



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:14 PM GMT

PDB ID : 4PLE
Title : Human Nuclear Receptor Liver Receptor Homologue-1, LRH-1, Bound to an E. Coli Phospholipid and a Fragment of TIF-2
Authors : Ortlund, E.A.; Musille, P.M.
Deposited on : 2014-05-16
Resolution : 1.75 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

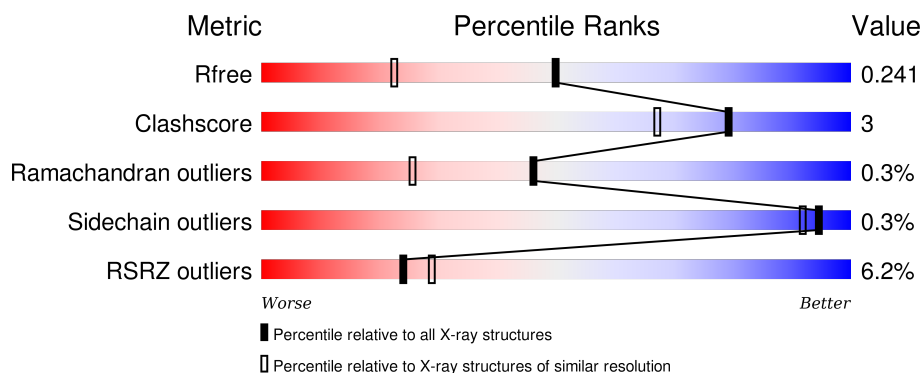
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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. 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	245	<div> <div>9%</div> <div>89%</div> <div>9%</div> </div>
1	C	245	<div> <div>4%</div> <div>89%</div> <div>9%</div> </div>
1	E	245	<div> <div>6%</div> <div>87%</div> <div>10%</div> </div>
1	G	245	<div> <div>4%</div> <div>91%</div> <div>7%</div> </div>
2	B	14	<div> <div>57%</div> <div>7%</div> <div>36%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	14	
2	F	14	
2	H	14	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9019 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 Nuclear receptor subfamily 5 group A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1953	1252	327	361	13			
1	C	239	Total	C	N	O	S	0	1	0
			1945	1249	324	358	14			
1	E	241	Total	C	N	O	S	0	1	0
			1958	1256	327	361	14			
1	G	241	Total	C	N	O	S	0	1	0
			1958	1256	327	361	14			

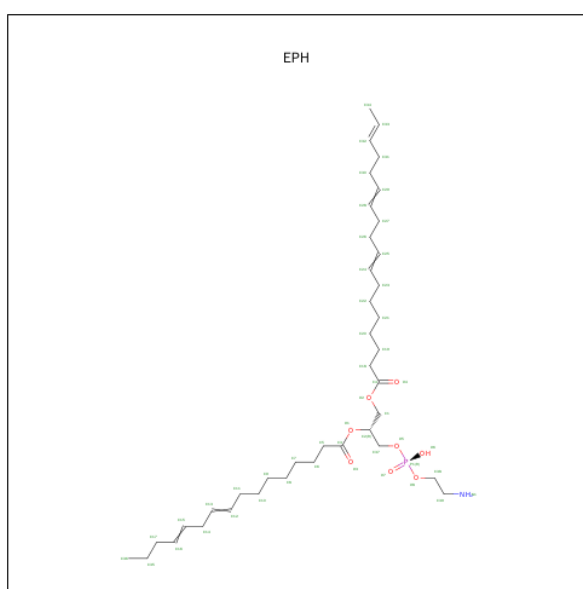
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	ALA	-	expression tag	UNP O00482
A	298	ALA	-	expression tag	UNP O00482
A	299	ALA	-	expression tag	UNP O00482
A	300	SER	-	expression tag	UNP O00482
C	297	ALA	-	expression tag	UNP O00482
C	298	ALA	-	expression tag	UNP O00482
C	299	ALA	-	expression tag	UNP O00482
C	300	SER	-	expression tag	UNP O00482
E	297	ALA	-	expression tag	UNP O00482
E	298	ALA	-	expression tag	UNP O00482
E	299	ALA	-	expression tag	UNP O00482
E	300	SER	-	expression tag	UNP O00482
G	297	ALA	-	expression tag	UNP O00482
G	298	ALA	-	expression tag	UNP O00482
G	299	ALA	-	expression tag	UNP O00482
G	300	SER	-	expression tag	UNP O00482

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

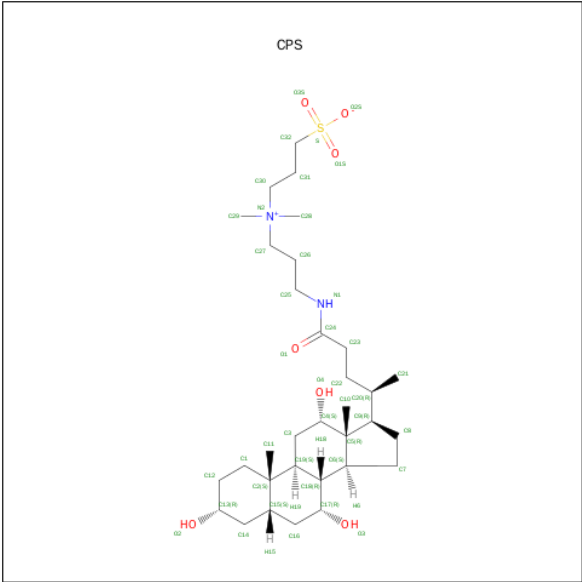
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			76	50	13	13			
2	D	10	Total	C	N	O	0	0	0
			85	56	15	14			
2	F	10	Total	C	N	O	0	0	0
			85	56	15	14			
2	H	10	Total	C	N	O	0	0	0
			85	56	15	14			

- Molecule 3 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			47	38	8	1		
3	C	1	Total	C	O	P	0	0
			47	38	8	1		
3	E	1	Total	C	O	P	0	0
			47	38	8	1		
3	G	1	Total	C	O	P	0	0
			47	38	8	1		

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	0	0	
			24	21	3			
4	A	1	Total	C	O	0	0	
			22	19	3			
4	A	1	Total	C	N	O	0	0
			29	24	1	4		
4	C	1	Total	C	O	0	0	
			25	22	3			
4	C	1	Total	C	O	0	0	
			24	21	3			
4	E	1	Total	C	O	0	0	
			26	23	3			
4	E	1	Total	C	N	O	0	0
			31	26	1	4		
4	E	1	Total	C	O	0	0	
			24	21	3			
4	E	1	Total	C	O	0	0	
			23	20	3			
4	E	1	Total	C	O	0	0	
			24	21	3			
4	G	1	Total	C	N	O	0	0
			30	25	1	4		
4	G	1	Total	C	O	0	0	
			23	20	3			

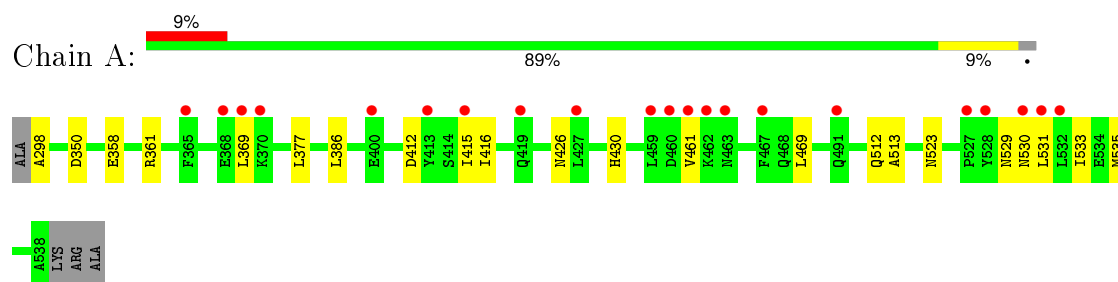
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total 90	O 90	0	0
5	C	103	Total 103	O 103	0	0
5	D	1	Total 1	O 1	0	0
5	E	94	Total 94	O 94	0	0
5	G	92	Total 92	O 92	0	0
5	H	1	Total 1	O 1	0	0

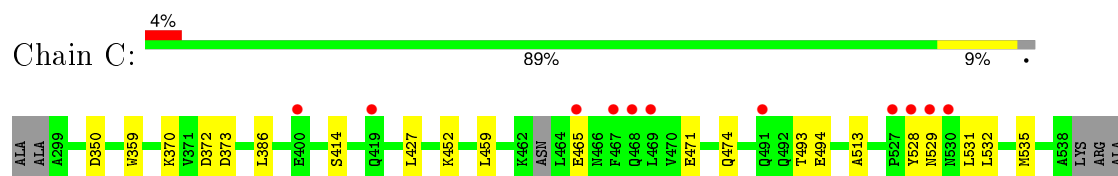
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

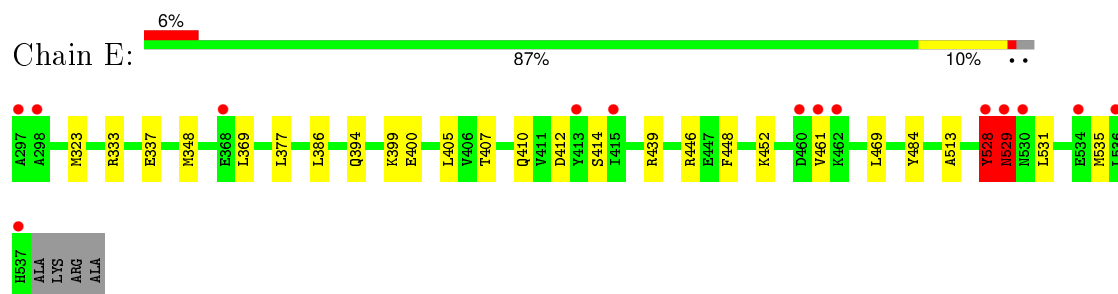
- Molecule 1: Nuclear receptor subfamily 5 group A member 2



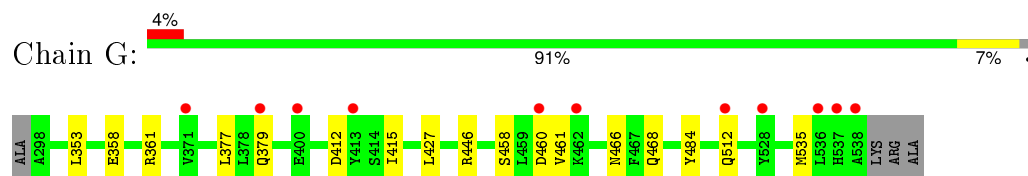
- Molecule 1: Nuclear receptor subfamily 5 group A member 2



- Molecule 1: Nuclear receptor subfamily 5 group A member 2



- Molecule 1: Nuclear receptor subfamily 5 group A member 2

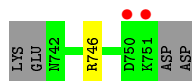


- Molecule 2: Nuclear receptor coactivator 2

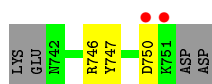




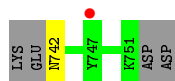
- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.95Å 76.89Å 108.48Å 90.00° 95.46° 90.00°	Depositor
Resolution (Å)	46.62 – 1.75 49.92 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.2 (46.62-1.75) 88.5 (49.92-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.214 , 0.236 0.219 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (2.13%)	DCC
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 100327 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9019	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.22 % 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 5.2742e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CPS, EPH

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	0.26	0/1989	0.42	0/2687
1	C	0.23	0/1983	0.37	0/2676
1	E	0.25	0/1997	0.41	0/2697
1	G	0.27	0/1997	0.40	0/2697
2	B	0.19	0/76	0.26	0/102
2	D	0.23	0/85	0.32	0/113
2	F	0.24	0/85	0.34	0/113
2	H	0.24	0/85	0.33	0/113
All	All	0.25	0/8297	0.40	0/11198

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1953	0	1962	17	0
1	C	1945	0	1959	14	1
1	E	1958	0	1971	18	1
1	G	1958	0	1971	11	0
2	B	76	0	80	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	85	0	93	2	0
2	F	85	0	93	3	0
2	H	85	0	93	1	0
3	A	47	0	61	3	0
3	C	47	0	61	2	0
3	E	47	0	61	2	0
3	G	47	0	61	0	0
4	A	75	0	103	0	0
4	C	49	0	69	0	0
4	E	128	0	178	0	0
4	G	53	0	71	0	0
5	A	90	0	0	3	0
5	C	103	0	0	1	0
5	D	1	0	0	0	0
5	E	94	0	0	0	0
5	G	92	0	0	0	0
5	H	1	0	0	0	0
All	All	9019	0	8887	61	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 3.

All (61) 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:G:379:GLN:HE22	2:H:742:ASN:HD22	1.37	0.73
1:C:372:ASP:OD2	2:D:746:ARG:NH2	2.23	0.69
1:C:529:ASN:HD21	2:F:747:TYR:HA	1.57	0.69
1:C:493:THR:HG23	1:C:494:GLU:HG3	1.74	0.68
1:A:358:GLU:OE1	1:A:361:ARG:NH2	2.16	0.67
1:G:358:GLU:OE1	1:G:361:ARG:NH2	2.31	0.63
1:C:528:TYR:OH	2:F:746:ARG:NH1	2.32	0.62
1:E:377:LEU:HD23	1:E:461:VAL:HG21	1.82	0.61
1:A:530:ASN:O	1:A:533:ILE:N	2.34	0.60
1:C:528:TYR:HE2	2:F:750:ASP:OD2	1.86	0.59
1:A:412:ASP:HB2	1:A:415:ILE:HD13	1.83	0.58
1:E:333:ARG:HB3	1:E:337:GLU:HG3	1.85	0.58
1:C:459:LEU:HG	1:C:474:GLN:HG3	1.84	0.58
1:A:361:ARG:NH1	2:B:748:LEU:O	2.37	0.57
1:E:412:ASP:OD2	1:E:414:SER:OG	2.22	0.57
1:A:426:ASN:O	1:A:430:HIS:HD2	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:O	1:A:535:MET:HG2	2.07	0.55
1:E:528:TYR:HD1	1:E:528:TYR:H	1.55	0.54
1:E:399:LYS:HG3	1:E:410:GLN:HE22	1.72	0.54
1:G:458:SER:OG	1:G:460:ASP:OD1	2.25	0.54
1:E:399:LYS:HG3	1:E:410:GLN:NE2	2.25	0.52
1:G:468:GLN:H	1:G:468:GLN:CD	2.13	0.52
1:A:386:LEU:HD13	3:A:601:EPH:H311	1.92	0.51
1:E:531:LEU:O	1:E:535:MET:HG2	2.11	0.50
1:G:377:LEU:HD23	1:G:461:VAL:HG21	1.94	0.50
1:G:353:LEU:HD21	1:G:535:MET:HG3	1.92	0.49
1:A:350:ASP:HB2	1:A:530:ASN:OD1	2.12	0.49
1:A:426:ASN:O	1:A:430:HIS:CD2	2.67	0.48
1:A:523:ASN:OD1	5:A:701:HOH:O	2.19	0.48
1:G:446:ARG:HD2	1:G:484:TYR:OH	2.14	0.48
1:A:369:LEU:HD21	1:A:469:LEU:HD22	1.95	0.47
1:A:426:ASN:OD1	1:A:512:GLN:NE2	2.46	0.47
5:A:701:HOH:O	1:G:458:SER:OG	2.20	0.47
1:E:446:ARG:HD2	1:E:484:TYR:CE1	2.49	0.47
1:G:427:LEU:HD21	1:G:512:GLN:HG2	1.97	0.46
1:A:513:ALA:HB1	3:A:601:EPH:H141	1.97	0.46
1:E:448:PHE:CZ	1:E:452:LYS:HD2	2.50	0.46
1:E:323[B]:MET:HG2	1:E:407:THR:HB	1.99	0.45
1:G:466:ASN:HA	1:G:468:GLN:OE1	2.16	0.45
2:D:746:ARG:HE	1:E:529:ASN:ND2	2.14	0.45
1:E:513:ALA:HB1	3:E:601:EPH:H141	1.99	0.45
1:A:426:ASN:ND2	1:A:430:HIS:NE2	2.66	0.44
1:E:369:LEU:HD21	1:E:469:LEU:HD22	1.99	0.44
1:E:394:GLN:O	1:E:439:ARG:NH2	2.51	0.43
1:E:386:LEU:HB3	3:E:601:EPH:H312	1.99	0.43
1:C:531:LEU:O	1:C:535:MET:HG2	2.19	0.42
1:C:427:LEU:HD21	1:C:513:ALA:HA	2.02	0.42
1:C:459:LEU:HD21	1:C:471:GLU:HA	2.02	0.41
1:E:348:MET:HE1	1:E:405:LEU:HD13	2.02	0.41
1:A:416:ILE:HA	3:A:601:EPH:O4	2.20	0.41
3:C:601:EPH:H221	3:C:601:EPH:H52	2.03	0.41
1:C:386:LEU:HB3	3:C:601:EPH:H311	2.03	0.41
1:C:350:ASP:HA	1:C:532:LEU:HD13	2.03	0.41
1:G:412:ASP:HB3	1:G:415:ILE:HG13	2.01	0.41
1:E:446:ARG:HD2	1:E:484:TYR:CZ	2.56	0.40
1:C:370:LYS:HG2	5:C:701:HOH:O	2.21	0.40
1:C:373:ASP:OD2	1:C:465:GLU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:LYS:NZ	1:E:410:GLN:HE22	2.19	0.40
1:A:377:LEU:HD23	1:A:461:VAL:HG21	2.02	0.40
1:C:359:TRP:CH2	1:C:452:LYS:HG2	2.57	0.40
1:A:298:ALA:N	5:A:710:HOH:O	2.53	0.40

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)
1:C:414:SER:OG	1:E:412:ASP:OD1[1_565]	2.17	0.03

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	239/245 (98%)	234 (98%)	4 (2%)	1 (0%)	39	19
1	C	236/245 (96%)	232 (98%)	4 (2%)	0	100	100
1	E	240/245 (98%)	237 (99%)	1 (0%)	2 (1%)	24	8
1	G	240/245 (98%)	237 (99%)	3 (1%)	0	100	100
2	B	7/14 (50%)	7 (100%)	0	0	100	100
2	D	8/14 (57%)	8 (100%)	0	0	100	100
2	F	8/14 (57%)	8 (100%)	0	0	100	100
2	H	8/14 (57%)	8 (100%)	0	0	100	100
All	All	986/1036 (95%)	971 (98%)	12 (1%)	3 (0%)	46	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	ASN

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Mol	Chain	Res	Type
1	E	528	TYR
1	E	529	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/218 (99%)	216 (100%)	0	100	100
1	C	216/218 (99%)	216 (100%)	0	100	100
1	E	217/218 (100%)	214 (99%)	3 (1%)	74	58
1	G	217/218 (100%)	217 (100%)	0	100	100
2	B	8/13 (62%)	8 (100%)	0	100	100
2	D	9/13 (69%)	9 (100%)	0	100	100
2	F	9/13 (69%)	9 (100%)	0	100	100
2	H	9/13 (69%)	9 (100%)	0	100	100
All	All	901/924 (98%)	898 (100%)	3 (0%)	94	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	400	GLU
1	E	528	TYR
1	E	529	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	529	ASN
1	E	410	GLN
1	E	529	ASN
2	H	742	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 ligands 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	$\# Z > 2$
3	EPH	A	601	-	46,46,48	0.30	0	47,51,53	0.56	0
4	CPS	A	602	-	27,27,45	0.20	0	43,44,70	0.43	0
4	CPS	A	603	-	25,25,45	0.25	0	37,41,70	0.38	0
4	CPS	A	604	-	32,32,45	0.15	0	51,51,70	0.31	0
3	EPH	C	601	-	46,46,48	0.29	0	47,51,53	0.54	0
4	CPS	C	602	-	28,28,45	0.19	0	46,46,70	0.38	0
4	CPS	C	603	-	27,27,45	0.21	0	43,44,70	0.43	0
3	EPH	E	601	-	46,46,48	0.28	0	47,51,53	0.56	0
4	CPS	E	602	-	29,29,45	0.16	0	47,47,70	0.36	0
4	CPS	E	603	-	34,34,45	0.17	0	53,53,70	0.32	0
4	CPS	E	604	-	27,27,45	0.18	0	43,44,70	0.39	0
4	CPS	E	605	-	26,26,45	0.19	0	42,43,70	0.29	0
4	CPS	E	606	-	27,27,45	0.18	0	43,44,70	0.40	0
3	EPH	G	601	-	46,46,48	0.29	0	47,51,53	0.57	0
4	CPS	G	602	-	33,33,45	0.14	0	52,52,70	0.32	0
4	CPS	G	603	-	26,26,45	0.20	0	42,43,70	0.32	0

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
3	EPH	A	601	-	-	0/50/50/52	0/0/0/0
4	CPS	A	602	-	-	0/2/67/90	0/4/4/4
4	CPS	A	603	-	-	0/0/61/90	0/4/4/4
4	CPS	A	604	-	-	0/9/74/90	0/4/4/4
3	EPH	C	601	-	-	0/50/50/52	0/0/0/0
4	CPS	C	602	-	-	0/4/69/90	0/4/4/4
4	CPS	C	603	-	-	0/2/67/90	0/4/4/4
3	EPH	E	601	-	-	0/50/50/52	0/0/0/0
4	CPS	E	602	-	-	0/6/71/90	0/4/4/4
4	CPS	E	603	-	-	0/12/77/90	0/4/4/4
4	CPS	E	604	-	-	0/2/67/90	0/4/4/4
4	CPS	E	605	-	-	0/0/65/90	0/4/4/4
4	CPS	E	606	-	-	0/2/67/90	0/4/4/4
3	EPH	G	601	-	-	0/50/50/52	0/0/0/0
4	CPS	G	602	-	-	0/11/76/90	0/4/4/4
4	CPS	G	603	-	-	0/0/65/90	0/4/4/4

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	EPH	3	0
3	C	601	EPH	2	0
3	E	601	EPH	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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	241/245 (98%)	0.64	21 (8%) 13 15	15, 29, 55, 92	0
1	C	239/245 (97%)	0.46	11 (4%) 36 42	14, 27, 50, 76	0
1	E	241/245 (98%)	0.51	14 (5%) 26 31	15, 28, 51, 88	0
1	G	241/245 (98%)	0.45	11 (4%) 36 42	15, 27, 49, 66	0
2	B	9/14 (64%)	0.51	0 100 100	31, 36, 42, 58	0
2	D	10/14 (71%)	1.23	2 (20%) 1 2	33, 38, 74, 82	0
2	F	10/14 (71%)	0.92	2 (20%) 1 2	34, 43, 66, 70	0
2	H	10/14 (71%)	0.87	1 (10%) 9 12	32, 42, 62, 65	0
All	All	1001/1036 (96%)	0.53	62 (6%) 24 29	14, 29, 53, 92	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	TYR	10.0
1	E	528	TYR	7.2
1	A	460	ASP	7.1
1	C	528	TYR	6.5
1	E	413	TYR	5.4
1	A	368	GLU	5.0
1	A	467	PHE	4.7
1	E	461	VAL	4.5
1	A	365	PHE	4.4
1	A	463	ASN	4.3
1	G	460	ASP	4.3
1	G	528	TYR	4.2
1	E	460	ASP	4.1
1	E	297	ALA	4.0
1	G	413	TYR	3.9
1	C	467	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	298	ALA	3.6
1	G	400	GLU	3.5
1	A	491	GLN	3.5
1	E	529	ASN	3.5
2	F	750	ASP	3.4
1	A	530	ASN	3.4
1	A	531	LEU	3.3
1	A	400	GLU	3.2
1	E	415	ILE	3.0
1	C	491	GLN	3.0
1	A	459	LEU	3.0
1	E	536	LEU	2.9
2	D	750	ASP	2.9
1	G	538	ALA	2.8
1	C	400	GLU	2.8
2	H	747	TYR	2.8
1	E	537	HIS	2.7
1	C	469	LEU	2.6
1	A	415	ILE	2.6
1	A	427	LEU	2.6
1	E	462	LYS	2.6
1	C	419	GLN	2.6
1	C	527	PRO	2.5
1	C	529	ASN	2.4
1	G	512	GLN	2.4
1	A	462	LYS	2.4
1	A	532	LEU	2.4
1	A	370	LYS	2.3
2	D	751	LYS	2.3
1	G	462	LYS	2.3
1	A	527	PRO	2.3
1	A	369	LEU	2.2
1	A	461	VAL	2.2
1	G	371	VAL	2.2
1	A	413	TYR	2.2
1	A	419	GLN	2.2
1	C	530	ASN	2.1
1	E	530	ASN	2.1
1	C	465	GLU	2.1
1	C	468	GLN	2.1
1	E	368	GLU	2.1
1	G	536	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	379	GLN	2.1
2	F	751	LYS	2.0
1	E	534	GLU	2.0
1	G	537	HIS	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	CPS	C	603	24/42	0.77	0.16	1.94	32,36,44,47	0
3	EPH	C	601	47/49	0.88	0.17	1.64	26,37,46,48	0
4	CPS	G	603	23/42	0.86	0.13	1.56	28,31,35,39	0
3	EPH	E	601	47/49	0.89	0.16	1.48	29,41,54,57	0
3	EPH	G	601	47/49	0.93	0.16	1.26	23,35,54,58	0
4	CPS	E	605	23/42	0.89	0.12	1.16	25,29,31,32	0
4	CPS	A	603	22/42	0.82	0.14	0.94	30,34,39,45	0
4	CPS	E	604	24/42	0.84	0.13	0.87	27,30,35,38	0
4	CPS	E	603	31/42	0.81	0.17	0.60	20,26,43,45	0
3	EPH	A	601	47/49	0.90	0.15	0.57	31,41,50,53	0
4	CPS	E	606	24/42	0.75	0.15	0.48	34,39,42,44	0
4	CPS	A	602	24/42	0.89	0.11	0.33	28,33,37,37	0
4	CPS	E	602	26/42	0.87	0.13	0.32	21,24,34,36	0
4	CPS	A	604	29/42	0.86	0.13	0.25	25,29,42,45	0
4	CPS	C	602	25/42	0.89	0.11	0.19	25,30,37,38	0
4	CPS	G	602	30/42	0.89	0.11	-0.35	19,25,40,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.