Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 05:00 PM EDT

PDB ID	:	3F5C
Title	:	Structure of Dax-1:LRH-1 complex
Authors	:	Fletterick, R.J.; Sablin, E.P.
Deposited on	:	2008-11-03
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

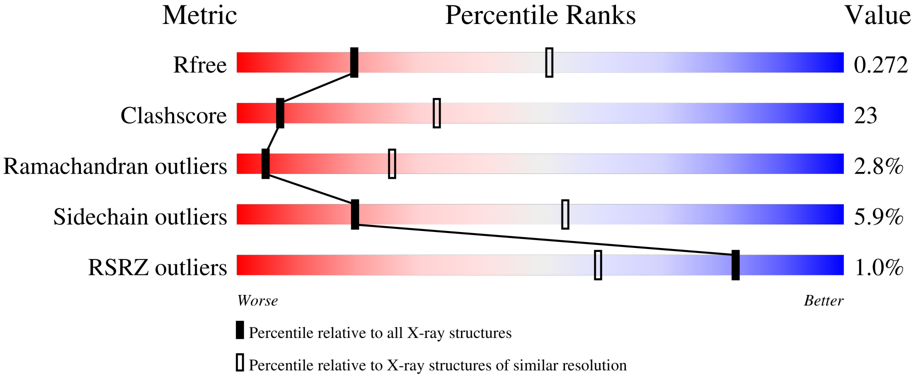
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

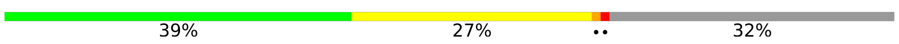
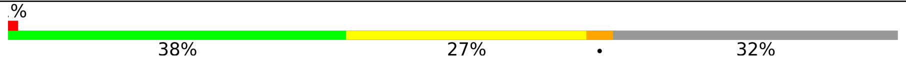
The reported resolution of this entry is 3.00 Å.

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	248	
2	B	268	
2	C	268	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4936 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
			Total	C	N	O	S			
1	A	243	1983	1270	337	367	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	525	LEU	ILE	engineered mutation	UNP P45448

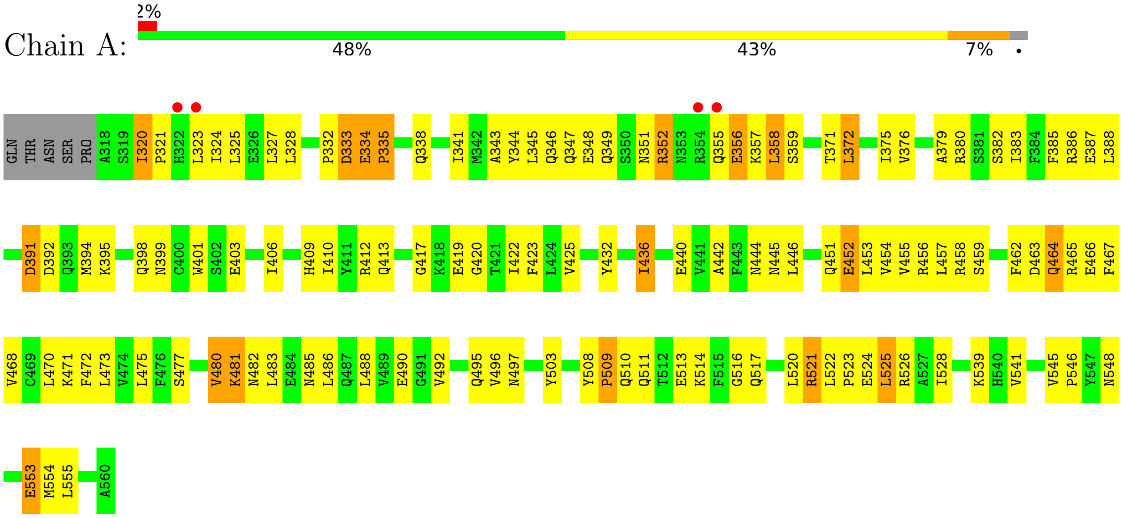
- Molecule 2 is a protein called Nuclear receptor subfamily 0 group B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	183	1485	970	243	257	15	0	0	0
2	C	181	1468	958	240	255	15	0	0	0

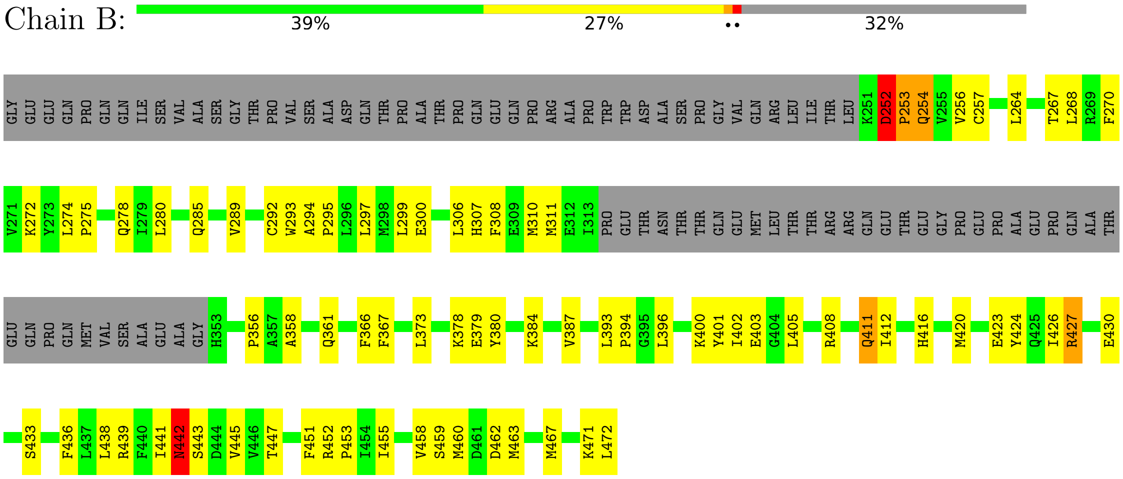
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

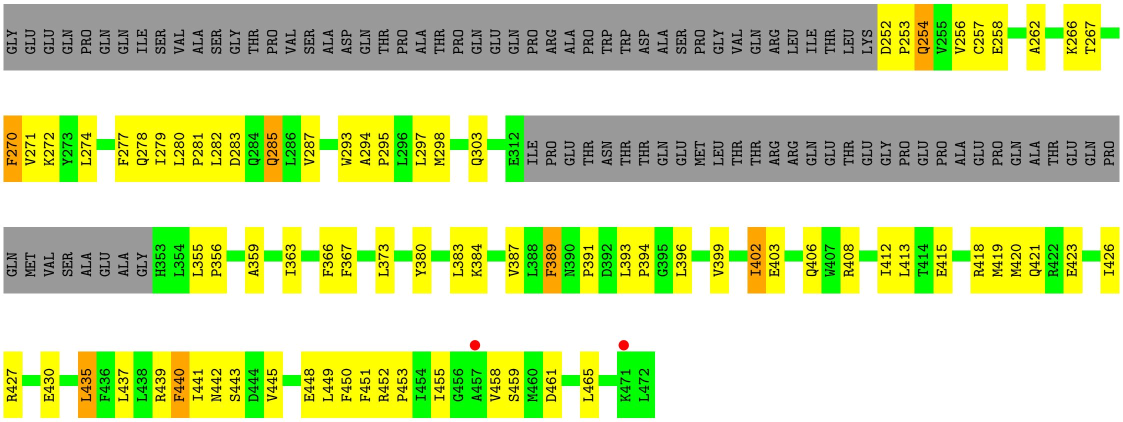
- Molecule 1: Nuclear receptor subfamily 5 group A member 2



- Molecule 2: Nuclear receptor subfamily 0 group B member 1



- Molecule 2: Nuclear receptor subfamily 0 group B member 1


GLY
GLU
GLU
GLN
PRO
GLN
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SER
VAL
ALA
SER
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THR
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GLY
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LEU
ILE
THR
LEU
LYS
D252
P253
Q254
V255
V256
C257
E258
A262
K266
T267
F270
V271
K272
Y273
L274
F277
Q278
I279
L280
P281
L282
D283
Q284
Q285
L286
V287
W293
A294
P295
L296
L297
M298
Q303
E312
ILE
PRO
GLU
THR
ASN
THR
THR
GLN
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MET
LEU
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THR
ARG
ARG
GLN
GLU
THR
GLU
GLY
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ALA
GLU
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ALA
THR
GLU
GLN
PRO
GLN
MET
VAL
SER
ALA
GLU
ALA
GLY
H353
L354
L355
P356
A359
I363
F366
F367
L373
Y380
L383
K384
V387
L388
F389
N390
P391
D392
L393
P394
G395
L396
V399
I402
E403
Q406
W407
R408
I412
L413
T414
E415
R418
M419
M420
Q421
R422
E423
I426
R427
E430
L435
F436
L437
L438
R439
F440
I441
N442
S443
D444
V445
E448
L449
F450
F451
R452
P453
I454
I455
G456
A457
V458
S459
M460
D461
L465
K471
L472

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	103.36Å 103.36Å 117.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.79 – 3.00 47.30 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.79-3.00) 98.3 (47.30-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.01Å)	Xtriage
Refinement program	PHENIX, CNS	Depositor
R, R_{free}	0.222 , 0.279 0.219 , 0.272	Depositor DCC
R_{free} test set	703 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å^2)	79.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4936	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.49	0/2019	0.63	1/2731 (0.0%)
2	B	0.56	0/1517	0.65	0/2050
2	C	0.51	0/1500	0.62	1/2028 (0.0%)
All	All	0.52	0/5036	0.63	2/6809 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	356	GLU	N-CA-C	5.79	126.62	111.00
2	C	389	PHE	CB-CA-C	-5.63	99.15	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1983	0	1997	100	0
2	B	1485	0	1523	65	0
2	C	1468	0	1499	64	0
All	All	4936	0	5019	226	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 23.

All (226) 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:358:LEU:HB2	1:A:359:SER:HA	1.44	0.99
1:A:356:GLU:O	1:A:356:GLU:HG2	1.64	0.98
1:A:333:ASP:O	1:A:334:GLU:HB2	1.65	0.94
2:C:282:LEU:HA	2:C:285:GLN:HB3	1.52	0.91
1:A:358:LEU:CB	1:A:359:SER:HA	2.00	0.86
1:A:419:GLU:HG3	1:A:420:GLY:H	1.41	0.85
2:B:442:ASN:O	2:B:443:SER:HB2	1.74	0.85
2:B:411:GLN:HE21	2:B:411:GLN:HA	1.43	0.82
1:A:548:ASN:O	2:B:275:PRO:HG3	1.81	0.81
2:B:442:ASN:HB3	2:B:445:VAL:HG23	1.63	0.79
2:C:294:ALA:HB3	2:C:295:PRO:HD3	1.68	0.75
1:A:442:ALA:HB2	2:C:281:PRO:HB3	1.70	0.73
1:A:511:GLN:HB3	1:A:514:LYS:HB2	1.68	0.73
2:B:294:ALA:HB3	2:B:295:PRO:HD3	1.70	0.73
1:A:324:ILE:HD12	1:A:324:ILE:H	1.54	0.72
1:A:444:ASN:C	1:A:446:LEU:H	1.93	0.72
2:B:254:GLN:CD	2:B:254:GLN:H	1.90	0.72
2:C:373:LEU:HD22	2:C:430:GLU:HG2	1.71	0.71
2:C:442:ASN:O	2:C:443:SER:HB3	1.90	0.71
1:A:356:GLU:O	1:A:356:GLU:CG	2.37	0.70
1:A:332:PRO:O	1:A:333:ASP:HB2	1.90	0.70
1:A:346:GLN:HA	1:A:349:GLN:HE21	1.55	0.70
2:B:378:LYS:HD3	2:B:416:HIS:CD2	2.27	0.69
2:B:424:TYR:CD2	2:B:424:TYR:O	2.45	0.69
2:B:252:ASP:O	2:B:256:VAL:HG22	1.93	0.69
2:C:461:ASP:O	2:C:465:LEU:HD13	1.93	0.69
1:A:333:ASP:O	1:A:334:GLU:CB	2.40	0.68
2:C:254:GLN:O	2:C:258:GLU:HB2	1.93	0.68
1:A:452:GLU:O	1:A:456:ARG:HB2	1.94	0.67
2:B:441:ILE:O	2:B:442:ASN:CB	2.44	0.65
1:A:332:PRO:O	1:A:333:ASP:CB	2.44	0.65
1:A:357:LYS:O	1:A:358:LEU:HB2	1.95	0.65
1:A:387:GLU:O	1:A:388:LEU:HB3	1.96	0.65
2:B:292:CYS:O	2:B:295:PRO:HD2	1.97	0.65
1:A:419:GLU:HG3	1:A:420:GLY:N	2.10	0.64
1:A:383:ILE:HA	1:A:386:ARG:HH21	1.63	0.63
1:A:486:LEU:O	1:A:490:GLU:HG2	1.99	0.63
2:C:281:PRO:O	2:C:282:LEU:HB3	1.98	0.63
2:B:455:ILE:HG12	2:B:458:VAL:HB	1.80	0.62
2:B:441:ILE:O	2:B:442:ASN:HB2	2.00	0.61
2:C:282:LEU:CA	2:C:285:GLN:HB3	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:CG	1:A:352:ARG:O	2.48	0.60
1:A:444:ASN:O	1:A:446:LEU:N	2.34	0.60
2:B:424:TYR:O	2:B:424:TYR:CG	2.53	0.60
2:C:391:PRO:HB2	2:C:399:VAL:HG13	1.82	0.60
1:A:371:THR:O	1:A:375:ILE:HG13	2.01	0.60
1:A:394:MET:O	1:A:398:GLN:HG3	2.02	0.60
1:A:480:VAL:HG12	1:A:481:LYS:N	2.18	0.59
2:C:426:ILE:O	2:C:430:GLU:HB2	2.03	0.59
1:A:372:LEU:O	1:A:376:VAL:HG23	2.03	0.59
1:A:409:HIS:HA	1:A:412:ARG:NH1	2.18	0.58
2:C:281:PRO:HB2	2:C:283:ASP:OD2	2.04	0.58
2:B:378:LYS:HD3	2:B:416:HIS:HD2	1.67	0.57
2:B:430:GLU:O	2:B:433:SER:HB3	2.05	0.57
2:B:300:GLU:OE2	2:B:384:LYS:HE2	2.05	0.57
2:C:420:MET:HG3	2:C:421:GLN:H	1.70	0.57
2:B:306:LEU:HD23	2:B:307:HIS:N	2.20	0.56
2:C:383:LEU:HD22	2:C:435:LEU:HD11	1.87	0.56
1:A:553:GLU:HG3	2:B:275:PRO:HB2	1.87	0.56
2:B:452:ARG:N	2:B:453:PRO:CD	2.69	0.56
2:C:423:GLU:HB3	2:C:426:ILE:HD12	1.88	0.56
1:A:388:LEU:HD13	1:A:485:ASN:HB3	1.89	0.55
1:A:516:GLY:O	1:A:520:LEU:HB2	2.05	0.55
2:B:292:CYS:C	2:B:295:PRO:HD2	2.26	0.55
2:C:295:PRO:HB2	2:C:387:VAL:HG11	1.88	0.55
2:C:274:LEU:O	2:C:277:PHE:HB3	2.07	0.55
1:A:403:GLU:HB3	1:A:525:LEU:HD21	1.88	0.54
1:A:444:ASN:C	1:A:446:LEU:N	2.55	0.54
2:B:411:GLN:HA	2:B:411:GLN:NE2	2.20	0.54
1:A:522:LEU:HB2	1:A:523:PRO:HD3	1.89	0.54
1:A:333:ASP:OD1	1:A:335:PRO:HD2	2.08	0.54
2:C:391:PRO:HG3	2:C:403:GLU:HG2	1.89	0.54
2:B:272:LYS:HZ1	2:B:472:LEU:HD23	1.74	0.53
1:A:324:ILE:O	1:A:328:LEU:HG	2.09	0.53
2:C:252:ASP:N	2:C:253:PRO:CD	2.71	0.53
2:C:452:ARG:HB2	2:C:453:PRO:HD3	1.90	0.53
1:A:436:ILE:HD13	1:A:436:ILE:O	2.09	0.53
1:A:467:PHE:CE2	1:A:471:LYS:HD2	2.44	0.53
1:A:513:GLU:O	1:A:517:GLN:HG2	2.08	0.53
1:A:403:GLU:OE1	1:A:526:ARG:HG2	2.09	0.53
1:A:462:PHE:HZ	1:A:467:PHE:HA	1.73	0.52
2:B:459:SER:HB2	2:B:462:ASP:CG	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:ALA:HB1	2:C:445:VAL:HG11	1.92	0.52
1:A:409:HIS:O	1:A:413:GLN:HG2	2.08	0.52
1:A:465:ARG:HD2	1:A:503:TYR:CE1	2.45	0.52
1:A:541:VAL:HG12	1:A:541:VAL:O	2.09	0.52
2:C:262:ALA:O	2:C:266:LYS:HB2	2.08	0.52
1:A:338:GLN:HG2	1:A:425:VAL:O	2.10	0.51
1:A:455:VAL:O	1:A:456:ARG:C	2.47	0.51
1:A:320:ILE:HG22	1:A:321:PRO:HD2	1.93	0.51
1:A:379:ALA:O	1:A:382:SER:HB3	2.11	0.51
1:A:401:TRP:CG	1:A:554:MET:HE2	2.46	0.51
2:B:268:LEU:O	2:B:272:LYS:HB2	2.10	0.50
2:C:303:GLN:HG3	2:C:380:TYR:CD2	2.46	0.50
1:A:352:ARG:O	1:A:352:ARG:HG2	2.10	0.50
2:C:448:GLU:HA	2:C:452:ARG:HG2	1.93	0.50
2:B:274:LEU:O	2:B:278:GLN:HG2	2.11	0.50
2:B:455:ILE:CG1	2:B:458:VAL:HB	2.40	0.50
1:A:524:GLU:O	1:A:528:ILE:HG13	2.12	0.50
1:A:321:PRO:O	1:A:325:LEU:HG	2.12	0.50
1:A:343:ALA:O	1:A:347:GLN:HB2	2.11	0.50
1:A:391:ASP:O	1:A:395:LYS:HG3	2.12	0.50
1:A:467:PHE:CZ	1:A:471:LYS:HD2	2.46	0.50
1:A:451:GLN:O	1:A:452:GLU:C	2.48	0.50
2:B:293:TRP:CH2	2:B:447:THR:HG22	2.46	0.50
1:A:388:LEU:HD11	1:A:392:ASP:CB	2.42	0.49
1:A:455:VAL:HG22	1:A:458:ARG:HH12	1.77	0.49
2:B:379:GLU:CD	2:B:427:ARG:HH12	2.15	0.49
2:B:361:GLN:HA	2:B:361:GLN:NE2	2.27	0.49
1:A:406:ILE:O	1:A:409:HIS:HB3	2.13	0.49
2:B:293:TRP:HH2	2:B:447:THR:HG22	1.78	0.49
2:C:458:VAL:O	2:C:459:SER:HB2	2.11	0.49
2:B:471:LYS:O	2:B:472:LEU:HG	2.12	0.49
2:B:358:ALA:O	2:B:361:GLN:HB3	2.12	0.49
2:C:298:MET:HA	2:C:298:MET:HE2	1.95	0.49
1:A:480:VAL:HG12	1:A:481:LYS:H	1.77	0.48
2:C:391:PRO:CB	2:C:399:VAL:HG13	2.43	0.48
1:A:511:GLN:CB	1:A:514:LYS:HB2	2.40	0.48
2:C:252:ASP:OD1	2:C:253:PRO:HD3	2.13	0.48
2:B:416:HIS:CE1	2:B:420:MET:HG3	2.49	0.48
2:B:426:ILE:O	2:B:430:GLU:HG3	2.13	0.48
2:B:295:PRO:HB2	2:B:387:VAL:HG11	1.95	0.48
2:B:280:LEU:HD21	2:B:401:TYR:CE2	2.49	0.48

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:488:LEU:O	1:A:492:VAL:HG22	2.14	0.48
2:B:452:ARG:N	2:B:453:PRO:HD2	2.30	0.47
1:A:324:ILE:HD12	1:A:324:ILE:N	2.28	0.47
1:A:464:GLN:HG2	1:A:464:GLN:O	2.15	0.47
2:C:355:LEU:O	2:C:356:PRO:C	2.52	0.47
2:C:380:TYR:O	2:C:384:LYS:HG3	2.15	0.47
1:A:323:LEU:O	1:A:327:LEU:HG	2.15	0.47
2:B:268:LEU:HD12	2:B:467:MET:HE2	1.96	0.47
2:B:400:LYS:O	2:B:403:GLU:HB2	2.15	0.47
1:A:413:GLN:O	1:A:417:GLY:HA3	2.15	0.47
2:C:383:LEU:HD22	2:C:435:LEU:CD1	2.45	0.46
1:A:468:VAL:O	1:A:472:PHE:HD1	1.98	0.46
2:C:455:ILE:HD11	2:C:458:VAL:HB	1.97	0.46
2:B:268:LEU:HD12	2:B:467:MET:HB3	1.98	0.46
2:C:280:LEU:HA	2:C:281:PRO:HD3	1.69	0.46
2:B:252:ASP:H	2:B:253:PRO:CD	2.29	0.46
2:C:451:PHE:O	2:C:455:ILE:HG22	2.15	0.46
2:C:441:ILE:O	2:C:442:ASN:HB2	2.14	0.46
2:C:427:ARG:O	2:C:427:ARG:HG3	2.15	0.46
2:C:448:GLU:HA	2:C:452:ARG:CG	2.46	0.46
2:B:268:LEU:N	2:B:268:LEU:HD23	2.31	0.45
2:B:285:GLN:O	2:B:289:VAL:HG23	2.17	0.45
2:C:279:ILE:O	2:C:280:LEU:HG	2.16	0.45
1:A:456:ARG:O	1:A:459:SER:HB2	2.17	0.45
2:C:449:LEU:HB3	2:C:450:PHE:CD1	2.50	0.45
1:A:492:VAL:HA	1:A:495:GLN:HB3	1.98	0.45
1:A:492:VAL:O	1:A:496:VAL:HG23	2.16	0.45
1:A:451:GLN:O	1:A:453:LEU:N	2.50	0.45
2:C:373:LEU:CD2	2:C:430:GLU:HG2	2.43	0.45
2:B:306:LEU:HD23	2:B:306:LEU:C	2.37	0.45
2:C:271:VAL:O	2:C:274:LEU:HB2	2.17	0.45
1:A:413:GLN:NE2	1:A:423:PHE:O	2.48	0.44
1:A:324:ILE:H	1:A:324:ILE:CD1	2.27	0.44
1:A:521:ARG:HD2	1:A:521:ARG:N	2.32	0.44
1:A:410:ILE:HG23	1:A:454:VAL:HG22	1.97	0.44
1:A:475:LEU:HD12	1:A:475:LEU:O	2.18	0.44
2:C:415:GLU:O	2:C:419:MET:HG2	2.17	0.44
2:B:451:PHE:O	2:B:455:ILE:HG22	2.17	0.44
1:A:451:GLN:C	1:A:453:LEU:N	2.70	0.44
2:B:293:TRP:CZ2	2:B:460:MET:HG2	2.52	0.44
2:B:306:LEU:CD2	2:B:308:PHE:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:389:PHE:O	2:C:406:GLN:NE2	2.51	0.44
1:A:345:LEU:O	1:A:349:GLN:HG2	2.18	0.44
1:A:508:TYR:HA	1:A:509:PRO:HD3	1.51	0.44
1:A:520:LEU:O	1:A:523:PRO:HD2	2.17	0.43
2:C:396:LEU:HD13	2:C:402:ILE:HD11	2.00	0.43
2:C:437:LEU:O	2:C:440:PHE:HD1	2.01	0.43
1:A:470:LEU:HD23	1:A:473:LEU:HD12	1.99	0.43
2:C:458:VAL:O	2:C:459:SER:CB	2.65	0.43
1:A:341:ILE:O	1:A:344:TYR:HB3	2.18	0.43
1:A:462:PHE:CZ	1:A:467:PHE:HA	2.53	0.43
2:B:436:PHE:O	2:B:439:ARG:HG3	2.18	0.43
2:C:256:VAL:HG23	2:C:257:CYS:N	2.33	0.43
2:C:393:LEU:HA	2:C:394:PRO:HD3	1.86	0.43
1:A:380:ARG:HA	1:A:385:PHE:CD2	2.54	0.43
2:C:277:PHE:CZ	2:C:285:GLN:HG3	2.53	0.43
2:B:267:THR:O	2:B:270:PHE:HB3	2.19	0.43
2:C:452:ARG:N	2:C:453:PRO:CD	2.82	0.43
1:A:463:ASP:CG	1:A:464:GLN:H	2.22	0.43
1:A:348:GLU:O	1:A:351:ASN:HB3	2.18	0.42
1:A:555:LEU:HD12	1:A:555:LEU:O	2.19	0.42
2:C:413:LEU:HD12	2:C:413:LEU:O	2.20	0.42
1:A:357:LYS:O	1:A:358:LEU:CB	2.65	0.42
1:A:388:LEU:HD11	1:A:392:ASP:HB2	2.00	0.42
1:A:422:ILE:HD11	1:A:451:GLN:HE21	1.83	0.42
2:C:458:VAL:O	2:C:458:VAL:HG12	2.19	0.42
2:C:298:MET:HB3	2:C:366:PHE:CE2	2.55	0.42
2:C:363:ILE:CG2	2:C:367:PHE:HE1	2.33	0.42
2:B:257:CYS:SG	2:B:453:PRO:HG2	2.60	0.42
2:C:408:ARG:O	2:C:412:ILE:HG22	2.20	0.42
1:A:481:LYS:HG3	1:A:482:ASN:ND2	2.34	0.41
2:C:280:LEU:C	2:C:282:LEU:H	2.22	0.41
2:B:436:PHE:O	2:B:439:ARG:CG	2.68	0.41
2:B:438:LEU:O	2:B:441:ILE:HG12	2.20	0.41
2:C:283:ASP:O	2:C:287:VAL:HG23	2.20	0.41
1:A:455:VAL:C	1:A:457:LEU:N	2.71	0.41
1:A:477:SER:O	1:A:480:VAL:HG23	2.20	0.41
1:A:440:GLU:OE2	1:A:539:LYS:HE2	2.20	0.41
2:B:463:MET:HE2	2:B:463:MET:HB2	1.88	0.41
2:C:293:TRP:CG	2:C:294:ALA:N	2.88	0.41
2:C:271:VAL:HG12	2:C:277:PHE:CE2	2.55	0.41
2:C:423:GLU:O	2:C:426:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TYR:CE2	1:A:451:GLN:HG3	2.55	0.41
2:B:451:PHE:C	2:B:453:PRO:HD2	2.40	0.41
1:A:462:PHE:CE1	1:A:466:GLU:HB2	2.56	0.41
2:B:366:PHE:CZ	2:B:438:LEU:HD13	2.56	0.41
2:B:272:LYS:NZ	2:B:472:LEU:HD23	2.36	0.41
2:B:401:TYR:CZ	2:B:405:LEU:HD11	2.56	0.41
2:B:452:ARG:HA	2:B:455:ILE:HG22	2.02	0.41
2:C:402:ILE:H	2:C:402:ILE:HG12	1.76	0.41
1:A:466:GLU:O	1:A:470:LEU:HG	2.21	0.41
1:A:488:LEU:O	1:A:488:LEU:HD12	2.21	0.41
2:B:393:LEU:HA	2:B:394:PRO:HD3	1.83	0.41
2:B:396:LEU:HD13	2:B:402:ILE:HD12	2.03	0.41
1:A:490:GLU:OE2	1:A:490:GLU:HA	2.20	0.40
2:B:380:TYR:O	2:B:384:LYS:HG3	2.22	0.40
2:C:267:THR:O	2:C:270:PHE:HB3	2.20	0.40
1:A:545:VAL:HA	1:A:546:PRO:HD3	1.91	0.40
2:C:363:ILE:O	2:C:367:PHE:HD1	2.05	0.40
2:B:373:LEU:O	2:B:427:ARG:NH2	2.55	0.40
2:C:437:LEU:HD13	2:C:437:LEU:HA	1.91	0.40
2:B:306:LEU:HB3	2:B:367:PHE:HE2	1.87	0.40
2:B:408:ARG:O	2:B:412:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	241/248 (97%)	205 (85%)	26 (11%)	10 (4%)	3	16
2	B	179/268 (67%)	154 (86%)	20 (11%)	5 (3%)	5	25
2	C	177/268 (66%)	144 (81%)	31 (18%)	2 (1%)	14	50
All	All	597/784 (76%)	503 (84%)	77 (13%)	17 (3%)	5	25

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	ASP
1	A	334	GLU
1	A	358	LEU
2	B	423	GLU
1	A	480	VAL
1	A	481	LYS
2	B	442	ASN
1	A	445	ASN
1	A	464	GLN
2	B	356	PRO
2	C	439	ARG
1	A	452	GLU
1	A	509	PRO
2	B	252	ASP
2	C	285	GLN
2	B	253	PRO
1	A	335	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/226 (98%)	208 (94%)	13 (6%)	19	54
2	B	164/235 (70%)	154 (94%)	10 (6%)	18	53
2	C	162/235 (69%)	153 (94%)	9 (6%)	21	56
All	All	547/696 (79%)	515 (94%)	32 (6%)	19	54

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	ILE
1	A	352	ARG
1	A	355	GLN
1	A	372	LEU

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Mol	Chain	Res	Type
1	A	391	ASP
1	A	399	ASN
1	A	436	ILE
1	A	483	LEU
1	A	497	ASN
1	A	510	GLN
1	A	521	ARG
1	A	525	LEU
1	A	553	GLU
2	B	252	ASP
2	B	254	GLN
2	B	264	LEU
2	B	297	LEU
2	B	299	LEU
2	B	310	MET
2	B	311	MET
2	B	411	GLN
2	B	427	ARG
2	B	442	ASN
2	C	254	GLN
2	C	270	PHE
2	C	272	LYS
2	C	278	GLN
2	C	297	LEU
2	C	402	ILE
2	C	418	ARG
2	C	435	LEU
2	C	440	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	A	349	GLN
1	A	355	GLN
1	A	370	GLN
1	A	398	GLN
1	A	399	ASN
1	A	444	ASN
1	A	482	ASN
1	A	497	ASN
1	A	510	GLN

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Mol	Chain	Res	Type
2	B	278	GLN
2	B	361	GLN
2	B	406	GLN
2	B	416	HIS
2	B	425	GLN
2	B	442	ASN
2	C	254	GLN
2	C	278	GLN
2	C	285	GLN
2	C	397	GLN
2	C	410	GLN

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 ⓘ

There are no ligands in this entry.

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	243/248 (97%)	-0.34	4 (1%)	72	44	68, 121, 197, 256	0
2	B	183/268 (68%)	-0.53	0	100	100	64, 97, 156, 190	0
2	C	181/268 (67%)	-0.41	2 (1%)	80	56	75, 105, 180, 207	0
All	All	607/784 (77%)	-0.42	6 (0%)	82	59	64, 108, 182, 256	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	457	ALA	4.3
1	A	355	GLN	4.0
1	A	354	ARG	3.2
1	A	323	LEU	3.1
1	A	322	HIS	2.9
2	C	471	LYS	2.5

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.