Q9H222
C	653	SER	-	expression tag	UNP Q9H222
C	654	HIS	-	expression tag	UNP Q9H222
C	655	HIS	-	expression tag	UNP Q9H222
C	656	HIS	-	expression tag	UNP Q9H222
C	657	HIS	-	expression tag	UNP Q9H222
C	658	HIS	-	expression tag	UNP Q9H222
C	659	HIS	-	expression tag	UNP Q9H222

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Chain	Residue	Modelled	Actual	Comment	Reference
C	660	GLY	-	expression tag	UNP Q9H222
C	661	HIS	-	expression tag	UNP Q9H222
C	662	HIS	-	expression tag	UNP Q9H222
C	663	HIS	-	expression tag	UNP Q9H222
C	664	HIS	-	expression tag	UNP Q9H222
C	665	HIS	-	expression tag	UNP Q9H222
C	666	HIS	-	expression tag	UNP Q9H222

- Molecule 2 is a protein called ATP-binding cassette sub-family G member 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	562	Total 4464	C 2905	N 756	O 775	S 28	0	0	0
2	D	571	Total 4529	C 2936	N 775	O 789	S 29	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP Q9H221
B	0	GLY	-	expression tag	UNP Q9H221
B	1	SER	-	expression tag	UNP Q9H221
B	674	ALA	-	expression tag	UNP Q9H221
B	675	SER	-	expression tag	UNP Q9H221
B	676	ASN	-	expression tag	UNP Q9H221
B	677	SER	-	expression tag	UNP Q9H221
B	678	LEU	-	expression tag	UNP Q9H221
B	679	GLU	-	expression tag	UNP Q9H221
B	680	VAL	-	expression tag	UNP Q9H221
B	681	LEU	-	expression tag	UNP Q9H221
B	682	PHE	-	expression tag	UNP Q9H221
B	683	GLN	-	expression tag	UNP Q9H221
D	-1	MET	-	initiating methionine	UNP Q9H221
D	0	GLY	-	expression tag	UNP Q9H221
D	1	SER	-	expression tag	UNP Q9H221
D	674	ALA	-	expression tag	UNP Q9H221
D	675	SER	-	expression tag	UNP Q9H221
D	676	ASN	-	expression tag	UNP Q9H221
D	677	SER	-	expression tag	UNP Q9H221
D	678	LEU	-	expression tag	UNP Q9H221
D	679	GLU	-	expression tag	UNP Q9H221
D	680	VAL	-	expression tag	UNP Q9H221

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Chain	Residue	Modelled	Actual	Comment	Reference
D	681	LEU	-	expression tag	UNP Q9H221
D	682	PHE	-	expression tag	UNP Q9H221
D	683	GLN	-	expression tag	UNP Q9H221

3 Residue-property plots ⓘ

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: ATP-binding cassette sub-family G member 5

• Molecule 1: ATP-binding cassette sub-family G member 5

• Molecule 2: ATP-binding cassette sub-family G member 8

Chain B:

A559 S560 F561 F562 L566 Y567 N568 S569 F570 Y571 L572 A573 G574 G575 F576 M577 I578 N579 L580 S581 S582 L583 W584 T585 V586 P587 A588 I590 S591 K592 V593 L596 R597 W598 C599 F600 E601 G602 L603 M604 Q607 F608 R610 R611 T612 Y613 K614 M615 P616 L617 G618 N619 L620 T621 I622

A623 V624 S625 G626 D627 K628 I629 L630 S631 V632 M633 E634 L635 D636 L640 I643 Y644 L645 I646 V647 I648 S651 G652 L657 Y658 V659 V660 S661 L662 R663 Q667 K668 Q671 D672 W673 ALA SER ASN SER LEU GLU VAL LEU PHE GLN

• Molecule 2: ATP-binding cassette sub-family G member 8

Chain D:

	.%			
	38%	39%	6% •	17%

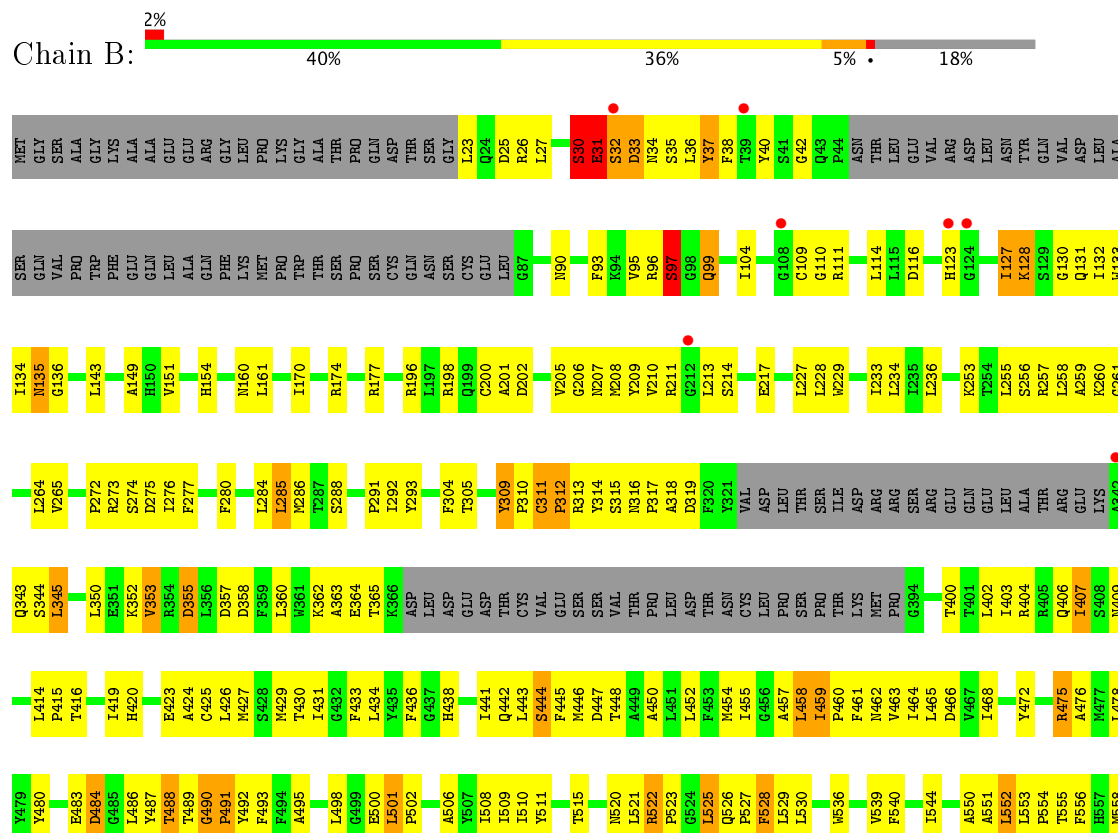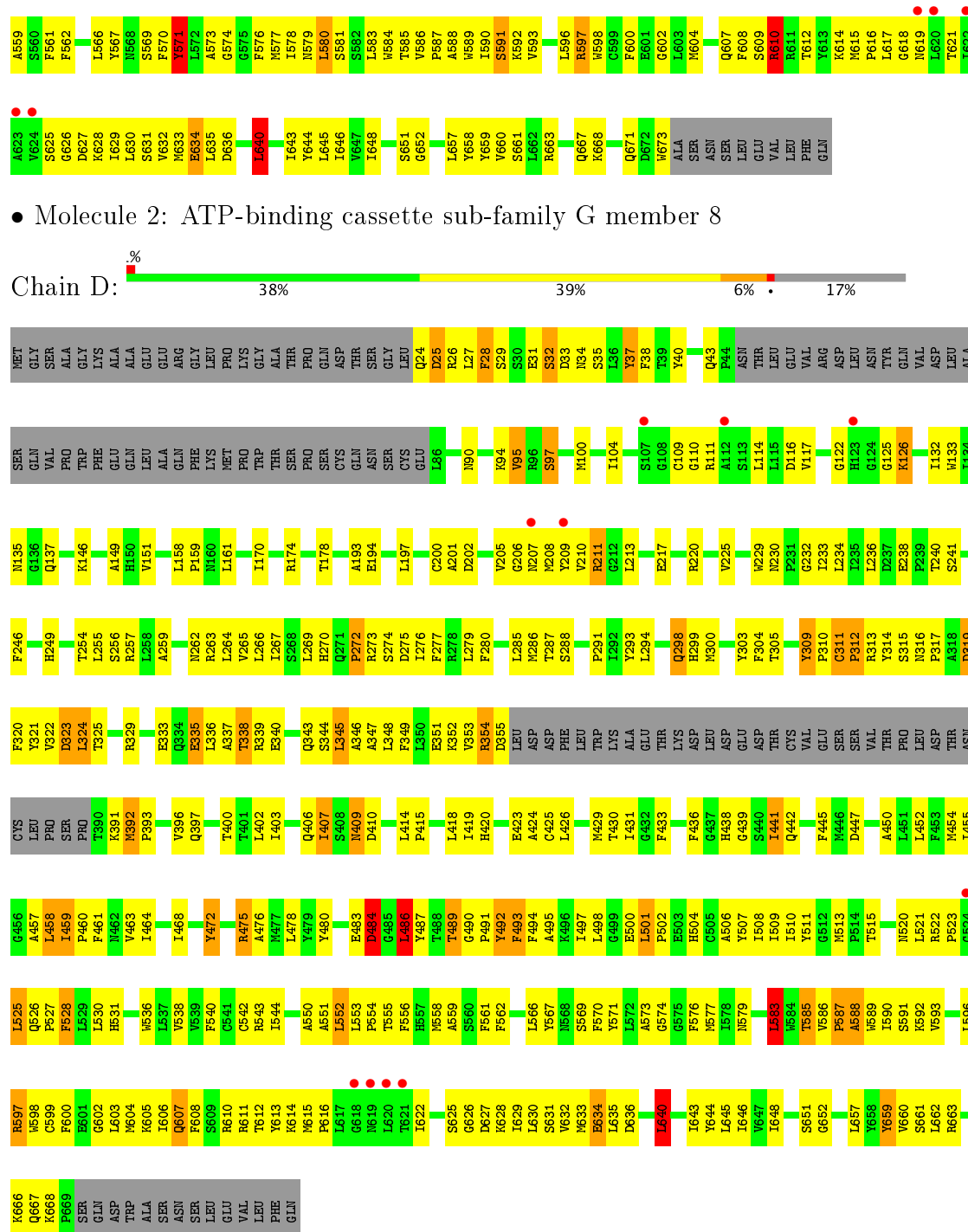MET GLY SER ALA GLY LYS ALA ALA GLU GLU ARG GLY LEU PRO LYS ALA THR PRO GLN ASP SER THR SER GLY LEU Q24 D25 R26 L27 F28 S29 S30 E31 S32 D33 N34 S35 L36 Y37 F38 T39 Y40 Q43 P44 ASN THR LEU GLU VAL ARG ASP LEU ASN TYR GLN VAL ASP LEU ALA

SER GLN VAL PRO TRP PHE GLU GLN LEU ALA GLN PHE LYS MET PRO TRP THR SER PRO SER CYS GLN ASN SER CYS GLU L86 N90 K94 V95 R96 S97 M100 I104 S107 G108 C109 G110 R111 A112 S113 L114 L115 D116 V117 G122 H123 G124 G125 K126 I132 W133 I134

N135 G136 Q137 K146 A149 H150 V151 L158 P159 N160 L161 I170 R174 T178 A193 E194 L197 C200 A201 D202 V205 G206 N207 M208 V209 Y210 R211 G212 L213 E217 R220 V225 W229 M230 P231 G232 I233 L234 I235 L236 D237 E238 P239 T240 S241

F246 H249 T254 L255 S256 R257 L258 A259 N262 R263 L264 V265 L266 I267 S268 L269 H270 Q271 P272 R273 S274 D275 I276 F277 R278 L279 F280 L285 M286 T287 S288 P291 I292 Y293 L294 Q298 H299 M300 Y303 F304 T305 Y309 P310 C311 P312 R313 Y314 S315 N316 P317 A318 D319

F320 Y321 V322 D323 L324 T325 R329 E333 Q334 E335 L336 A337 T338 R339 E340 Q343 S344 L345 A346 A347 L348 F349 L350 K352 V353 R354 D355 LEU ASP ASP PHE LEU TRP LYS ALA GLU THR LYS ASP LEU ASP GLU ASP CYS VAL GLU SER SER VAL THR PRO LEU ASP THR ASN

CYS LEU PRO SER PRO T390 K391 M392 P393 V396 Q397 T400 T401 L402 I403 Q406 I407 S408 N409 D410 L414 P415 L418 I419 H420 E423 A424 C425 L426 M429 T430 I431 G432 F433 F436 G437 H438 G439 S440 I441 Q442 F445 M446 D447 A450 L451 L452 F453 M454 I455

G456 A457 L458 I459 P460 F461 N462 V463 I464 I468 Y472 Y479 R475 A476 M477 L478 Y479 Y480 E483 D484 G485 L486 Y487 T488 T489 G490 P491 Y492 F493 F494 A495 K496 L497 L498 G499 E500 L501 P502 E503 H504 C505 A506 Y507 I508 I509 I510 S511 G512 M513 P514 T515 N520 L521 R522 P523 G524

L525 Q526 P527 F528 L529 L530 H531 W536 L537 V538 V539 F540 C541 C542 R543 I544 A550 A551 L552 L553 P554 T555 F556 H557 M558 A559 S560 F561 F562 L566 Y567 N568 S569 F570 L571 L572 A573 G574 F576 M577 I578 N579 I583 W584 T585 V586 P587 A588 W589 I590 S591 K592 V593 L596

R597 W598 C599 F600 E601 G602 L603 M604 K605 I606 Q607 F608 R610 R611 T612 Y613 K614 M615 P616 L617 G618 N619 L620 T621 I622 S625 G626 D627 K628 I629 L630 S631 V632 M633 E634 L635 D636 L640 I643 Y644 L645 I646 V647 I648 S651 G652 L657 Y658 Y659 V660 S661 L662 R663

K666 Q667 K668 P669 SER GLN ASP TRP ALA SER ASN SER LEU GLU VAL LEU PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	173.55Å 224.80Å 253.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.93	Depositor
	24.96 – 3.94	EDS
% Data completeness	82.5 (25.00-3.93)	Depositor
(in resolution range)	83.5 (24.96-3.94)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.97Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.245 , 0.329	Depositor
	0.250 , 0.327	DCC
R_{free} test set	1845 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.0	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	18150	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.54	0/4697	0.82	4/6355 (0.1%)
1	C	0.52	0/4639	0.79	2/6272 (0.0%)
2	B	0.54	0/4572	0.84	4/6192 (0.1%)
2	D	0.55	0/4634	0.84	2/6273 (0.0%)
All	All	0.54	0/18542	0.82	12/25092 (0.0%)

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	8
1	C	0	3
2	B	0	3
2	D	0	6
All	All	0	20

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	37	TYR	CA-CB-CG	8.16	128.91	113.40
2	B	571	TYR	CA-CB-CG	7.90	128.41	113.40
1	A	81	ILE	CB-CA-C	-6.54	98.52	111.60
2	D	486	LEU	CA-CB-CG	5.79	128.61	115.30
1	A	190	LEU	CA-CB-CG	5.56	128.09	115.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLY	Peptide
1	A	186	GLY	Peptide
1	A	192	GLY	Peptide
1	A	308	ASP	Peptide
1	A	34	GLU	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	4606	0	4747	323	0
1	C	4551	0	4682	287	0
2	B	4464	0	4528	321	1
2	D	4529	0	4615	327	1
All	All	18150	0	18572	1233	1

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 34.

The worst 5 of 1233 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:75:TYR:CZ	1:C:77:GLU:OE2	1.85	1.30
1:A:81:ILE:CD1	1:A:260:PHE:HA	1.60	1.29
2:B:36:LEU:CB	2:B:95:VAL:HG21	1.63	1.26
1:A:81:ILE:HD11	1:A:261:ASP:N	1.53	1.20
1:C:140:SER:HA	1:C:185:ILE:HD11	1.17	1.12

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:ASP:OD1	2:D:339:ARG:NH2[6_454]	2.09	0.11

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	579/666 (87%)	468 (81%)	101 (17%)	10 (2%)	11	52
1	C	571/666 (86%)	465 (81%)	92 (16%)	14 (2%)	6	44
2	B	554/685 (81%)	445 (80%)	91 (16%)	18 (3%)	5	39
2	D	565/685 (82%)	443 (78%)	101 (18%)	21 (4%)	4	36
All	All	2269/2702 (84%)	1821 (80%)	385 (17%)	63 (3%)	6	42

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	557	ILE
2	B	127	ILE
2	B	135	ASN
2	B	484	ASP
2	B	491	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	512/582 (88%)	474 (93%)	38 (7%)	16	52
1	C	505/582 (87%)	467 (92%)	38 (8%)	16	52
2	B	481/591 (81%)	441 (92%)	40 (8%)	13	47
2	D	490/591 (83%)	449 (92%)	41 (8%)	13	47
All	All	1988/2346 (85%)	1831 (92%)	157 (8%)	14	50

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	579	ASN
2	D	202	ASP
1	C	444	VAL
2	B	597	ARG
2	D	28	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	667	GLN
2	D	420	HIS
1	C	470	HIS
2	B	438	HIS
1	C	528	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	585/666 (87%)	-0.53	6 (1%)	82	74	20, 64, 145, 252	0
1	C	579/666 (86%)	-0.48	6 (1%)	82	74	20, 65, 143, 220	0
2	B	562/685 (82%)	-0.39	12 (2%)	64	54	20, 77, 157, 247	0
2	D	571/685 (83%)	-0.52	10 (1%)	69	59	20, 49, 139, 234	0
All	All	2297/2702 (85%)	-0.48	34 (1%)	74	64	20, 63, 147, 252	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	621	THR	4.8
2	D	620	LEU	4.4
2	D	619	ASN	4.3
1	A	587	CYS	3.9
1	C	589	SER	3.7

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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.