Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:06 AM EDT

PDB ID	:	1ZH7
Title	:	Structural and Biochemical Basis for Selective Repression of the Orphan Nuclear Receptor LRH-1 by SHP
Authors	:	Li, Y.; Choi, M.; Suino, K.; Kovach, A.; Daugherty, J.; Kliewer, S.A.; Xu, H.E.
Deposited on	:	2005-04-22
Resolution	:	2.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

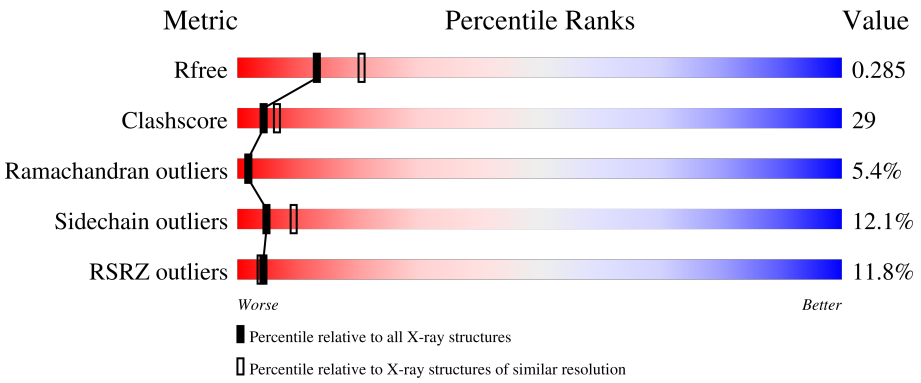
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	243	9%, 57%, 31%, 11% •
1	B	243	12%, 52%, 38%, 8% •
2	C	11	27%, 36%, 45%, 18%
2	D	11	36%, 45%, 36%, 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4315 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 Orphan nuclear receptor NR5A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1984	1270	337	368	9	0	0	0
1	B	243	1984	1270	337	368	9	0	0	0

- Molecule 2 is a protein called nuclear receptor subfamily 0, group B, member 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	11	88	58	13	17	0	0	0
2	D	11	88	58	13	17	0	0	0

- Molecule 3 is water.

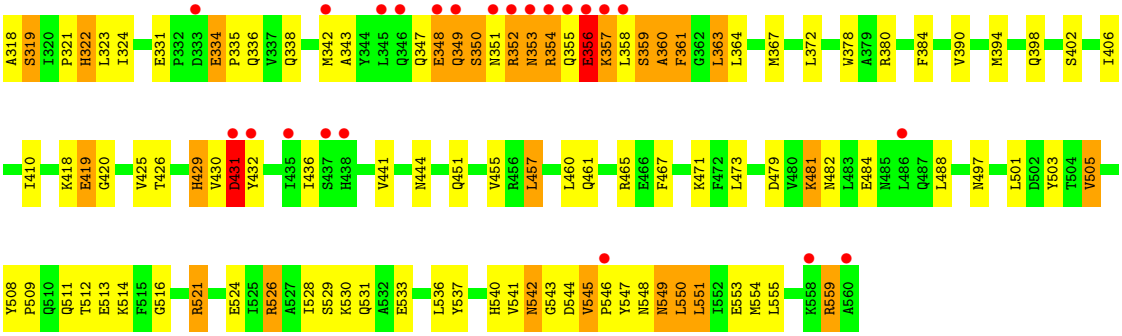
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	71	71	71	0	0
3	B	91	91	91	0	0
3	C	2	2	2	0	0
3	D	7	7	7	0	0

3 Residue-property plots (i)

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

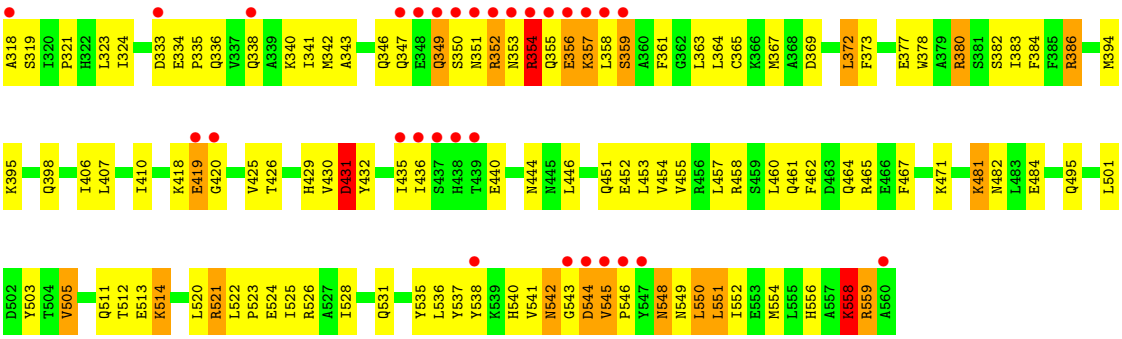
• Molecule 1: Orphan nuclear receptor NR5A2

Chain A:



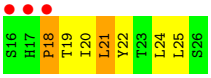
• Molecule 1: Orphan nuclear receptor NR5A2

Chain B:



• Molecule 2: nuclear receptor subfamily 0, group B, member 2

Chain C:



• Molecule 2: nuclear receptor subfamily 0, group B, member 2

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.77Å 35.13Å 134.21Å 90.00° 92.61° 90.00°	Depositor
Resolution (Å)	30.20 – 2.50 30.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.20-2.50) 99.3 (30.17-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.285 0.226 , 0.285	Depositor DCC
R_{free} test set	1659 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 69.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4315	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (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	0.39	0/2020	0.59	0/2731
1	B	0.36	0/2020	0.57	0/2731
2	C	0.40	0/90	0.66	0/122
2	D	0.39	0/90	0.67	0/122
All	All	0.37	0/4220	0.59	0/5706

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	1984	0	1997	118	3
1	B	1984	0	1997	118	1
2	C	88	0	90	13	0
2	D	88	0	90	7	0
3	A	71	0	0	11	2
3	B	91	0	0	2	1
3	C	2	0	0	0	0
3	D	7	0	0	0	0
All	All	4315	0	4174	242	4

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 29.

All (242) 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:B:357:LYS:HE3	1:B:359:SER:HB3	1.35	1.04
1:A:549:ASN:HD22	2:C:20:ILE:HG13	1.22	1.04
1:B:354:ARG:HE	1:B:355:GLN:HB3	1.26	1.01
1:A:352:ARG:HH12	1:A:358:LEU:HG	1.25	0.98
1:A:349:GLN:HG2	1:A:358:LEU:HD11	1.47	0.96
1:B:352:ARG:HH12	1:B:358:LEU:HG	1.33	0.91
1:A:357:LYS:C	1:A:357:LYS:HE2	1.95	0.86
1:A:536:LEU:HD23	1:A:555:LEU:HD22	1.61	0.83
2:D:18:PRO:O	2:D:22:TYR:HB2	1.80	0.82
1:A:334:GLU:HB3	1:A:335:PRO:HD3	1.61	0.81
1:A:354:ARG:HE	1:A:355:GLN:HB3	1.45	0.79
1:A:357:LYS:HE3	1:A:359:SER:H	1.47	0.79
1:B:355:GLN:O	1:B:356:GLU:HB2	1.83	0.79
2:C:19:THR:HG23	2:C:20:ILE:H	1.46	0.78
1:B:352:ARG:HG2	1:B:352:ARG:O	1.83	0.78
1:B:342:MET:HG2	1:B:426:THR:HB	1.64	0.78
1:B:558:LYS:NZ	1:B:558:LYS:HB3	1.99	0.77
1:B:382:SER:O	1:B:386:ARG:HG2	1.85	0.77
1:A:352:ARG:O	1:A:352:ARG:HG2	1.86	0.75
1:B:377:GLU:HA	1:B:380:ARG:HH12	1.50	0.75
1:A:349:GLN:HE21	1:A:349:GLN:C	1.90	0.74
1:A:559:ARG:HA	1:A:559:ARG:NE	2.02	0.73
1:A:338:GLN:O	1:A:342:MET:HB2	1.89	0.73
1:B:436:ILE:HG23	1:B:444:ASN:ND2	2.05	0.72
1:B:343:ALA:O	1:B:347:GLN:HG2	1.89	0.72
1:A:512:THR:HA	3:A:111:HOH:O	1.88	0.72
1:B:540:HIS:HA	1:B:545:VAL:HG23	1.71	0.72
1:A:432:TYR:HE2	1:A:451:GLN:HG3	1.55	0.72
1:B:338:GLN:O	1:B:342:MET:HB2	1.90	0.71
1:B:321:PRO:HG2	1:B:324:ILE:HD12	1.72	0.71
1:A:357:LYS:HE2	1:A:357:LYS:O	1.92	0.69
1:A:349:GLN:CG	1:A:358:LEU:HD11	2.21	0.69
1:B:365:CYS:SG	1:B:545:VAL:HG13	2.32	0.69
1:A:548:ASN:HB2	1:A:551:LEU:HB2	1.74	0.69
1:B:558:LYS:HD2	1:B:558:LYS:O	1.93	0.68
1:A:501:LEU:O	1:A:505:VAL:HG12	1.94	0.68
1:B:349:GLN:HE21	1:B:349:GLN:C	1.97	0.68
1:A:549:ASN:HD22	2:C:20:ILE:CG1	2.04	0.67
1:A:553:GLU:OE2	2:C:20:ILE:HB	1.94	0.67
1:A:343:ALA:O	1:A:347:GLN:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:HIS:HA	1:B:545:VAL:CG2	2.24	0.67
3:B:89:HOH:O	2:D:18:PRO:HB3	1.93	0.66
1:B:548:ASN:N	1:B:548:ASN:ND2	2.44	0.66
1:A:354:ARG:HD2	1:A:355:GLN:N	2.10	0.66
1:A:457:LEU:HD21	1:A:521:ARG:HG2	1.78	0.66
1:B:395:LYS:HE2	1:B:482:ASN:HB2	1.77	0.66
1:A:349:GLN:HE21	1:A:350:SER:N	1.93	0.66
1:B:394:MET:SD	2:D:18:PRO:HB2	2.36	0.65
1:B:378:TRP:CZ2	1:B:471:LYS:HE2	2.31	0.65
1:B:451:GLN:O	1:B:455:VAL:HG23	1.96	0.64
1:B:432:TYR:O	1:B:436:ILE:HG12	1.98	0.64
1:B:377:GLU:HA	1:B:380:ARG:NH1	2.13	0.64
1:A:540:HIS:HA	1:A:545:VAL:HG23	1.80	0.64
1:B:548:ASN:HD22	1:B:552:ILE:CD1	2.11	0.64
1:A:402:SER:OG	1:A:529:SER:HB2	1.98	0.63
1:A:357:LYS:HE3	1:A:359:SER:N	2.11	0.63
1:A:419:GLU:HG3	1:A:420:GLY:H	1.64	0.63
1:A:529:SER:O	1:A:533:GLU:HG3	1.98	0.63
1:B:333:ASP:OD2	1:B:336:GLN:HB2	1.99	0.62
1:A:352:ARG:NH1	1:A:358:LEU:HG	2.06	0.62
1:B:453:LEU:O	1:B:457:LEU:HD23	1.97	0.62
1:A:321:PRO:HG2	1:A:324:ILE:HD12	1.80	0.62
1:A:331:GLU:OE2	1:A:471:LYS:NZ	2.28	0.62
1:B:436:ILE:HG23	1:B:444:ASN:HD22	1.63	0.62
1:A:338:GLN:HB3	1:A:426:THR:O	1.99	0.62
1:B:334:GLU:HB3	1:B:335:PRO:HD3	1.81	0.62
1:A:354:ARG:HD2	1:A:354:ARG:C	2.19	0.62
1:B:373:PHE:O	1:B:377:GLU:HG3	2.00	0.62
1:A:467:PHE:CZ	1:A:471:LYS:HD2	2.35	0.61
1:A:541:VAL:HG12	1:A:541:VAL:O	2.00	0.61
1:A:353:ASN:HD22	1:A:354:ARG:N	1.97	0.61
1:B:465:ARG:HD2	1:B:503:TYR:CZ	2.35	0.61
1:B:548:ASN:HD22	1:B:552:ILE:HD13	1.65	0.61
1:A:537:TYR:CD1	1:A:559:ARG:HD2	2.36	0.61
1:B:520:LEU:O	1:B:523:PRO:HD2	2.00	0.60
1:A:355:GLN:O	1:A:356:GLU:HB2	2.01	0.60
1:B:349:GLN:HE21	1:B:350:SER:N	1.98	0.60
1:B:524:GLU:O	1:B:528:ILE:HG13	2.01	0.60
1:A:323:LEU:HD11	1:A:384:PHE:HZ	1.67	0.59
1:B:352:ARG:HH22	1:B:358:LEU:HA	1.67	0.59
1:B:465:ARG:HD2	1:B:503:TYR:OH	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:HIS:H	1:A:429:HIS:CD2	2.19	0.59
1:B:558:LYS:O	1:B:559:ARG:HB3	2.02	0.59
2:C:18:PRO:O	2:C:22:TYR:HB2	2.03	0.58
1:A:488:LEU:HD12	1:A:488:LEU:O	2.02	0.58
1:B:354:ARG:NE	1:B:355:GLN:HB3	2.07	0.58
1:A:322:HIS:HD2	3:A:33:HOH:O	1.86	0.58
1:A:342:MET:HG2	1:A:426:THR:HB	1.86	0.57
1:A:531:GLN:NE2	3:A:92:HOH:O	2.37	0.57
1:A:394:MET:HG2	2:C:25:LEU:HD12	1.87	0.57
1:A:429:HIS:CD2	1:A:429:HIS:N	2.73	0.57
1:A:432:TYR:CE2	1:A:451:GLN:HG3	2.38	0.57
1:B:419:GLU:HG3	1:B:420:GLY:H	1.70	0.57
2:C:19:THR:HG23	2:C:20:ILE:N	2.19	0.57
1:B:349:GLN:C	1:B:349:GLN:NE2	2.58	0.57
1:B:513:GLU:HG3	1:B:513:GLU:O	2.04	0.57
1:B:432:TYR:HE2	1:B:451:GLN:HG3	1.69	0.57
1:B:349:GLN:CG	1:B:358:LEU:HD11	2.35	0.56
1:B:467:PHE:CZ	1:B:471:LYS:HD2	2.40	0.56
1:B:357:LYS:CE	1:B:359:SER:HB3	2.21	0.56
1:B:457:LEU:HD12	1:B:462:PHE:CG	2.40	0.56
1:A:430:VAL:HG12	1:A:430:VAL:O	2.05	0.56
1:A:441:VAL:HB	1:B:542:ASN:HB3	1.88	0.56
1:A:398:GLN:OE1	2:C:18:PRO:CG	2.55	0.55
1:A:323:LEU:HD11	1:A:384:PHE:CZ	2.41	0.55
1:A:349:GLN:C	1:A:349:GLN:NE2	2.59	0.55
1:A:550:LEU:O	1:A:554:MET:HG2	2.07	0.55
1:B:341:ILE:HG22	1:B:426:THR:HG22	1.89	0.55
1:B:380:ARG:HH11	1:B:380:ARG:HB3	1.72	0.55
1:B:522:LEU:HB2	1:B:523:PRO:HD3	1.89	0.54
1:B:558:LYS:HB3	1:B:558:LYS:HZ2	1.70	0.54
1:A:322:HIS:NE2	3:A:121:HOH:O	2.33	0.54
1:B:511:GLN:HG2	1:B:514:LYS:HB2	1.89	0.54
1:B:537:TYR:CD1	1:B:559:ARG:HD2	2.42	0.54
1:B:383:ILE:HA	1:B:386:ARG:CZ	2.38	0.54
1:A:398:GLN:OE1	2:C:18:PRO:HG3	2.07	0.54
1:A:540:HIS:HA	1:A:545:VAL:CG2	2.38	0.53
1:A:394:MET:HG2	2:C:21:LEU:HD13	1.91	0.53
1:B:354:ARG:C	1:B:354:ARG:HD2	2.28	0.53
1:B:446:LEU:HD21	1:B:531:GLN:HB3	1.89	0.53
1:B:453:LEU:HD11	1:B:524:GLU:OE2	2.07	0.53
1:B:430:VAL:HG12	1:B:435:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ARG:NE	1:A:355:GLN:HB3	2.20	0.53
1:B:349:GLN:HG2	1:B:358:LEU:HD21	1.90	0.53
1:B:323:LEU:HD22	1:B:495:GLN:HG3	1.92	0.52
1:A:530:LYS:HD2	3:A:59:HOH:O	2.08	0.52
1:B:349:GLN:HG2	1:B:358:LEU:HD11	1.90	0.52
2:D:19:THR:HG23	2:D:20:ILE:N	2.24	0.52
1:A:406:ILE:O	1:A:410:ILE:HG13	2.10	0.52
1:B:372:LEU:HD13	1:B:550:LEU:HD13	1.90	0.52
1:B:548:ASN:N	1:B:548:ASN:HD22	2.07	0.52
1:A:394:MET:SD	2:C:18:PRO:HB2	2.51	0.51
1:B:318:ALA:O	1:B:319:SER:HB2	2.10	0.51
1:A:378:TRP:CZ2	1:A:471:LYS:HE2	2.45	0.51
1:A:473:LEU:HD11	1:A:497:ASN:ND2	2.25	0.51
1:A:537:TYR:O	1:A:541:VAL:HG23	2.11	0.51
1:B:352:ARG:HH12	1:B:358:LEU:CG	2.14	0.51
1:B:542:ASN:O	1:B:544:ASP:N	2.44	0.50
1:A:419:GLU:HG3	1:A:420:GLY:N	2.27	0.50
1:A:432:TYR:CE1	1:A:436:ILE:HG13	2.46	0.50
1:A:430:VAL:O	1:A:431:ASP:O	2.29	0.50
1:B:354:ARG:HE	1:B:355:GLN:CB	2.10	0.50
2:C:21:LEU:HD22	2:C:25:LEU:HG	1.93	0.50
1:B:372:LEU:HD11	1:B:554:MET:HG3	1.92	0.50
1:A:357:LYS:CE	1:A:359:SER:N	2.75	0.50
1:A:513:GLU:CD	1:A:516:GLY:H	2.14	0.50
1:B:364:LEU:O	1:B:367:MET:HG2	2.13	0.49
1:B:429:HIS:CD2	1:B:429:HIS:H	2.30	0.49
1:B:537:TYR:O	1:B:541:VAL:HG23	2.12	0.49
1:A:336:GLN:HA	1:A:336:GLN:OE1	2.12	0.49
1:A:436:ILE:HG23	1:A:444:ASN:ND2	2.26	0.49
1:B:430:VAL:O	1:B:431:ASP:C	2.50	0.49
1:A:360:ALA:O	1:A:361:PHE:C	2.50	0.49
1:A:524:GLU:O	1:A:528:ILE:HG13	2.13	0.49
1:B:457:LEU:HD21	1:B:521:ARG:HG2	1.95	0.49
1:B:549:ASN:HD22	2:D:20:ILE:HG13	1.78	0.49
1:A:357:LYS:CE	1:A:359:SER:H	2.21	0.48
1:B:380:ARG:HH11	1:B:380:ARG:CB	2.26	0.48
1:B:432:TYR:CE1	1:B:436:ILE:HG13	2.48	0.48
1:A:542:ASN:ND2	3:A:37:HOH:O	2.46	0.48
1:A:429:HIS:H	1:A:429:HIS:HD2	1.61	0.48
1:A:530:LYS:HE2	3:A:101:HOH:O	2.13	0.48
1:B:556:HIS:C	1:B:558:LYS:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:VAL:HG22	1:A:425:VAL:O	2.14	0.48
1:A:559:ARG:HA	1:A:559:ARG:HE	1.79	0.47
1:B:429:HIS:CD2	1:B:429:HIS:N	2.82	0.47
1:B:481:LYS:H	1:B:481:LYS:HG2	1.52	0.47
1:A:457:LEU:N	1:A:457:LEU:HD23	2.29	0.47
1:B:501:LEU:O	1:B:505:VAL:HG13	2.15	0.47
1:A:318:ALA:O	1:A:319:SER:HB2	2.14	0.47
1:B:548:ASN:HB2	1:B:551:LEU:HB2	1.96	0.46
1:B:418:LYS:O	1:B:419:GLU:O	2.33	0.46
1:B:383:ILE:HG12	1:B:384:PHE:CD1	2.51	0.46
1:B:352:ARG:HH22	1:B:358:LEU:HD23	1.80	0.46
1:B:321:PRO:CG	1:B:324:ILE:HD12	2.45	0.46
1:A:441:VAL:CG2	1:B:542:ASN:HB3	2.46	0.46
1:B:430:VAL:HG11	1:B:435:ILE:HD11	1.98	0.46
1:B:334:GLU:O	1:B:338:GLN:HG3	2.15	0.46
1:B:367:MET:HE2	1:B:425:VAL:HG12	1.98	0.46
1:B:407:LEU:HD13	1:B:525:ILE:CD1	2.46	0.46
1:B:538:TYR:HE2	3:B:151:HOH:O	1.97	0.45
1:A:338:GLN:HG2	1:A:425:VAL:O	2.15	0.45
1:A:352:ARG:HG2	1:A:352:ARG:HH11	1.81	0.45
1:A:526:ARG:NE	3:A:98:HOH:O	2.49	0.45
1:B:548:ASN:O	1:B:549:ASN:C	2.55	0.45
1:A:334:GLU:HB3	1:A:335:PRO:CD	2.41	0.45
1:A:418:LYS:O	1:A:419:GLU:C	2.55	0.45
1:B:452:GLU:O	1:B:455:VAL:HB	2.17	0.45
1:A:541:VAL:O	1:A:541:VAL:CG1	2.65	0.45
1:A:549:ASN:O	1:A:553:GLU:HB2	2.17	0.44
1:A:521:ARG:HA	1:A:521:ARG:HD3	1.69	0.44
1:A:430:VAL:O	1:A:431:ASP:C	2.56	0.44
1:B:558:LYS:HB3	1:B:558:LYS:HZ3	1.78	0.44
1:A:457:LEU:HD21	1:A:521:ARG:CG	2.47	0.43
1:A:451:GLN:O	1:A:455:VAL:HG23	2.18	0.43
1:B:372:LEU:CD1	1:B:550:LEU:HD13	2.48	0.43
1:B:464:GLN:O	1:B:467:PHE:HB3	2.19	0.43
1:B:398:GLN:OE1	2:D:18:PRO:CG	2.66	0.43
1:A:357:LYS:HE3	1:A:359:SER:CB	2.49	0.43
1:A:419:GLU:CG	1:A:420:GLY:H	2.25	0.43
1:A:481:LYS:O	1:A:482:ASN:HB2	2.19	0.43
1:B:336:GLN:OE1	1:B:336:GLN:HA	2.16	0.43
1:A:513:GLU:HA	1:A:513:GLU:OE1	2.19	0.43
2:D:24:LEU:HD12	2:D:24:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:PHE:CE2	1:A:471:LYS:HD2	2.53	0.43
1:B:369:ASP:CG	1:B:548:ASN:HB3	2.40	0.43
1:B:342:MET:HE1	1:B:346:GLN:OE1	2.18	0.42
1:A:548:ASN:CB	1:A:551:LEU:HB2	2.45	0.42
1:B:373:PHE:CD1	1:B:550:LEU:HD12	2.54	0.42
1:B:407:LEU:HD13	1:B:525:ILE:HD13	2.00	0.42
1:B:513:GLU:OE1	1:B:513:GLU:HA	2.19	0.42
1:A:488:LEU:HD12	1:A:488:LEU:C	2.39	0.42
1:A:465:ARG:HD2	1:A:503:TYR:OH	2.19	0.42
1:A:513:GLU:O	1:A:513:GLU:HG3	2.19	0.42
1:A:526:ARG:CZ	3:A:98:HOH:O	2.67	0.42
1:B:460:LEU:O	1:B:461:GLN:HB2	2.19	0.42
1:A:481:LYS:H	1:A:481:LYS:HG2	1.69	0.42
1:A:348:GLU:O	1:A:349:GLN:C	2.58	0.42
1:B:465:ARG:HD2	1:B:503:TYR:CE1	2.54	0.42
1:A:465:ARG:NH1	3:A:122:HOH:O	2.52	0.42
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.93	0.42
1:A:360:ALA:O	1:A:363:LEU:N	2.38	0.42
1:A:363:LEU:HD22	1:A:363:LEU:O	2.20	0.42
1:B:338:GLN:HG2	1:B:425:VAL:O	2.19	0.42
1:B:383:ILE:HG12	1:B:384:PHE:CE1	2.55	0.42
1:B:536:LEU:HD21	1:B:551:LEU:HD22	2.02	0.41
1:B:406:ILE:O	1:B:410:ILE:HD13	2.21	0.41
1:A:460:LEU:O	1:A:461:GLN:HB2	2.19	0.41
1:B:513:GLU:O	1:B:513:GLU:CG	2.68	0.41
1:A:508:TYR:N	1:A:509:PRO:CD	2.83	0.41
1:B:430:VAL:HG12	1:B:430:VAL:O	2.21	0.41
1:A:549:ASN:ND2	2:C:20:ILE:HG13	2.07	0.41
1:B:361:PHE:HE1	1:B:535:TYR:HE2	1.68	0.41
1:A:321:PRO:CG	1:A:324:ILE:HD12	2.48	0.41
1:A:548:ASN:O	1:A:550:LEU:N	2.54	0.41
1:A:436:ILE:O	1:A:436:ILE:HG22	2.20	0.41
1:A:361:PHE:O	1:A:364:LEU:HB2	2.21	0.40
1:A:390:VAL:HG23	3:A:52:HOH:O	2.21	0.40
1:A:418:LYS:O	1:A:419:GLU:O	2.39	0.40
1:B:454:VAL:O	1:B:458:ARG:HB2	2.21	0.40
1:B:338:GLN:HB3	1:B:426:THR:O	2.21	0.40
1:B:418:LYS:O	1:B:419:GLU:C	2.60	0.40

All (4) 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:A:347:GLN:NE2	3:A:146:HOH:O[1_545]	1.12	1.08
1:A:336:GLN:NE2	3:A:136:HOH:O[1_545]	1.83	0.37
1:A:547:TYR:CD1	3:B:68:HOH:O[1_545]	1.99	0.21
1:B:340:LYS:NZ	1:B:452:GLU:OE1[1_565]	2.02	0.18

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	241/243 (99%)	205 (85%)	24 (10%)	12 (5%)	2 2
1	B	241/243 (99%)	205 (85%)	23 (10%)	13 (5%)	2 2
2	C	9/11 (82%)	7 (78%)	1 (11%)	1 (11%)	0 0
2	D	9/11 (82%)	8 (89%)	0	1 (11%)	0 0
All	All	500/508 (98%)	425 (85%)	48 (10%)	27 (5%)	2 2

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	GLU
1	A	360	ALA
1	A	419	GLU
1	A	431	ASP
1	A	546	PRO
1	B	356	GLU
1	B	419	GLU
1	B	546	PRO
1	A	359	SER
1	A	361	PHE
1	B	359	SER
1	B	512	THR
1	B	543	GLY
1	B	558	LYS

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Mol	Chain	Res	Type
1	A	351	ASN
1	A	543	GLY
1	A	549	ASN
1	B	354	ARG
1	B	357	LYS
2	C	18	PRO
2	D	18	PRO
1	B	351	ASN
1	B	431	ASP
1	B	559	ARG
1	A	334	GLU
1	A	350	SER
1	B	440	GLU

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	221/221 (100%)	191 (86%)	30 (14%)	3 7
1	B	221/221 (100%)	199 (90%)	22 (10%)	7 15
2	C	11/11 (100%)	9 (82%)	2 (18%)	1 3
2	D	11/11 (100%)	9 (82%)	2 (18%)	1 3
All	All	464/464 (100%)	408 (88%)	56 (12%)	5 9

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	SER
1	A	322	HIS
1	A	348	GLU
1	A	349	GLN
1	A	352	ARG
1	A	353	ASN
1	A	354	ARG
1	A	356	GLU

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Mol	Chain	Res	Type
1	A	357	LYS
1	A	363	LEU
1	A	367	MET
1	A	372	LEU
1	A	380	ARG
1	A	429	HIS
1	A	431	ASP
1	A	457	LEU
1	A	479	ASP
1	A	481	LYS
1	A	484	GLU
1	A	505	VAL
1	A	511	GLN
1	A	514	LYS
1	A	521	ARG
1	A	526	ARG
1	A	542	ASN
1	A	544	ASP
1	A	545	VAL
1	A	550	LEU
1	A	551	LEU
1	A	559	ARG
1	B	349	GLN
1	B	352	ARG
1	B	353	ASN
1	B	354	ARG
1	B	363	LEU
1	B	372	LEU
1	B	380	ARG
1	B	386	ARG
1	B	431	ASP
1	B	481	LYS
1	B	484	GLU
1	B	505	VAL
1	B	514	LYS
1	B	521	ARG
1	B	526	ARG
1	B	542	ASN
1	B	544	ASP
1	B	545	VAL
1	B	548	ASN
1	B	550	LEU

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Mol	Chain	Res	Type
1	B	551	LEU
1	B	558	LYS
2	C	21	LEU
2	C	24	LEU
2	D	21	LEU
2	D	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	353	ASN
1	A	429	HIS
1	A	461	GLN
1	A	497	ASN
1	A	511	GLN
1	A	549	ASN
1	B	349	GLN
1	B	429	HIS
1	B	451	GLN
1	B	497	ASN
1	B	548	ASN
1	B	549	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 monosaccharides 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	243/243 (100%)	0.54	23 (9%)	8	8	44, 75, 137, 183	0
1	B	243/243 (100%)	0.72	30 (12%)	4	3	45, 77, 138, 181	0
2	C	11/11 (100%)	2.08	3 (27%)	0	0	71, 80, 153, 154	0
2	D	11/11 (100%)	2.75	4 (36%)	0	0	67, 75, 154, 155	0
All	All	508/508 (100%)	0.71	60 (11%)	4	4	44, 77, 148, 183	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	16	SER	11.1
2	C	16	SER	10.4
1	B	353	ASN	9.1
1	A	358	LEU	8.3
1	B	354	ARG	8.1
2	D	17	HIS	8.0
2	D	18	PRO	7.8
1	B	356	GLU	7.5
1	A	354	ARG	7.5
1	B	419	GLU	7.4
1	A	352	ARG	7.4
1	B	357	LYS	7.4
1	B	438	HIS	6.9
1	B	352	ARG	6.8
1	B	437	SER	6.6
2	C	17	HIS	6.5
1	A	353	ASN	6.2
1	B	355	GLN	6.0
1	B	350	SER	5.7
2	C	18	PRO	5.5
1	A	356	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	349	GLN	5.4
1	B	347	GLN	4.9
1	A	349	GLN	4.8
1	B	436	ILE	4.8
1	A	355	GLN	4.7
1	A	342	MET	4.7
1	A	560	ALA	4.6
1	B	435	ILE	4.4
1	A	486	LEU	4.4
1	A	346	GLN	4.3
1	B	338	GLN	4.3
1	B	545	VAL	4.1
1	B	439	THR	3.6
1	A	546	PRO	3.6
1	B	543	GLY	3.6
1	A	345	LEU	3.5
1	B	348	GLU	3.4
1	A	558	LYS	3.3
1	B	358	LEU	3.2
1	B	538	TYR	3.1
1	A	357	LYS	3.1
1	A	435	ILE	3.1
1	B	547	TYR	2.9
1	B	546	PRO	2.7
1	B	560	ALA	2.7
1	B	544	ASP	2.6
1	B	351	ASN	2.6
1	B	420	GLY	2.4
2	D	19	THR	2.4
1	A	333	ASP	2.4
1	B	333	ASP	2.4
1	A	351	ASN	2.4
1	A	437	SER	2.2
1	B	318	ALA	2.2
1	A	431	ASP	2.1
1	A	348	GLU	2.1
1	A	432	TYR	2.1
1	A	438	HIS	2.1
1	B	359	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.