



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:30 AM UTC

PDB ID : 3P0U / pdb_00003p0u
Title : Crystal Structure of the ligand binding domain of human testicular receptor 4
Authors : Zhou, X.E.; Suino-Powell, K.M.; Xu, Y.; Chan, C.-W.; Kruse, S.W.; Reynolds, R.; Engel, J.D.; Xu, H.E.
Deposited on : 2010-09-29
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

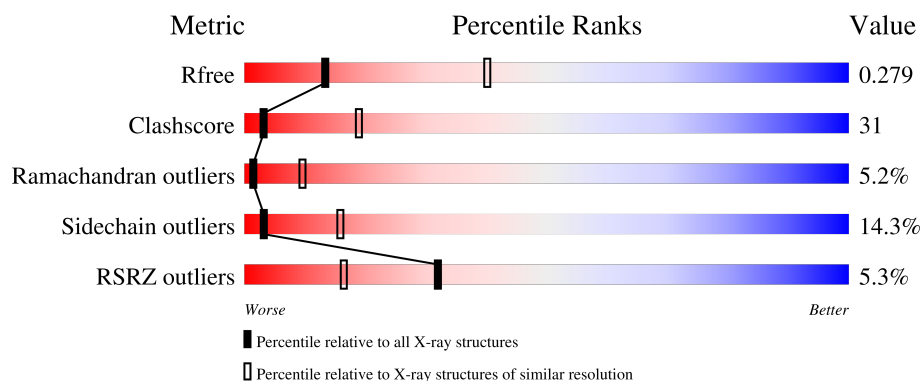
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	249	3% 45% 36% 8% 11%
1	B	249	6% 39% 36% 10% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3558 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 2 group C member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1764	1131	289	330	14			
1	B	216	Total	C	N	O	S	0	0	0
			1721	1105	280	323	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	539	ALA	LYS	engineered mutation	UNP P49116
A	550	ALA	LYS	engineered mutation	UNP P49116
B	539	ALA	LYS	engineered mutation	UNP P49116
B	550	ALA	LYS	engineered mutation	UNP P49116

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	42	Total	O	0	0
			42	42		

4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.48Å 140.96Å 184.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-3.00) 99.6 (30.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.258 , 0.287 0.255 , 0.279	Depositor DCC
R_{free} test set	1228 reflections (6.97%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 122.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3558	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.98	1/1799 (0.1%)	1.00	1/2439 (0.0%)
1	B	0.93	0/1758	0.96	1/2388 (0.0%)
All	All	0.96	1/3557 (0.0%)	0.98	2/4827 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	530	THR	CA-CB	6.25	1.64	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ASN	N-CA-C	5.80	118.65	108.56
1	A	400	LEU	N-CA-C	5.43	122.36	110.80

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	1764	0	1762	113	0
1	B	1721	0	1715	110	0
2	A	31	0	0	7	0
2	B	42	0	0	11	0
All	All	3558	0	3477	217	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 31.

All (217) 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:455:GLN:NE2	1:A:456:VAL:HG13	1.57	1.17
1:B:486:GLN:HA	2:B:23:HOH:O	1.54	1.05
1:A:455:GLN:HE22	1:A:456:VAL:CG1	1.75	0.98
1:A:455:GLN:C	1:A:455:GLN:HE21	1.75	0.94
1:B:508:GLY:HA2	2:B:59:HOH:O	1.68	0.92
1:A:374:ILE:HD12	1:A:376:VAL:CG1	1.99	0.92
1:A:455:GLN:NE2	1:A:456:VAL:CG1	2.31	0.92
1:A:455:GLN:CD	1:A:456:VAL:HG13	1.97	0.90
1:B:450:LEU:HD23	1:B:494:LEU:HD11	1.54	0.89
1:A:455:GLN:HE22	1:A:456:VAL:HG13	1.29	0.86
1:A:402:VAL:HG22	1:A:403:HIS:H	1.40	0.86
1:B:452:GLN:HB2	2:B:2:HOH:O	1.76	0.85
1:A:374:ILE:HD12	1:A:376:VAL:HG12	1.61	0.83
1:A:486:GLN:HA	2:A:56:HOH:O	1.79	0.82
1:A:431:GLN:O	1:A:435:THR:HG22	1.80	0.79
1:B:377:GLU:OE2	1:B:377:GLU:N	2.16	0.79
1:B:391:THR:HG22	1:B:393:PRO:HD3	1.65	0.76
1:A:392:MET:HG3	1:A:415:LEU:HD21	1.68	0.76
1:B:449:GLY:O	1:B:452:GLN:HB3	1.86	0.75
1:B:421:ARG:NH1	1:B:598:ILE:HG22	2.03	0.73
1:A:542:MET:HG3	1:B:557:TYR:CE2	2.23	0.72
1:B:420:ALA:O	1:B:423:ILE:HG22	1.90	0.72
1:A:585:LEU:N	1:A:585:LEU:HD12	2.06	0.71
1:B:413:LEU:HG	1:B:417:MET:HE2	1.73	0.70
1:B:460:SER:O	1:B:462:ILE:HG23	1.91	0.70
1:A:459:LEU:HB3	1:A:461:THR:HG23	1.74	0.70
1:B:501:MET:HE1	1:B:565:ARG:HG3	1.74	0.69
1:B:560:ALA:O	1:B:564:VAL:HG23	1.92	0.69
1:A:455:GLN:HE22	1:A:456:VAL:HG12	1.57	0.69
1:B:402:VAL:HG22	1:B:403:HIS:H	1.58	0.69
1:B:586:ILE:O	1:B:589:VAL:HG22	1.94	0.67
1:B:462:ILE:O	1:B:463:LEU:O	2.12	0.67
1:A:455:GLN:NE2	1:A:455:GLN:C	2.50	0.66
1:A:392:MET:HE2	1:A:415:LEU:HG	1.78	0.66
1:B:423:ILE:HG23	1:B:426:PHE:HB2	1.78	0.66
1:B:374:ILE:HD12	1:B:376:VAL:HG23	1.78	0.65
1:B:373:ILE:HD12	1:B:373:ILE:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ILE:HD13	1:B:424:PRO:N	2.11	0.65
1:A:458:SER:HA	2:A:3:HOH:O	1.97	0.64
1:A:402:VAL:HG13	1:A:403:HIS:N	2.13	0.64
1:A:452:GLN:HE22	1:A:515:LYS:NZ	1.95	0.64
1:A:586:ILE:HG13	1:A:594:ILE:CD1	2.27	0.64
1:A:402:VAL:HG22	1:A:403:HIS:N	2.12	0.64
1:B:402:VAL:HG13	1:B:403:HIS:N	2.11	0.63
1:A:522:PRO:HD2	2:B:30:HOH:O	1.97	0.63
1:B:448:LEU:HD23	1:B:515:LYS:HG2	1.80	0.63
1:A:503:LYS:NZ	1:B:367:ARG:HB3	2.13	0.63
1:A:455:GLN:NE2	1:A:456:VAL:N	2.46	0.62
1:A:503:LYS:HZ1	1:B:367:ARG:HD3	1.63	0.62
1:B:593:SER:O	1:B:596:PRO:HD2	2.00	0.61
1:A:591:ILE:HA	1:A:594:ILE:HD12	1.83	0.61
1:B:389:LYS:C	1:B:390:LEU:HD22	2.25	0.61
1:B:392:MET:HE2	1:B:415:LEU:HG	1.81	0.61
1:B:423:ILE:HD13	1:B:423:ILE:C	2.25	0.61
1:B:530:THR:O	1:B:534:GLU:HG3	2.01	0.61
1:A:390:LEU:HD13	1:A:509:TYR:CE1	2.36	0.61
1:B:379:PRO:HD2	1:B:532:GLN:NE2	2.15	0.60
1:B:485:LYS:N	2:B:16:HOH:O	2.35	0.59
1:B:576:ILE:HG22	1:B:580:LEU:HD22	1.83	0.59
1:B:378:GLY:HA3	2:B:17:HOH:O	2.01	0.59
1:B:391:THR:HG22	1:B:393:PRO:CD	2.32	0.59
1:A:530:THR:O	2:A:5:HOH:O	2.16	0.58
1:B:374:ILE:CD1	1:B:376:VAL:HG23	2.33	0.58
1:A:461:THR:HA	2:A:9:HOH:O	2.01	0.58
1:A:439:ARG:HD3	1:A:592:ASP:OD2	2.03	0.58
1:A:538:GLU:O	1:A:542:MET:HB2	2.04	0.58
1:A:418:HIS:HA	1:A:421:ARG:HG2	1.86	0.58
1:A:439:ARG:HD3	1:A:592:ASP:CG	2.28	0.58
1:A:529:SER:O	2:A:5:HOH:O	2.17	0.57
1:B:535:LYS:HE2	2:B:71:HOH:O	2.04	0.57
1:B:448:LEU:HD13	1:B:569:LEU:HD11	1.86	0.57
1:A:427:GLN:N	2:A:20:HOH:O	2.37	0.57
1:A:425:ALA:HB1	1:A:536:PHE:CE1	2.39	0.56
1:A:421:ARG:HA	1:A:426:PHE:CD2	2.40	0.56
1:A:405:ILE:HD12	1:A:459:LEU:HD11	1.88	0.56
1:A:459:LEU:HB3	1:A:461:THR:CG2	2.36	0.56
1:B:511:TYR:O	1:B:515:LYS:HG3	2.05	0.56
1:B:376:VAL:HG12	1:B:377:GLU:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD22	1:A:417:MET:HE3	1.88	0.55
1:A:452:GLN:HE22	1:A:515:LYS:HZ2	1.53	0.55
1:A:389:LYS:HB3	1:A:419:TRP:NE1	2.21	0.55
1:A:389:LYS:HB3	1:A:419:TRP:HE1	1.70	0.55
1:B:446:PHE:O	1:B:450:LEU:HB2	2.06	0.55
1:B:563:LEU:O	1:B:566:LEU:HD23	2.07	0.55
1:A:450:LEU:HD13	1:A:494:LEU:HD11	1.88	0.55
1:B:434:ASN:C	1:B:436:SER:H	2.14	0.54
1:B:437:LEU:CD1	1:B:527:LEU:HD21	2.37	0.54
1:B:557:TYR:HB2	1:B:561:ARG:HH21	1.72	0.54
1:B:551:THR:O	1:B:551:THR:HG22	2.07	0.54
1:A:513:TYR:O	1:A:516:ALA:HB3	2.08	0.53
1:B:373:ILE:HD12	1:B:373:ILE:N	2.24	0.53
1:B:379:PRO:HD2	1:B:532:GLN:HE22	1.72	0.53
1:A:420:ALA:HB1	1:A:519:LEU:HD11	1.89	0.53
1:A:576:ILE:O	1:A:580:LEU:HD13	2.09	0.53
1:B:372:PRO:HD2	1:B:376:VAL:O	2.09	0.53
1:B:591:ILE:O	1:B:595:ILE:HG13	2.08	0.53
1:A:384:THR:HG23	1:A:384:THR:O	2.09	0.52
1:B:595:ILE:HB	1:B:596:PRO:HD3	1.90	0.52
1:B:501:MET:HE2	1:B:501:MET:HA	1.92	0.52
1:B:450:LEU:C	1:B:452:GLN:H	2.17	0.52
1:A:392:MET:HE2	1:A:415:LEU:CD2	2.41	0.51
1:A:372:PRO:HG2	1:A:374:ILE:HG13	1.93	0.51
1:A:595:ILE:HB	1:A:596:PRO:HD3	1.92	0.51
1:B:444:GLU:HG2	1:B:569:LEU:HB3	1.91	0.51
1:A:376:VAL:HG13	1:A:377:GLU:H	1.76	0.51
1:A:392:MET:HE2	1:A:415:LEU:CG	2.40	0.51
1:A:442:TRP:CE2	1:A:591:ILE:HD11	2.46	0.50
1:A:504:LEU:HB2	1:A:506:ILE:CD1	2.41	0.50
1:B:548:VAL:HG13	1:B:558:ARG:HD3	1.93	0.50
1:A:368:ASP:OD1	1:A:368:ASP:C	2.55	0.50
1:A:586:ILE:HG13	1:A:594:ILE:HD13	1.94	0.50
1:B:403:HIS:NE2	1:B:583:THR:HG23	2.27	0.50
1:A:529:SER:OG	1:A:530:THR:N	2.38	0.50
1:A:503:LYS:HZ3	1:B:367:ARG:HB3	1.77	0.49
1:A:588:ASN:OD1	1:A:588:ASN:N	2.45	0.49
1:B:389:LYS:HE2	1:B:423:ILE:HA	1.94	0.49
1:B:505:ASP:O	1:B:558:ARG:NH2	2.46	0.49
1:B:598:ILE:HA	2:B:6:HOH:O	2.11	0.49
1:B:400:LEU:HG	1:B:401:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ALA:HA	1:B:542:MET:HE3	1.93	0.49
1:B:556:THR:HG23	1:B:557:TYR:CD1	2.47	0.49
1:A:459:LEU:N	1:A:459:LEU:HD22	2.28	0.49
1:A:434:ASN:O	1:A:435:THR:C	2.56	0.48
1:A:544:LEU:HD13	1:A:559:LEU:HD21	1.93	0.48
1:B:396:MET:SD	1:B:455:GLN:HB3	2.53	0.48
1:A:583:THR:HA	1:A:587:GLY:HA3	1.95	0.48
1:A:402:VAL:HG13	1:A:404:TYR:H	1.78	0.48
1:A:373:ILE:HG12	1:A:530:THR:CG2	2.43	0.48
1:A:396:MET:SD	1:A:456:VAL:HG11	2.53	0.48
1:A:593:SER:O	1:A:596:PRO:HD2	2.14	0.48
1:B:501:MET:HE1	1:B:565:ARG:CG	2.43	0.48
1:A:374:ILE:CD1	1:A:376:VAL:CG1	2.85	0.47
1:A:503:LYS:HZ1	1:B:367:ARG:HB3	1.78	0.47
1:A:589:VAL:HG12	1:A:589:VAL:O	2.14	0.47
1:B:397:PRO:HG3	1:B:411:ARG:NH2	2.29	0.47
1:B:558:ARG:O	1:B:559:LEU:C	2.57	0.47
1:B:586:ILE:HG12	1:B:589:VAL:HG21	1.97	0.47
1:A:372:PRO:O	1:A:374:ILE:O	2.33	0.47
1:B:585:LEU:HD13	1:B:589:VAL:HG23	1.96	0.47
1:A:472:ASN:N	1:A:472:ASN:HD22	2.13	0.47
1:B:566:LEU:HB2	1:B:567:PRO:HD3	1.95	0.47
1:A:537:GLN:O	1:A:541:GLN:HG2	2.15	0.46
1:B:463:LEU:HD12	1:B:463:LEU:C	2.40	0.46
1:A:413:LEU:HD22	1:A:413:LEU:O	2.15	0.46
1:A:544:LEU:HD13	1:A:559:LEU:CD2	2.45	0.46
1:A:417:MET:HG3	1:A:598:ILE:HG21	1.98	0.46
1:B:423:ILE:C	1:B:423:ILE:CD1	2.89	0.45
1:B:544:LEU:HG	1:B:559:LEU:HD21	1.99	0.45
1:B:506:ILE:HG23	1:B:510:GLU:HB2	1.96	0.45
1:A:442:TRP:NE1	1:A:591:ILE:HD11	2.31	0.45
1:A:513:TYR:CE2	1:A:543:GLU:HB2	2.51	0.45
1:B:402:VAL:HG22	1:B:403:HIS:N	2.30	0.45
1:A:585:LEU:N	1:A:585:LEU:CD1	2.79	0.45
1:B:443:ASN:HB3	2:B:18:HOH:O	2.16	0.45
1:A:506:ILE:HD12	1:A:506:ILE:N	2.32	0.44
1:A:548:VAL:HG13	1:A:558:ARG:HD3	1.99	0.44
1:B:397:PRO:HG3	1:B:411:ARG:HH21	1.82	0.44
1:A:591:ILE:O	1:A:595:ILE:HG12	2.17	0.44
1:B:506:ILE:O	1:B:506:ILE:HG22	2.17	0.44
1:A:413:LEU:O	1:A:417:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:LYS:HG3	1:B:488:MET:HG2	1.99	0.44
1:A:560:ALA:O	1:A:564:VAL:HG23	2.17	0.44
1:A:520:PHE:O	1:A:537:GLN:HB2	2.16	0.44
1:B:563:LEU:O	1:B:566:LEU:CD2	2.66	0.44
1:B:420:ALA:HB1	1:B:519:LEU:HD21	1.99	0.43
1:B:387:THR:HG22	1:B:387:THR:O	2.18	0.43
1:B:557:TYR:HB2	1:B:561:ARG:NH2	2.33	0.43
1:A:586:ILE:HG12	1:A:591:ILE:HG22	1.99	0.43
1:B:390:LEU:HD13	1:B:509:TYR:HB3	1.99	0.43
1:B:423:ILE:CG2	1:B:426:PHE:HB2	2.48	0.43
1:A:500:SER:O	1:A:504:LEU:HD12	2.18	0.43
1:A:583:THR:O	1:A:584:GLY:C	2.62	0.43
1:B:546:ASP:O	1:B:550:ALA:HB3	2.19	0.43
1:A:372:PRO:O	1:A:373:ILE:C	2.62	0.43
1:A:564:VAL:HG12	1:A:564:VAL:O	2.19	0.43
1:A:585:LEU:HD12	1:A:585:LEU:H	1.83	0.43
1:B:585:LEU:HD13	1:B:589:VAL:CG2	2.49	0.43
1:A:447:THR:HA	1:A:450:LEU:HB2	2.01	0.42
1:B:367:ARG:O	1:B:368:ASP:HB2	2.19	0.42
1:B:548:VAL:HG21	1:B:559:LEU:HD23	2.01	0.42
1:B:431:GLN:O	1:B:434:ASN:HB2	2.19	0.42
1:B:437:LEU:HD13	1:B:527:LEU:HD21	1.99	0.42
1:A:503:LYS:HZ1	1:B:367:ARG:CD	2.30	0.42
1:B:563:LEU:C	1:B:565:ARG:H	2.27	0.42
1:A:459:LEU:HD12	1:A:461:THR:CG2	2.50	0.42
1:B:371:THR:HG23	1:B:376:VAL:O	2.19	0.42
1:B:376:VAL:HG12	1:B:377:GLU:N	2.34	0.42
1:A:424:PRO:C	2:A:20:HOH:O	2.63	0.42
1:B:544:LEU:O	1:B:548:VAL:HG23	2.19	0.42
1:B:564:VAL:HG12	1:B:564:VAL:O	2.20	0.42
1:A:396:MET:HA	1:A:397:PRO:HD3	1.84	0.41
1:A:426:PHE:O	1:A:434:ASN:OD1	2.38	0.41
1:A:423:ILE:HB	1:A:426:PHE:HB2	2.01	0.41
1:B:389:LYS:HE3	1:B:422:SER:OG	2.20	0.41
1:A:506:ILE:HG23	1:A:510:GLU:HB2	2.02	0.41
1:A:392:MET:SD	1:A:515:LYS:NZ	2.93	0.41
1:A:455:GLN:OE1	1:A:456:VAL:HG13	2.18	0.41
1:B:389:LYS:HD2	1:B:389:LYS:N	2.36	0.41
1:A:539:ALA:O	1:A:543:GLU:HG3	2.21	0.41
1:B:367:ARG:HB2	2:B:29:HOH:O	2.20	0.41
1:A:489:GLU:O	1:A:493:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:N	1:A:567:PRO:CD	2.84	0.41
1:B:434:ASN:O	1:B:438:VAL:HG12	2.21	0.41
1:B:490:HIS:CG	1:B:576:ILE:HG21	2.55	0.41
1:A:457:MET:HG3	1:A:457:MET:O	2.21	0.41
1:A:487:VAL:O	1:A:491:ILE:HG13	2.21	0.41
1:B:572:MET:HE3	1:B:572:MET:HB2	1.97	0.41
1:B:524:HIS:HA	1:B:525:PRO:HD3	1.96	0.40
1:A:399:TYR:HD1	1:A:400:LEU:H	1.69	0.40
1:B:459:LEU:HD23	2:B:1:HOH:O	2.21	0.40
1:A:389:LYS:HE3	1:A:423:ILE:HD13	2.03	0.40
1:A:595:ILE:N	1:A:596:PRO:CD	2.85	0.40
1:B:372:PRO:HD3	1:B:377:GLU:HA	2.03	0.40
1:B:438:VAL:HG13	1:B:439:ARG:N	2.36	0.40
1:A:374:ILE:HD12	1:A:376:VAL:HG13	1.96	0.40
1:B:460:SER:O	1:B:462:ILE:N	2.54	0.40
1:B:536:PHE:O	1:B:539:ALA:HB3	2.22	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	214/249 (86%)	177 (83%)	29 (14%)	8 (4%)	2	15
1	B	212/249 (85%)	163 (77%)	35 (16%)	14 (7%)	1	5
All	All	426/498 (86%)	340 (80%)	64 (15%)	22 (5%)	1	9

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	LEU
1	A	401	ASN

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Mol	Chain	Res	Type
1	A	402	VAL
1	A	457	MET
1	B	386	VAL
1	B	397	PRO
1	B	463	LEU
1	A	385	HIS
1	A	397	PRO
1	A	584	GLY
1	B	374	ILE
1	B	402	VAL
1	B	368	ASP
1	B	461	THR
1	B	505	ASP
1	B	593	SER
1	B	373	ILE
1	B	376	VAL
1	B	589	VAL
1	A	571	LEU
1	B	586	ILE
1	B	456	VAL

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	198/220 (90%)	173 (87%)	25 (13%)	4	20
1	B	193/220 (88%)	162 (84%)	31 (16%)	2	12
All	All	391/440 (89%)	335 (86%)	56 (14%)	3	16

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

Mol	Chain	Res	Type
1	A	367	ARG
1	A	377	GLU
1	A	380	LEU

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Mol	Chain	Res	Type
1	A	399	TYR
1	A	403	HIS
1	A	412	LEU
1	A	413	LEU
1	A	421	ARG
1	A	450	LEU
1	A	455	GLN
1	A	484	ILE
1	A	486	GLN
1	A	495	GLN
1	A	496	GLU
1	A	507	ASP
1	A	514	LEU
1	A	519	LEU
1	A	529	SER
1	A	571	LEU
1	A	574	SER
1	A	583	THR
1	A	585	LEU
1	A	590	SER
1	A	591	ILE
1	A	601	MET
1	B	373	ILE
1	B	376	VAL
1	B	390	LEU
1	B	392	MET
1	B	398	GLU
1	B	399	TYR
1	B	403	HIS
1	B	404	TYR
1	B	423	ILE
1	B	429	LEU
1	B	431	GLN
1	B	452	GLN
1	B	455	GLN
1	B	456	VAL
1	B	460	SER
1	B	484	ILE
1	B	507	ASP
1	B	527	LEU
1	B	530	THR
1	B	535	LYS

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Mol	Chain	Res	Type
1	B	537	GLN
1	B	549	GLN
1	B	556	THR
1	B	559	LEU
1	B	566	LEU
1	B	570	ARG
1	B	571	LEU
1	B	580	LEU
1	B	586	ILE
1	B	588	ASN
1	B	599	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	369	GLN
1	A	385	HIS
1	A	434	ASN
1	A	452	GLN
1	A	455	GLN
1	A	490	HIS
1	A	499	ASN
1	A	549	GLN
1	A	575	ASN
1	B	427	GLN
1	B	499	ASN
1	B	532	GLN
1	B	537	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 oligosaccharides 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	222/249 (89%)	0.13	7 (3%)	50 29	44, 78, 127, 179	0
1	B	216/249 (86%)	0.27	16 (7%)	20 10	49, 87, 147, 159	0
All	All	438/498 (87%)	0.20	23 (5%)	32 16	44, 82, 143, 179	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	ASN	4.6
1	B	588	ASN	4.1
1	A	403	HIS	3.6
1	B	400	LEU	3.5
1	A	373	ILE	3.4
1	B	385	HIS	3.4
1	A	394	SER	3.2
1	B	507	ASP	2.9
1	B	394	SER	2.9
1	B	373	ILE	2.9
1	B	552	TYR	2.8
1	A	377	GLU	2.8
1	B	463	LEU	2.7
1	B	462	ILE	2.6
1	A	400	LEU	2.6
1	B	464	ALA	2.3
1	B	403	HIS	2.3
1	B	392	MET	2.3
1	A	401	ASN	2.3
1	A	379	PRO	2.2
1	B	377	GLU	2.2
1	B	384	THR	2.1
1	B	386	VAL	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 oligosaccharides 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.