Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:26 AM GMT

PDB ID	:	3P0U
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

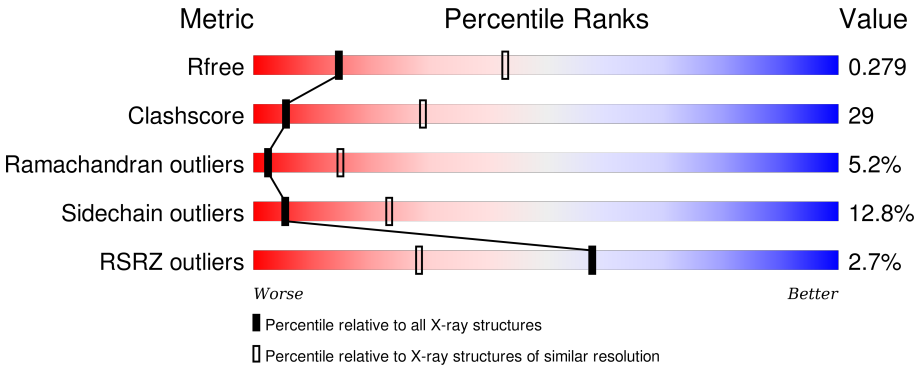
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	249	% 46% 36% 6% 11%
1	B	249	4% 41% 35% 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.

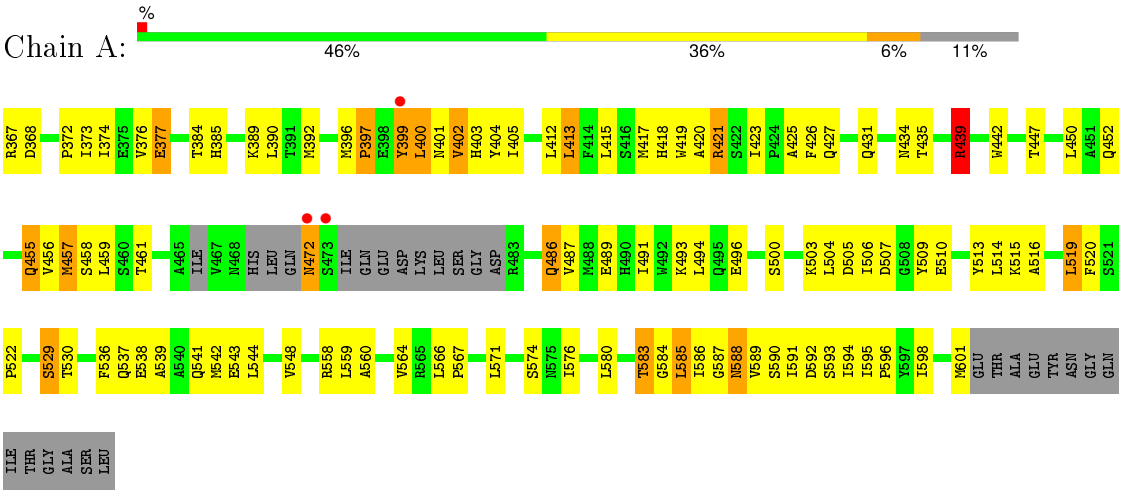
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	42	Total	O	0	0
			42	42		

3 Residue-property plots (i)

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.

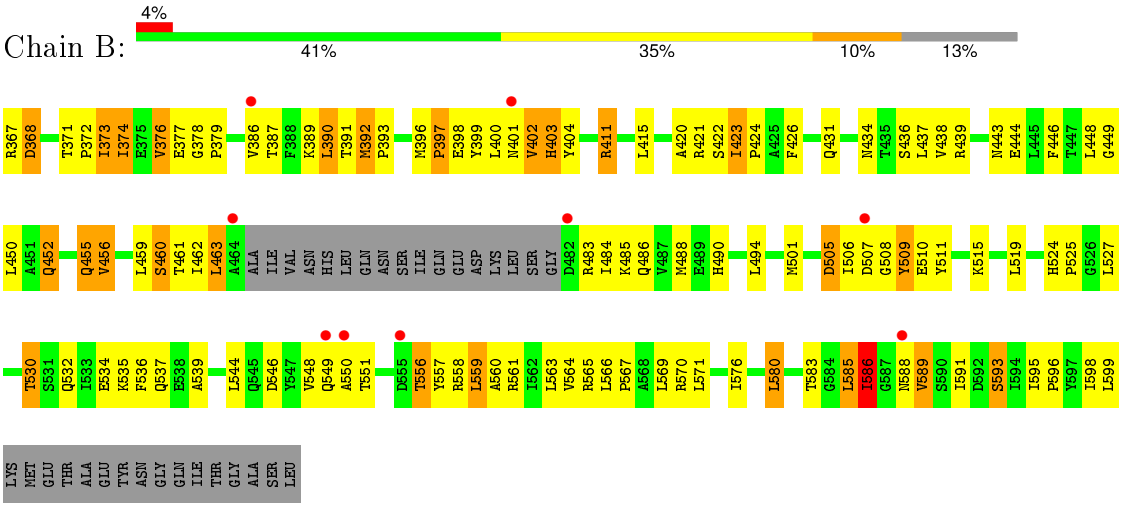
- Molecule 1: Nuclear receptor subfamily 2 group C member 2

Chain A:



- Molecule 1: Nuclear receptor subfamily 2 group C member 2

Chain B:



4 Data and refinement statistics (i)

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 38.65 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-3.00) 98.3 (38.65-2.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.258 , 0.287 0.254 , 0.279	Depositor DCC
R_{free} test set	1228 reflections (7.76%)	DCC
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 , 96.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 17570 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.77	0/1799	0.75	1/2439 (0.0%)
1	B	0.71	0/1758	0.71	0/2388
All	All	0.74	0/3557	0.73	1/4827 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	439	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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	1764	0	1762	107	0
1	B	1721	0	1715	104	0
2	A	31	0	0	6	0
2	B	42	0	0	11	0
All	All	3558	0	3477	205	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 29.

All (205) 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: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:B:450:LEU:HD23	1:B:494:LEU:HD11	1.54	0.89
1:A:455:GLN:HE21	1:A:455:GLN:C	1.75	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:455:GLN:CD	1:A:456:VAL:HG13	1.97	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:B:420:ALA:O	1:B:423:ILE:HG22	1.90	0.72
1:A:542:MET:HG3	1:B:557:TYR:CE2	2.23	0.72
1:A:585:LEU:HD12	1:A:585:LEU:N	2.06	0.71
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: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: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:H	1:B:373:ILE:HD12	1.61	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:593:SER:O	1:B:596:PRO:HD2	2.00	0.61
1:A:503:LYS:HZ1	1:B:367:ARG:HD3	1.64	0.61
1:A:591:ILE:HA	1:A:594:ILE:HD12	1.83	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:A:455:GLN:NE2	1:A:455:GLN:C	2.50	0.59
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:B:374:ILE:CD1	1:B:376:VAL:HG23	2.33	0.58
1:A:530:THR:O	2:A:5:HOH:O	2.16	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: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:A:529:SER:OG	1:A:530:THR:N	2.38	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:B:396:MET:HE3	1:B:397:PRO:HD2	1.87	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:B:389:LYS:C	1:B:390:LEU:HD22	2.25	0.56
1:B:423:ILE:HD13	1:B:423:ILE:C	2.25	0.56
1:A:459:LEU:HB3	1:A:461:THR:CG2	2.36	0.56
1:A:405:ILE:HD12	1:A:459:LEU:HD11	1.88	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
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:B:446:PHE:O	1:B:450:LEU:HB2	2.06	0.55
1:A:389:LYS:HB3	1:A:419:TRP:HE1	1.70	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:A:503:LYS:HZ3	1:B:367:ARG:HB3	1.72	0.54
1:B:437:LEU:CD1	1:B:527:LEU:HD21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:TYR:HB2	1:B:561:ARG:HH21	1.72	0.54
1:B:551:THR:HG22	1:B:551:THR:O	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:A:439:ARG:HD3	1:A:592:ASP:CG	2.28	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:A:455:GLN:HE21	1:A:456:VAL:N	2.08	0.52
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: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: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:B:434:ASN:C	1:B:436:SER:H	2.14	0.50
1:A:588:ASN:OD1	1:A:588:ASN:N	2.45	0.49
1:B:598:ILE:HA	2:B:6:HOH:O	2.11	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:556:THR:HG23	1:B:557:TYR:CD1	2.47	0.49
1:B:400:LEU:HG	1:B:401:ASN:H	1.77	0.49
1:A:459:LEU:N	1:A:459:LEU:HD22	2.28	0.49
1:B:396:MET:SD	1:B:455:GLN:HB3	2.53	0.48
1:A:544:LEU:HD13	1:A:559:LEU:HD21	1.93	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:B:501:MET:HE3	1:B:565:ARG:HB3	1.95	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:A:374:ILE:CD1	1:A:376:VAL:CG1	2.85	0.47
1:B:397:PRO:HG3	1:B:411:ARG:NH2	2.29	0.47
1:A:589:VAL:HG12	1:A:589:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:C	1:B:452:GLN:H	2.17	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: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:A:368:ASP:C	1:A:368:ASP:OD1	2.55	0.46
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:N	1:A:506:ILE:HD12	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:HG22	1:B:506:ILE:O	2.17	0.44
1:B:485:LYS:HG3	1:B:488:MET:HG2	1.99	0.44
1:A:413:LEU:O	1:A:417:MET:HG2	2.18	0.44
1:A:560:ALA:O	1:A:564:VAL:HG23	2.17	0.44
1:A:434:ASN:O	1:A:435:THR:C	2.56	0.44
1:B:563:LEU:O	1:B:566:LEU:CD2	2.66	0.44
1:A:520:PHE:O	1:A:537:GLN:HB2	2.16	0.44
1:B:420:ALA:HB1	1:B:519:LEU:HD21	1.99	0.43
1:B:557:TYR:HB2	1:B:561:ARG:NH2	2.33	0.43
1:B:387:THR:HG22	1:B:387:THR:O	2.18	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:B:546:ASP:O	1:B:550:ALA:HB3	2.19	0.43
1:A:564:VAL:O	1:A:564:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ARG:O	1:B:559:LEU:C	2.57	0.42
1:A:503:LYS:HZ1	1:B:367:ARG:HB3	1.83	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:437:LEU:HD13	1:B:527:LEU:HD21	1.99	0.42
1:B:431:GLN:O	1:B:434:ASN:HB2	2.19	0.42
1:B:392:MET:CE	1:B:415:LEU:HG	2.49	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:459:LEU:HD12	1:A:461:THR:CG2	2.50	0.42
1:A:503:LYS:HZ1	1:B:367:ARG:CD	2.31	0.42
1:B:564:VAL:O	1:B:564:VAL:HG12	2.20	0.42
1:B:544:LEU:O	1:B:548:VAL:HG23	2.19	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:455:GLN:OE1	1:A:456:VAL:HG13	2.18	0.41
1:A:392:MET:SD	1:A:515:LYS:NZ	2.93	0.41
1:B:389:LYS:N	1:B:389:LYS:HD2	2.36	0.41
1:B:367:ARG:HB2	2:B:29:HOH:O	2.20	0.41
1:A:539:ALA:O	1:A:543:GLU:HG3	2.21	0.41
1:A:489:GLU:O	1:A:493:LYS:HG3	2.21	0.41
1:B:463:LEU:HD12	1:B:463:LEU:C	2.40	0.41
1:B:490:HIS:CG	1:B:576:ILE:HG21	2.55	0.41
1:B:434:ASN:O	1:B:438:VAL:HG12	2.21	0.41
1:A:566:LEU:N	1:A:567:PRO:CD	2.84	0.41
1:A:487:VAL:O	1:A:491:ILE:HG13	2.21	0.41
1:A:457:MET:HG3	1:A:457:MET:O	2.21	0.41
1:B:524:HIS:HA	1:B:525:PRO:HD3	1.96	0.40
1:B:459:LEU:HD23	2:B:1:HOH:O	2.21	0.40
1:A:399:TYR:HD1	1:A:400:LEU:H	1.69	0.40
1:A:389:LYS:HE3	1:A:423:ILE:HD13	2.03	0.40
1:B:372:PRO:HD3	1:B:377:GLU:HA	2.03	0.40
1:A:595:ILE:N	1:A:596:PRO:CD	2.85	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%)	4 23
1	B	212/249 (85%)	163 (77%)	35 (16%)	14 (7%)	1 8
All	All	426/498 (86%)	340 (80%)	64 (15%)	22 (5%)	2 15

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	LEU
1	A	401	ASN
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 (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	198/220 (90%)	176 (89%)	22 (11%)	8 29
1	B	193/220 (88%)	165 (86%)	28 (14%)	4 18
All	All	391/440 (89%)	341 (87%)	50 (13%)	5 23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ARG
1	A	377	GLU
1	A	399	TYR
1	A	412	LEU
1	A	413	LEU
1	A	421	ARG
1	A	439	ARG
1	A	455	GLN
1	A	472	ASN
1	A	486	GLN
1	A	496	GLU
1	A	505	ASP
1	A	507	ASP
1	A	514	LEU
1	A	519	LEU
1	A	529	SER
1	A	574	SER
1	A	583	THR
1	A	585	LEU
1	A	588	ASN
1	A	590	SER
1	A	601	MET
1	B	390	LEU
1	B	392	MET
1	B	398	GLU
1	B	399	TYR
1	B	403	HIS

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Mol	Chain	Res	Type
1	B	404	TYR
1	B	411	ARG
1	B	423	ILE
1	B	452	GLN
1	B	455	GLN
1	B	456	VAL
1	B	460	SER
1	B	483	ARG
1	B	484	ILE
1	B	507	ASP
1	B	509	TYR
1	B	530	THR
1	B	537	GLN
1	B	549	GLN
1	B	556	THR
1	B	559	LEU
1	B	570	ARG
1	B	571	LEU
1	B	580	LEU
1	B	585	LEU
1	B	586	ILE
1	B	588	ASN
1	B	599	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	GLN
1	A	434	ASN
1	A	452	GLN
1	A	455	GLN
1	A	541	GLN
1	A	549	GLN
1	A	575	ASN
1	B	427	GLN
1	B	434	ASN
1	B	452	GLN
1	B	499	ASN
1	B	532	GLN
1	B	537	GLN
1	B	545	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 carbohydrates 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, 95^{th} 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%)	-0.37	3 (1%) 78 51	44, 78, 127, 179	0
1	B	216/249 (86%)	-0.27	9 (4%) 40 16	49, 87, 147, 159	0
All	All	438/498 (87%)	-0.32	12 (2%) 58 28	44, 82, 143, 179	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	550	ALA	3.8
1	A	472	ASN	3.7
1	B	401	ASN	3.5
1	A	473	SER	3.4
1	B	588	ASN	3.3
1	B	386	VAL	3.1
1	B	555	ASP	2.9
1	B	464	ALA	2.4
1	B	482	ASP	2.3
1	B	549	GLN	2.2
1	A	399	TYR	2.2
1	B	507	ASP	2.2

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 carbohydrates 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.