Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:22 AM GMT

PDB ID	:	2QH6
Title	:	Crystal Structure of the Estrogen Receptor Alpha Ligand Binding Domain Complexed with an Oxabicyclic diarylethylene Compound
Authors	:	Nettles, K.W.; Bruning, J.B.; Nowak, J.; Sharma, S.K.; Hahm, J.B.; Shi, Y.; Kulp, K.; Hochberg, R.B.; Zhou, H.; Katzenellenbogen, J.A.; Katzenellenbogen, B.S.; Kim, Y.; Joachmiak, A.; Greene, G.L.
Deposited on	:	2007-06-29
Resolution	:	2.70 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:

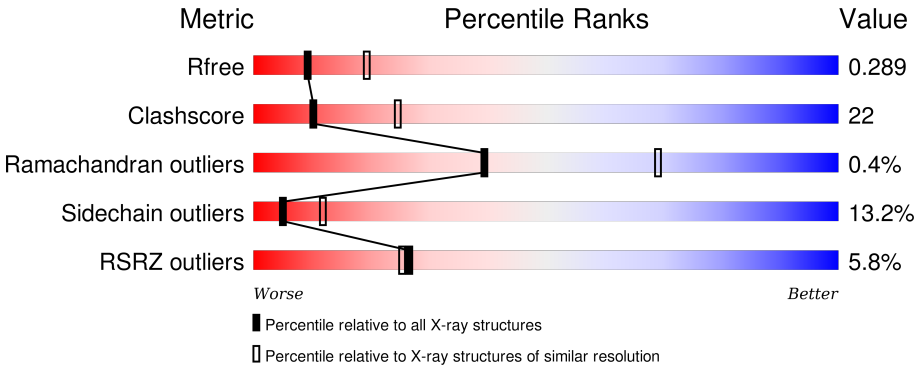
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	258	6% 52% 31% 5% • 10%
1	B	258	4% 54% 28% 7% 12%
2	C	13	8% 38% 31% 8% 23%
2	D	13	15% 38% 23% 15% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ODE	A	700	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3945 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	5	0
			1884	1205	331	329	19			
1	B	228	Total	C	N	O	S	0	2	0
			1818	1165	308	326	19			

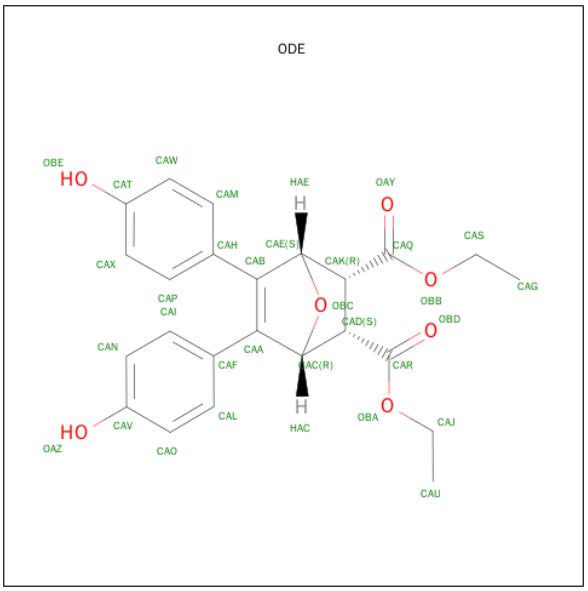
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	SER	-	EXPRESSION TAG	UNP P03372
A	537	SER	TYR	ENGINEERED	UNP P03372
B	297	SER	-	EXPRESSION TAG	UNP P03372
B	537	SER	TYR	ENGINEERED	UNP P03372

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			89	57	19	13			
2	D	10	Total	C	N	O	0	0	0
			89	57	19	13			

- Molecule 3 is DIETHYL (1R,2S,3R,4S)-5,6-BIS(4-HYDROXYPHENYL)-7-OXABICYCLO[2.2.1]HEPT-5-ENE-2,3-DICARBOXYLATE (three-letter code: ODE) (formula: $C_{24}H_{24}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 31 24 7	0	0
3	B	1	Total C O 31 24 7	0	0

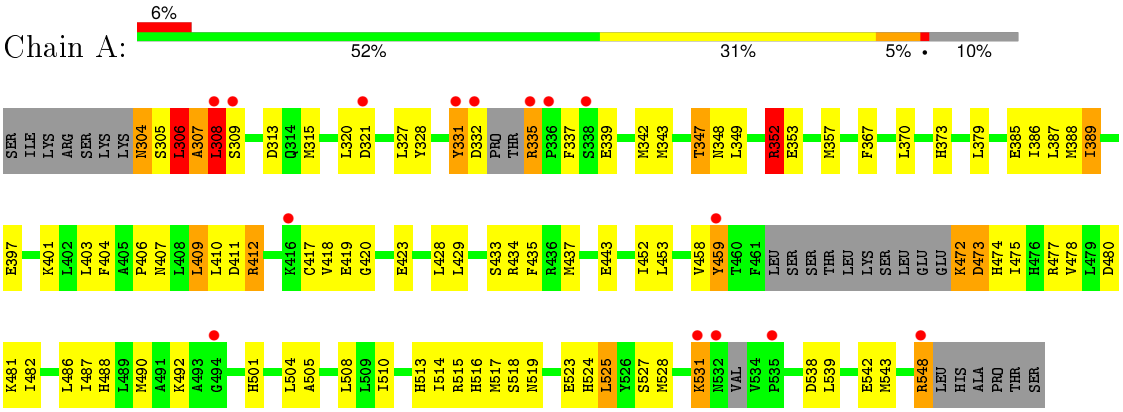
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	2	Total O 2 2	0	0

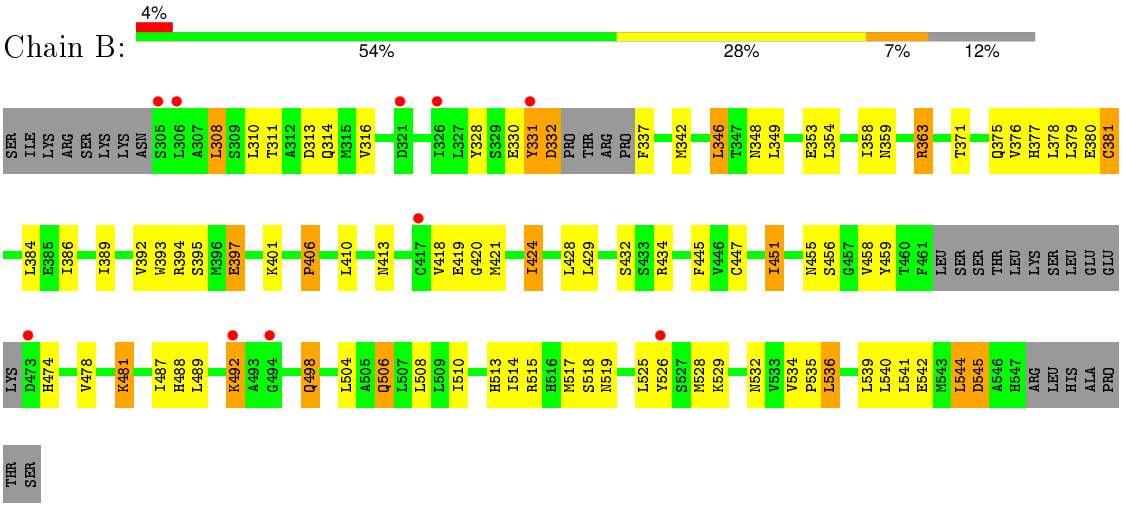
3 Residue-property plots (i)

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.

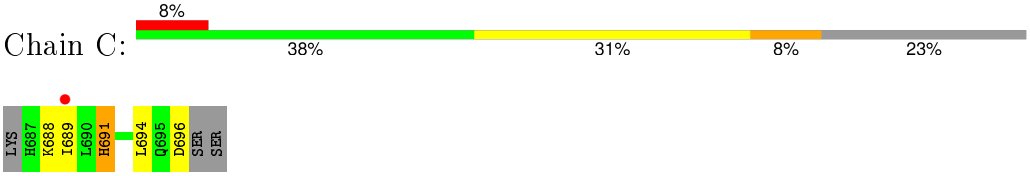
- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor

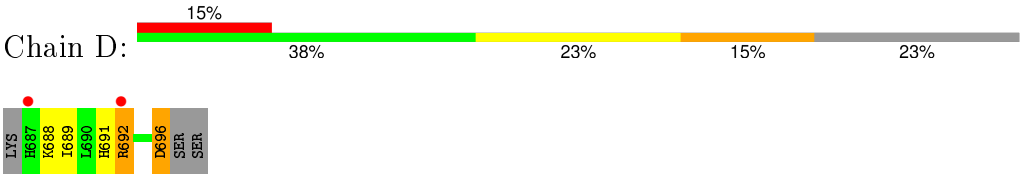


- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.77Å 81.72Å 58.31Å 90.00° 109.90° 90.00°	Depositor
Resolution (Å)	19.73 – 2.70 19.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.73-2.70) 97.7 (19.73-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	4.35 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.291 0.203 , 0.289	Depositor DCC
R_{free} test set	691 reflections (5.49%)	DCC
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.2	EDS
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 13275 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3945	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ODE

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	0.82	0/1940	0.90	6/2615 (0.2%)
1	B	0.84	1/1858 (0.1%)	0.87	1/2508 (0.0%)
2	C	0.75	0/90	0.72	0/119
2	D	0.59	0/90	0.74	0/119
All	All	0.83	1/3978 (0.0%)	0.88	7/5361 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	397	GLU	CB-CG	5.32	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352[A]	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	352[B]	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	352[A]	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	352[B]	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	515	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	B	429	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	A	480	ASP	CB-CG-OD1	5.13	122.92	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	305	SER	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	ASN	Peptide
1	A	306	LEU	Peptide

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	1884	0	1918	94	0
1	B	1818	0	1857	76	0
2	C	89	0	95	4	0
2	D	89	0	95	5	0
3	A	31	0	22	16	0
3	B	31	0	22	7	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
All	All	3945	0	4009	173	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 22.

All (173) 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)
3:A:700:ODE:CAE	3:A:700:ODE:HAG3	1.81	1.11
1:A:305:SER:HB2	1:A:308:LEU:HD11	1.22	1.10
1:A:343:MET:O	1:A:347:THR:HG22	1.53	1.08
3:A:700:ODE:HAG3	3:A:700:ODE:HAE	1.33	1.07
1:A:519:ASN:HD22	1:B:519:ASN:ND2	1.58	1.02
1:A:519:ASN:ND2	1:B:519:ASN:HD22	1.59	1.01
1:B:363:ARG:HG3	1:B:363:ARG:HH21	1.24	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:700:ODE:HAE	3:A:700:ODE:CAG	1.98	0.93
3:A:700:ODE:HAG3	3:A:700:ODE:CAK	2.01	0.90
1:B:342:MET:HE1	1:B:410:LEU:HD11	1.51	0.90
1:A:305:SER:HB2	1:A:308:LEU:CD1	2.01	0.89
1:A:305:SER:OG	1:A:306:LEU:HA	1.76	0.86
1:A:305:SER:CB	1:A:308:LEU:HD11	2.07	0.83
1:B:363:ARG:HG3	1:B:363:ARG:NH2	1.88	0.81
1:A:458:VAL:HG13	1:A:459:TYR:CD2	2.17	0.80
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.65	0.78
1:A:525:LEU:HD13	3:A:700:ODE:HAG1	1.65	0.78
1:A:305:SER:OG	1:A:308:LEU:HD12	1.86	0.76
1:B:342:MET:CE	1:B:410:LEU:HD11	2.14	0.76
1:B:534:VAL:HG22	1:B:535:PRO:HD2	1.66	0.74
1:A:459:TYR:HB2	1:B:513:HIS:CD2	2.22	0.74
1:A:389:ILE:HD13	1:A:452:ILE:HD11	1.71	0.72
1:A:305:SER:CB	1:A:308:LEU:CD1	2.66	0.72
1:A:307:ALA:O	1:A:309:SER:N	2.23	0.71
1:B:420:GLY:O	1:B:424:ILE:HD13	1.94	0.68
1:B:359:ASN:HB3	1:B:363:ARG:HH12	1.59	0.68
1:A:458:VAL:HG13	1:A:459:TYR:HD2	1.58	0.67
1:B:310:LEU:HD22	1:B:314:GLN:HG3	1.76	0.67
2:D:696:ASP:OD2	2:D:696:ASP:N	2.24	0.66
1:A:513[A]:HIS:CE1	1:B:459:TYR:CD1	2.84	0.66
1:A:538:ASP:O	1:A:542:GLU:HG3	1.95	0.65
2:D:689:ILE:HA	2:D:692:ARG:HG3	1.78	0.65
1:B:363:ARG:CG	1:B:363:ARG:HH21	2.04	0.65
3:A:700:ODE:HAG3	3:A:700:ODE:HAK	1.78	0.64
1:B:487:ILE:HD11	1:B:504:LEU:HD22	1.80	0.64
1:B:349:LEU:O	1:B:353:GLU:HG3	1.97	0.64
1:B:358:ILE:HD12	1:B:379:LEU:HD13	1.80	0.64
1:B:359:ASN:HB3	1:B:363:ARG:NH1	2.14	0.62
1:B:342:MET:HE3	1:B:346:LEU:CD2	2.29	0.62
1:B:332:ASP:N	1:B:332:ASP:OD1	2.32	0.62
1:A:514:ILE:HD13	1:A:517:MET:CE	2.30	0.62
1:A:331:TYR:CD2	1:A:337:PHE:HZ	2.18	0.62
1:A:331:TYR:CE1	1:A:407:ASN:O	2.53	0.62
1:A:343:MET:O	1:A:347:THR:CG2	2.40	0.62
1:A:343:MET:HE1	3:A:700:ODE:HAS1	1.81	0.60
3:A:700:ODE:CAG	3:A:700:ODE:CAK	2.78	0.60
1:B:421:MET:HG3	3:B:800:ODE:HAU2	1.84	0.60
1:A:339:GLU:HG3	1:A:418:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ALA:C	1:A:309:SER:H	2.05	0.60
1:B:447:CYS:O	1:B:451:ILE:HG12	2.02	0.59
1:A:420:GLY:HA2	1:A:423:GLU:OE2	2.01	0.59
1:A:305:SER:OG	1:A:306:LEU:CA	2.51	0.59
1:A:331:TYR:HD2	1:A:337:PHE:HZ	1.51	0.59
1:B:514:ILE:HA	1:B:517:MET:HE3	1.85	0.58
1:A:473:ASP:O	1:A:477:ARG:HG3	2.03	0.58
1:B:384:LEU:HD11	3:B:800:ODE:OBC	2.04	0.58
1:B:354:LEU:O	1:B:358:ILE:HG12	2.02	0.58
1:A:404:PHE:CE2	1:A:410:LEU:HD22	2.38	0.58
1:A:487:ILE:HD11	1:A:504:LEU:HD22	1.87	0.57
1:B:474:HIS:O	1:B:478:VAL:HG23	2.03	0.57
1:B:342:MET:HE3	1:B:346:LEU:HD22	1.87	0.57
3:B:800:ODE:OAY	3:B:800:ODE:HAG2	2.05	0.57
1:A:539:LEU:HA	2:C:689:ILE:HG21	1.87	0.57
1:A:505:ALA:HA	1:B:508:LEU:CD1	2.34	0.56
1:A:388:MET:HG2	1:A:428:LEU:HD21	1.87	0.56
3:A:700:ODE:CAR	3:A:700:ODE:OAY	2.54	0.56
1:A:401:LYS:HB3	1:A:409:LEU:HD23	1.90	0.54
1:B:310:LEU:HA	1:B:314:GLN:HE21	1.72	0.54
1:B:371:THR:O	1:B:375:GLN:HG3	2.08	0.53
1:B:342:MET:CE	1:B:410:LEU:CD1	2.85	0.53
1:A:305:SER:OG	1:A:308:LEU:CD1	2.55	0.53
1:A:459:TYR:CD2	1:B:513:HIS:CE1	2.96	0.52
1:A:488:HIS:CE1	1:A:492:LYS:HD2	2.45	0.52
1:A:523:GLU:HG3	1:A:524[B]:HIS:HD2	1.75	0.52
1:A:524[A]:HIS:ND1	3:A:700:ODE:HAS2	2.25	0.51
1:A:304:ASN:O	1:A:305:SER:HB2	2.11	0.51
1:B:395[B]:SER:OG	1:B:401:LYS:O	2.28	0.51
3:B:800:ODE:CAG	3:B:800:ODE:OAY	2.59	0.50
1:A:331:TYR:CD1	1:A:407:ASN:O	2.65	0.50
1:B:428:LEU:HD23	1:B:517:MET:SD	2.51	0.50
1:B:456:SER:HA	1:B:515:ARG:NH2	2.26	0.50
1:A:435:PHE:HE1	1:A:510:ILE:HD13	1.77	0.49
1:A:304:ASN:O	1:A:305:SER:CB	2.60	0.49
1:A:418:VAL:CG1	1:A:524[A]:HIS:HE1	2.25	0.49
1:A:385:GLU:HG2	1:A:514:ILE:HG22	1.95	0.48
1:A:403:LEU:HD23	1:A:403:LEU:O	2.13	0.48
3:A:700:ODE:HAL	3:A:700:ODE:CAH	2.44	0.48
1:A:418:VAL:HG12	1:A:524[A]:HIS:CE1	2.48	0.48
1:B:331:TYR:CE2	1:B:337:PHE:HE2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ILE:HD12	1:B:424:ILE:N	2.29	0.48
1:B:455:ASN:O	1:B:458:VAL:HG12	2.14	0.48
1:B:424:ILE:N	1:B:424:ILE:CD1	2.77	0.47
1:B:542:GLU:OE2	2:D:689:ILE:HD12	2.14	0.47
1:A:459:TYR:CE1	1:B:510:ILE:HG12	2.50	0.47
1:A:434:ARG:NE	1:B:459:TYR:OH	2.46	0.47
1:A:459:TYR:CD2	1:B:513:HIS:NE2	2.82	0.47
1:A:458:VAL:HG13	1:A:459:TYR:CE2	2.50	0.47
2:C:688:LYS:O	2:C:691:HIS:HB2	2.15	0.47
1:A:474:HIS:O	1:A:478:VAL:HG23	2.15	0.46
1:B:392:VAL:HG13	1:B:432:SER:HA	1.96	0.46
1:A:519:ASN:HD22	1:B:519:ASN:HD22	0.74	0.46
1:A:352[A]:ARG:HG2	1:A:352[A]:ARG:HH11	1.80	0.46
1:B:525:LEU:HD13	3:B:800:ODE:HAE	1.98	0.46
1:A:305:SER:CB	1:A:308:LEU:HD12	2.42	0.46
1:A:348:ASN:OD1	1:A:352[B]:ARG:NH1	2.49	0.46
1:A:459:TYR:CE1	1:B:434:ARG:HG2	2.51	0.45
1:A:328:TYR:CE1	1:A:406:PRO:HB2	2.51	0.45
1:A:434:ARG:NH1	1:A:437:MET:SD	2.87	0.45
1:A:513[A]:HIS:CE1	1:B:459:TYR:CE1	3.04	0.45
1:A:548:ARG:C	1:A:548:ARG:HD3	2.36	0.45
1:A:353:GLU:OE1	3:A:700:ODE:OAZ	2.35	0.45
1:B:377:HIS:O	1:B:381:CYS:HB2	2.17	0.45
1:A:516:HIS:HA	1:B:519:ASN:HD21	1.82	0.44
3:B:800:ODE:CAA	3:B:800:ODE:OBD	2.65	0.44
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.98	0.44
1:A:434:ARG:HA	1:A:437:MET:HG2	1.99	0.44
1:A:459:TYR:HE1	1:B:434:ARG:HG2	1.83	0.44
1:A:357:MET:HE1	1:A:387:LEU:HG	1.99	0.44
1:B:394:ARG:HH11	1:B:394:ARG:HG3	1.83	0.44
1:A:332:ASP:HB3	1:A:335:ARG:HB2	2.00	0.44
1:B:506:GLN:HE21	1:B:506:GLN:HB3	1.63	0.44
1:A:349:LEU:O	1:A:353:GLU:HG3	2.18	0.43
1:A:418:VAL:HG12	1:A:524[A]:HIS:HE1	1.83	0.43
1:B:376:VAL:O	1:B:380:GLU:HG2	2.18	0.43
1:B:534:VAL:HG22	1:B:535:PRO:CD	2.41	0.43
1:B:331:TYR:CE2	1:B:337:PHE:CE2	3.07	0.43
2:D:689:ILE:HD12	2:D:689:ILE:H	1.84	0.43
1:A:411:ASP:O	1:A:412:ARG:C	2.56	0.43
1:A:523:GLU:CG	1:A:524[B]:HIS:HD2	2.30	0.43
1:A:342:MET:HE3	1:A:417:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:HD13	3:A:700:ODE:CAG	2.42	0.42
1:B:392:VAL:HG13	1:B:432:SER:CA	2.49	0.42
1:B:330:GLU:OE1	1:B:348:ASN:ND2	2.52	0.42
1:B:541:LEU:O	1:B:545:ASP:HB3	2.18	0.42
1:B:386:ILE:HA	1:B:389:ILE:HG22	2.01	0.42
1:B:358:ILE:CD1	1:B:379:LEU:HD13	2.49	0.42
1:B:393:TRP:HB2	1:B:445:PHE:CE2	2.54	0.42
1:A:539:LEU:O	1:A:543:MET:HG2	2.19	0.42
1:A:401:LYS:HB3	1:A:409:LEU:CD2	2.49	0.42
1:A:327:LEU:HD22	1:A:352[A]:ARG:NH2	2.34	0.42
1:B:418:VAL:O	1:B:419:GLU:C	2.57	0.42
1:B:498:GLN:HB2	1:B:498:GLN:HE21	1.66	0.42
1:A:435:PHE:CE1	1:A:510:ILE:HD13	2.54	0.42
1:B:526:TYR:HD2	1:B:544:LEU:HD13	1.84	0.42
1:A:367:PHE:CE1	1:A:453:LEU:HD11	2.54	0.42
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.70	0.42
1:B:328:TYR:CE2	1:B:406:PRO:HB2	2.55	0.42
1:A:472:LYS:HG2	1:A:473:ASP:N	2.33	0.42
1:B:492:LYS:HA	1:B:492:LYS:HD2	1.74	0.42
1:B:536:LEU:HD12	1:B:536:LEU:HA	1.90	0.42
1:A:486:LEU:HD22	1:A:490:MET:HE3	2.02	0.41
1:A:434:ARG:HG2	1:B:459:TYR:CZ	2.54	0.41
1:B:311:THR:H	1:B:314:GLN:NE2	2.18	0.41
1:A:386:ILE:O	1:A:389:ILE:HG22	2.20	0.41
1:A:524[A]:HIS:ND1	3:A:700:ODE:CAS	2.84	0.41
3:B:800:ODE:OAY	3:B:800:ODE:CAR	2.66	0.41
1:A:379:LEU:HD12	2:C:694:LEU:HD11	2.03	0.41
1:A:352[A]:ARG:HG2	1:A:352[A]:ARG:NH1	2.35	0.41
1:A:528:MET:CE	1:A:531:LYS:HD2	2.50	0.41
1:A:478:VAL:O	1:A:482:ILE:HG13	2.20	0.41
1:B:342:MET:HE2	1:B:410:LEU:CD1	2.51	0.41
1:A:459:TYR:OH	1:B:510:ILE:HG13	2.21	0.41
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.89	0.41
1:B:541:LEU:HD23	1:B:541:LEU:HA	1.91	0.41
1:A:320:LEU:HD11	1:A:443:GLU:HG3	2.03	0.41
1:A:477:ARG:NH2	1:A:477:ARG:HG2	2.36	0.40
1:A:342:MET:CE	1:A:417:CYS:HB2	2.51	0.40
1:B:308:LEU:O	1:B:481:LYS:HD2	2.20	0.40
3:A:700:ODE:CAA	3:A:700:ODE:OBD	2.68	0.40
1:B:534:VAL:CG2	1:B:535:PRO:HD2	2.44	0.40
3:A:700:ODE:HAE	3:A:700:ODE:CAS	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LEU:HA	2:C:689:ILE:CG2	2.49	0.40
2:D:688:LYS:HG2	2:D:691:HIS:ND1	2.36	0.40

There are no symmetry-related clashes.

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	229/258 (89%)	219 (96%)	8 (4%)	2 (1%)	21 49
1	B	224/258 (87%)	210 (94%)	14 (6%)	0	100 100
2	C	8/13 (62%)	8 (100%)	0	0	100 100
2	D	8/13 (62%)	8 (100%)	0	0	100 100
All	All	469/542 (86%)	445 (95%)	22 (5%)	2 (0%)	39 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ALA
1	A	308	LEU

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	213/233 (91%)	183 (86%)	30 (14%)	4 10
1	B	206/233 (88%)	180 (87%)	26 (13%)	5 13
2	C	10/13 (77%)	8 (80%)	2 (20%)	1 4
2	D	10/13 (77%)	8 (80%)	2 (20%)	1 4
All	All	439/492 (89%)	379 (86%)	60 (14%)	5 11

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	308	LEU
1	A	313	ASP
1	A	315	MET
1	A	321	ASP
1	A	331	TYR
1	A	335	ARG
1	A	347	THR
1	A	352[A]	ARG
1	A	352[B]	ARG
1	A	373[A]	HIS
1	A	373[B]	HIS
1	A	389	ILE
1	A	397	GLU
1	A	409	LEU
1	A	412	ARG
1	A	419	GLU
1	A	433	SER
1	A	459	TYR
1	A	472	LYS
1	A	473	ASP
1	A	481	LYS
1	A	501[A]	HIS
1	A	501[B]	HIS
1	A	508	LEU
1	A	518	SER
1	A	525	LEU
1	A	527	SER
1	A	531	LYS
1	A	548	ARG
1	B	308	LEU
1	B	313	ASP
1	B	331	TYR

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Mol	Chain	Res	Type
1	B	332	ASP
1	B	346	LEU
1	B	363	ARG
1	B	381	CYS
1	B	397	GLU
1	B	406	PRO
1	B	413	ASN
1	B	424	ILE
1	B	451	ILE
1	B	481	LYS
1	B	488	HIS
1	B	492	LYS
1	B	498	GLN
1	B	506	GLN
1	B	518	SER
1	B	528	MET
1	B	529	LYS
1	B	532	ASN
1	B	536	LEU
1	B	539	LEU
1	B	540	LEU
1	B	544	LEU
1	B	545	ASP
2	C	691	HIS
2	C	696	ASP
2	D	692	ARG
2	D	696	ASP

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

Mol	Chain	Res	Type
1	A	314	GLN
1	A	488	HIS
1	B	314	GLN
1	B	377	HIS
1	B	414	GLN
1	B	488	HIS
1	B	498	GLN
1	B	506	GLN
1	B	513	HIS
1	B	519	ASN
1	B	547	HIS

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Mol	Chain	Res	Type
2	C	691	HIS
2	D	687	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	ODE	A	700	-	34,34,34	1.99	9 (26%)	37,49,49	2.87	11 (29%)
3	ODE	B	800	-	34,34,34	1.91	9 (26%)	37,49,49	2.44	12 (32%)

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	ODE	A	700	-	-	0/22/50/50	0/2/4/4
3	ODE	B	800	-	-	0/22/50/50	0/2/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	ODE	CAF-CAA	-4.69	1.38	1.48
3	A	700	ODE	CAH-CAB	-4.28	1.39	1.48
3	B	800	ODE	CAH-CAB	-3.87	1.40	1.48
3	A	700	ODE	CAF-CAA	-3.82	1.40	1.48
3	B	800	ODE	OBA-CAJ	-3.05	1.36	1.46
3	B	800	ODE	CAD-CAR	-2.79	1.46	1.51
3	A	700	ODE	CAD-CAR	-2.55	1.47	1.51
3	A	700	ODE	CAK-CAE	2.11	1.58	1.54
3	B	800	ODE	CAB-CAA	2.24	1.39	1.34
3	A	700	ODE	CAB-CAA	2.45	1.40	1.34
3	A	700	ODE	OBB-CAQ	2.60	1.38	1.33
3	B	800	ODE	OBB-CAQ	3.15	1.40	1.33
3	B	800	ODE	CAE-CAB	3.18	1.55	1.51
3	B	800	ODE	OBC-CAC	3.54	1.48	1.43
3	A	700	ODE	CAK-CAQ	4.30	1.58	1.51
3	A	700	ODE	CAE-CAB	4.34	1.57	1.51
3	B	800	ODE	CAK-CAQ	4.35	1.58	1.51
3	A	700	ODE	OBC-CAC	4.36	1.49	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	700	ODE	OBB-CAQ-OAY	-5.46	112.92	124.05
3	A	700	ODE	OBA-CAJ-CAU	-4.74	90.61	108.42
3	A	700	ODE	OBD-CAR-CAD	-4.34	117.35	125.03
3	B	800	ODE	OBA-CAJ-CAU	-4.04	93.25	108.42
3	A	700	ODE	OBC-CAE-CAK	-4.02	91.28	103.08
3	B	800	ODE	CAI-CAF-CAA	-3.83	115.85	120.90
3	B	800	ODE	OBC-CAE-CAK	-3.82	91.87	103.08
3	B	800	ODE	OBD-CAR-CAD	-3.69	118.49	125.03
3	B	800	ODE	CAK-CAD-CAR	-3.51	106.22	114.66
3	B	800	ODE	CAP-CAH-CAB	-3.14	116.76	120.90
3	A	700	ODE	CAP-CAH-CAB	-3.07	116.85	120.90
3	B	800	ODE	OAY-CAQ-CAK	-2.63	120.37	125.03
3	A	700	ODE	CAK-CAD-CAR	-2.55	108.54	114.66
3	A	700	ODE	OAY-CAQ-CAK	-2.53	120.55	125.03
3	B	800	ODE	CAW-CAM-CAH	-2.47	117.90	120.76
3	A	700	ODE	CAI-CAN-CAV	-2.38	117.12	119.87
3	B	800	ODE	CAJ-OBA-CAR	-2.16	111.32	116.68
3	A	700	ODE	CAM-CAH-CAB	2.19	123.78	120.90
3	B	800	ODE	CAL-CAF-CAA	3.13	125.02	120.90
3	A	700	ODE	OBA-CAR-CAD	6.14	119.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	800	ODE	OBB-CAQ-CAK	6.16	119.39	111.07
3	B	800	ODE	OBA-CAR-CAD	6.59	119.97	111.07
3	A	700	ODE	OBB-CAQ-CAK	11.37	126.43	111.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	ODE	16	0
3	B	800	ODE	7	0

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

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	232/258 (89%)	0.08	15 (6%)	22	20	2, 14, 46, 60	0
1	B	228/258 (88%)	-0.02	10 (4%)	38	37	2, 13, 38, 51	1 (0%)
2	C	10/13 (76%)	1.11	1 (10%)	9	7	24, 30, 37, 40	0
2	D	10/13 (76%)	0.60	2 (20%)	1	1	21, 30, 38, 39	0
All	All	480/542 (88%)	0.06	28 (5%)	26	25	2, 13, 44, 60	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	LEU	9.0
1	A	531	LYS	6.2
1	A	331	TYR	4.0
1	A	532	ASN	3.9
1	A	548	ARG	3.6
1	B	331	TYR	3.1
2	D	687	HIS	3.0
1	A	416	LYS	2.9
1	A	332	ASP	2.8
1	B	305	SER	2.4
1	B	492	LYS	2.4
1	B	526	TYR	2.3
1	A	309	SER	2.3
1	A	494	GLY	2.3
1	A	308	LEU	2.3
2	D	692	ARG	2.3
1	B	494	GLY	2.2
1	B	321	ASP	2.1
1	B	417	CYS	2.1
1	B	473	ASP	2.1
1	A	535	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	ASP	2.1
1	B	326	ILE	2.1
1	A	335	ARG	2.1
1	A	338	SER	2.1
1	A	459	TYR	2.0
1	A	336	PRO	2.0
2	C	689	ILE	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, 95^{th} 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
3	ODE	A	700	31/31	0.90	0.19	0.49	12,32,40,43	0
3	ODE	B	800	31/31	0.91	0.17	0.21	10,25,39,42	0

6.5 Other polymers (i)

There are no such residues in this entry.