Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:04 PM GMT

PDB ID	:	4QUV
Title	:	Structure of an integral membrane delta(14)-sterol reductase
Authors	:	Li, X.; Blobel, G.
Deposited on	:	2014-07-12
Resolution	:	2.74 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:

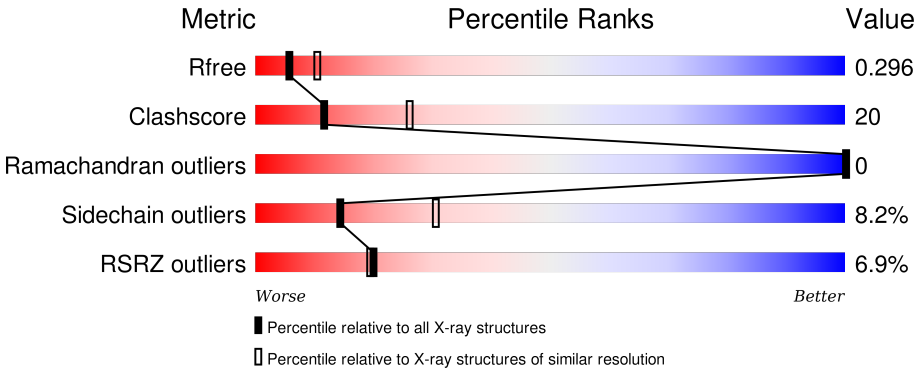
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	427	7% 61% 29% • 8%
1	B	427	5% 57% 30% • 9%

2 Entry composition (i)

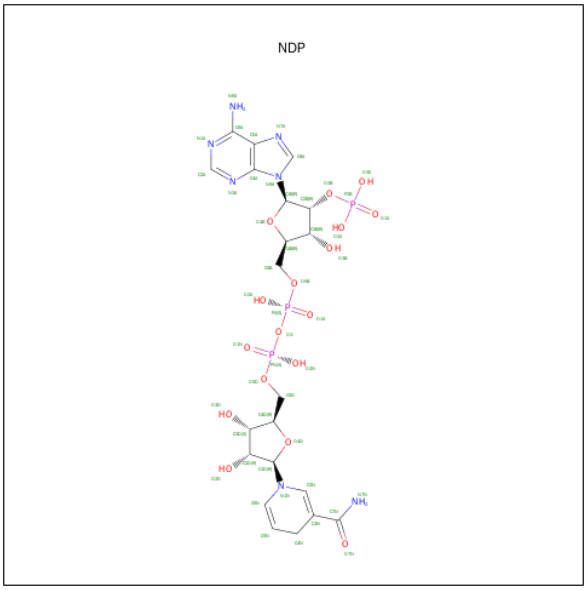
There are 2 unique types of molecules in this entry. The entry contains 6490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Delta(14)-sterol reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3235	2181	520	516	18			
1	B	389	Total	C	N	O	S	0	0	0
			3193	2149	515	511	18			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



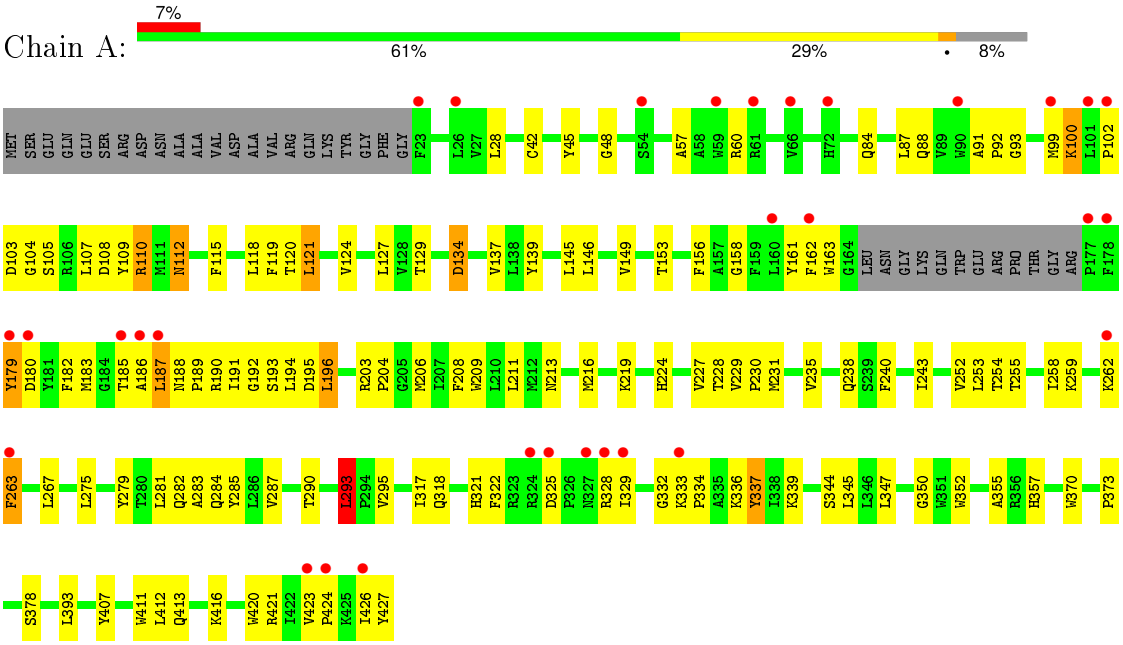
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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.

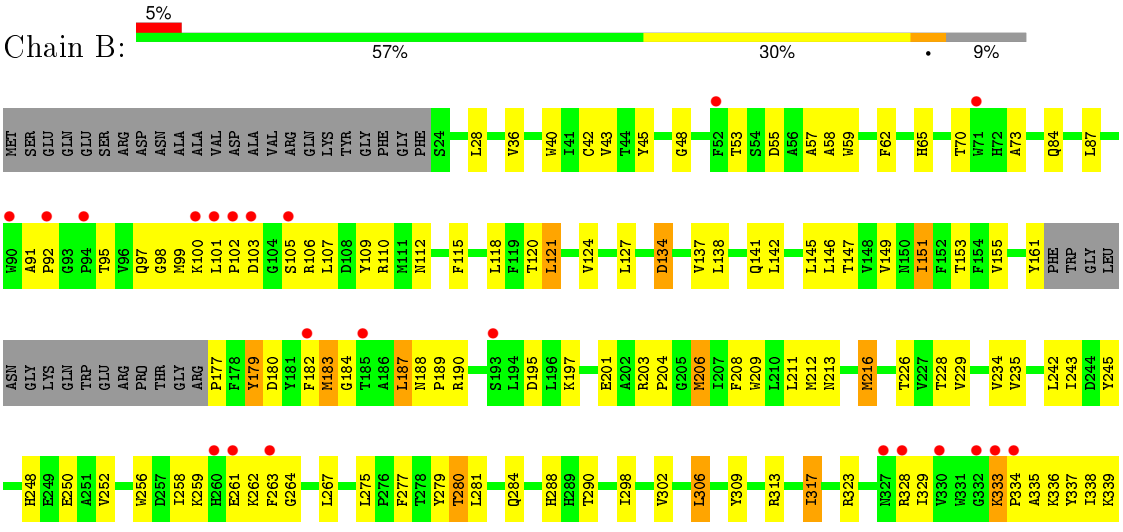
- Molecule 1: Delta(14)-sterol reductase

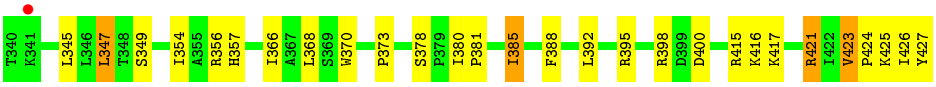
Chain A:



- Molecule 1: Delta(14)-sterol reductase

Chain B:




T340
K341
L345
L346
L347
T348
S349
I354
A355
R356
H357
I366
A367
L368
S369
W370
P373
S378
P379
I380
P381
I385
F388
L392
R395
R398
D399
D400
R415
K416
K417
R421
T422
V423
P424
K425
I426
Y427

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.66Å 74.61Å 79.55Å 66.00° 90.37° 86.86°	Depositor
Resolution (Å)	37.26 – 2.74 37.26 – 2.74	Depositor EDS
% Data completeness (in resolution range)	74.5 (37.26-2.74) 73.9 (37.26-2.74)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.233 , 0.284 0.248 , 0.296	Depositor DCC
R_{free} test set	1523 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 30554 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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: NDP

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	0.47	0/3360	0.66	1/4590 (0.0%)
1	B	0.51	0/3314	0.72	1/4527 (0.0%)
All	All	0.49	0/6674	0.69	2/9117 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	293	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	423	VAL	C-N-CD	5.89	140.77	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3235	0	3203	149	0
1	B	3193	0	3168	116	0
2	A	31	0	11	2	0
2	B	31	0	11	1	0
All	All	6490	0	6393	261	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 20.

All (261) 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:158:GLY:O	1:A:162:PHE:CD2	1.93	1.21
1:A:190:ARG:NH1	1:A:195:ASP:HB2	1.54	1.21
1:A:190:ARG:CZ	1:A:195:ASP:HB2	1.73	1.17
1:A:107:LEU:HD21	1:A:190:ARG:NH2	1.61	1.15
1:A:107:LEU:HD11	1:A:190:ARG:HE	1.13	1.03
1:A:107:LEU:CD2	1:A:190:ARG:NH2	2.25	0.99
1:A:333:LYS:HE2	1:A:336:LYS:HZ3	1.30	0.95
1:B:333:LYS:CG	1:B:334:PRO:HD2	1.97	0.94
1:A:103:ASP:HB3	1:A:105:SER:CB	1.99	0.93
1:A:104:GLY:N	1:A:105:SER:HB3	1.85	0.92
1:A:118:LEU:HD13	1:B:121:LEU:HB3	1.52	0.91
1:A:187:LEU:O	1:A:189:PRO:HD3	1.69	0.91
1:A:158:GLY:O	1:A:162:PHE:HD2	1.41	0.91
1:A:420:TRP:CB	1:A:424:PRO:HB2	1.99	0.90
1:B:188:ASN:OD1	1:B:197:LYS:CD	2.20	0.90
1:A:333:LYS:CE	1:A:336:LYS:HZ3	1.87	0.88
1:A:107:LEU:CD2	1:A:190:ARG:HH21	1.86	0.88
1:A:91:ALA:HB1	1:A:112:ASN:HB3	1.56	0.88
1:A:420:TRP:CD2	1:A:424:PRO:O	2.28	0.86
1:A:57:ALA:HA	1:A:60:ARG:HD3	1.58	0.85
1:A:206:MET:HG3	1:A:275:LEU:HD21	1.59	0.84
1:A:190:ARG:NH1	1:A:195:ASP:CB	2.41	0.83
1:A:333:LYS:HE2	1:A:336:LYS:NZ	1.92	0.82
1:A:107:LEU:HD11	1:A:190:ARG:NE	1.95	0.82
1:B:333:LYS:CD	1:B:334:PRO:HD2	2.10	0.81
1:B:187:LEU:O	1:B:189:PRO:HD3	1.79	0.81
1:A:192:GLY:O	1:A:193:SER:OG	1.99	0.80
1:B:188:ASN:OD1	1:B:197:LYS:HD3	1.79	0.80
1:B:328:ARG:O	1:B:335:ALA:N	2.14	0.80
1:A:355:ALA:HB2	1:A:424:PRO:HB3	1.62	0.79
1:B:99:MET:HG3	1:B:259:LYS:HD3	1.65	0.78
1:B:92:PRO:O	1:B:112:ASN:ND2	2.16	0.78
1:B:188:ASN:OD1	1:B:197:LYS:HD2	1.81	0.78
1:A:420:TRP:HB2	1:A:424:PRO:HB2	1.64	0.77
1:A:107:LEU:HD22	1:A:109:TYR:CZ	2.21	0.76
1:A:333:LYS:HG2	1:A:334:PRO:HD2	1.67	0.75
1:A:103:ASP:HB3	1:A:105:SER:HB3	1.66	0.75
1:A:321:HIS:NE2	1:B:226:THR:HG22	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:OD2	1:A:105:SER:HB2	1.87	0.74
1:B:333:LYS:HD3	1:B:334:PRO:HD2	1.68	0.74
1:A:84:GLN:HE21	1:A:203:ARG:HB3	1.53	0.73
1:A:420:TRP:CB	1:A:424:PRO:CB	2.67	0.72
1:A:91:ALA:O	1:A:110:ARG:CZ	2.37	0.72
1:A:107:LEU:HD21	1:A:190:ARG:CZ	2.20	0.71
1:A:107:LEU:HD22	1:A:109:TYR:CE2	2.25	0.71
1:A:190:ARG:NH2	1:A:195:ASP:HB2	2.04	0.71
1:A:355:ALA:HB2	1:A:424:PRO:CB	2.19	0.71
1:A:337:TYR:HD1	1:A:337:TYR:H	1.39	0.70
1:B:55:ASP:O	1:B:57:ALA:N	2.20	0.70
1:A:355:ALA:HB2	1:A:424:PRO:HG3	1.73	0.70
1:A:333:LYS:CD	1:A:336:LYS:NZ	2.55	0.70
1:A:190:ARG:HH12	1:A:195:ASP:HB2	1.52	0.69
1:B:28:LEU:HD23	1:B:182:PHE:HZ	1.57	0.69
1:A:329:ILE:HG22	1:A:332:GLY:O	1.93	0.69
1:A:423:VAL:HG23	1:A:427:TYR:C	2.12	0.69
1:A:337:TYR:CD2	1:A:345:LEU:HD22	2.28	0.69
1:A:103:ASP:HB3	1:A:105:SER:HB2	1.75	0.68
1:B:333:LYS:HG2	1:B:334:PRO:HD2	1.75	0.68
1:A:99:MET:HG3	1:A:259:LYS:HG2	1.76	0.67
1:B:180:ASP:O	1:B:184:GLY:N	2.28	0.67
1:A:355:ALA:CB	1:A:424:PRO:HB3	2.25	0.67
1:B:99:MET:CE	1:B:259:LYS:HD3	2.24	0.66
1:B:336:LYS:HB2	1:B:349:SER:HB3	1.77	0.66
1:B:333:LYS:CB	1:B:334:PRO:HD2	2.26	0.66
1:A:91:ALA:HB1	1:A:112:ASN:CB	2.25	0.66
1:A:149:VAL:O	1:A:153:THR:HG23	1.96	0.65
1:A:355:ALA:HB2	1:A:424:PRO:CG	2.26	0.65
1:A:333:LYS:CD	1:A:336:LYS:HZ3	2.10	0.65
1:B:187:LEU:HD22	1:B:262:LYS:HG2	1.80	0.65
1:A:420:TRP:HB3	1:A:424:PRO:CB	2.27	0.64
1:A:206:MET:O	1:A:209:TRP:HB3	1.98	0.64
1:B:99:MET:HG3	1:B:259:LYS:CD	2.28	0.64
1:B:99:MET:HE2	1:B:259:LYS:HD3	1.79	0.63
1:A:420:TRP:CG	1:A:424:PRO:O	2.50	0.63
1:A:158:GLY:C	1:A:162:PHE:CD2	2.71	0.63
1:A:423:VAL:HG11	1:A:426:ILE:HB	1.80	0.63
1:B:213:ASN:HB3	1:B:235:VAL:HG22	1.80	0.63
1:A:158:GLY:O	1:A:162:PHE:CE2	2.50	0.62
1:A:216:MET:SD	1:A:284:GLN:HG3	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:MET:HA	1:B:264:GLY:HA3	1.80	0.62
1:B:101:LEU:N	1:B:102:PRO:HD2	2.14	0.61
1:A:107:LEU:HD23	1:A:108:ASP:O	2.00	0.61
1:A:420:TRP:CE3	1:A:424:PRO:O	2.54	0.61
1:B:252:VAL:O	1:B:258:ILE:HG13	2.00	0.61
1:A:91:ALA:O	1:A:110:ARG:NE	2.33	0.61
1:A:104:GLY:H	1:A:105:SER:HB3	1.64	0.60
1:A:158:GLY:C	1:A:162:PHE:HD2	2.04	0.60
1:B:425:LYS:HB3	1:B:426:ILE:HD12	1.84	0.60
1:B:58:ALA:O	1:B:62:PHE:N	2.32	0.60
1:A:121:LEU:HB3	1:B:118:LEU:HD13	1.84	0.59
1:A:107:LEU:HD22	1:A:190:ARG:HH21	1.66	0.58
1:B:395:ARG:HG3	1:B:398:ARG:HH22	1.67	0.58
1:B:112:ASN:OD1	1:B:115:PHE:HB3	2.03	0.58
1:B:206:MET:HG3	1:B:275:LEU:HD21	1.85	0.58
1:B:149:VAL:O	1:B:153:THR:HG23	2.04	0.58
1:A:139:TYR:HD2	1:A:216:MET:HG2	1.70	0.57
1:A:420:TRP:CG	1:A:424:PRO:HB2	2.40	0.57
1:B:161:TYR:HE1	1:B:180:ASP:HB2	1.68	0.57
1:A:337:TYR:N	1:A:337:TYR:CD1	2.72	0.57
1:A:161:TYR:HE1	1:A:180:ASP:HB2	1.68	0.57
1:A:93:GLY:N	1:A:112:ASN:OD1	2.28	0.57
1:A:99:MET:CE	1:A:259:LYS:HD3	2.35	0.56
1:B:216:MET:SD	1:B:284:GLN:HG3	2.45	0.56
1:A:107:LEU:HD22	1:A:190:ARG:NH2	2.17	0.56
1:A:423:VAL:CG2	1:A:427:TYR:H	2.19	0.56
1:B:97:GLN:HB3	1:B:106:ARG:HG2	1.86	0.56
1:A:134:ASP:O	1:A:137:VAL:HG23	2.06	0.56
1:B:147:THR:O	1:B:151:ILE:HG23	2.06	0.56
1:B:124:VAL:HG11	1:B:211:LEU:HD22	1.88	0.56
1:A:185:THR:O	1:A:186:ALA:HB3	2.06	0.56
1:A:420:TRP:HB2	1:A:424:PRO:CB	2.31	0.55
1:A:183:MET:O	1:A:262:LYS:O	2.24	0.55
1:B:357:HIS:N	1:B:421:ARG:O	2.39	0.55
1:A:333:LYS:HD3	1:A:336:LYS:NZ	2.22	0.55
1:A:100:LYS:HB3	1:A:105:SER:HG	1.72	0.55
1:B:101:LEU:N	1:B:102:PRO:CD	2.68	0.55
1:B:378:SER:O	1:B:381:PRO:HD2	2.07	0.55
1:B:102:PRO:O	1:B:103:ASP:HB3	2.07	0.54
1:A:190:ARG:CZ	1:A:195:ASP:CB	2.67	0.54
1:B:43:VAL:HA	1:B:48:GLY:HA2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:MET:HE2	1:B:259:LYS:CD	2.38	0.54
1:A:333:LYS:CE	1:A:336:LYS:NZ	2.58	0.54
1:A:240:PHE:HA	1:A:243:ILE:HD12	1.89	0.53
1:B:146:LEU:HD13	1:B:277:PHE:CD2	2.43	0.53
1:A:329:ILE:CG2	1:A:332:GLY:O	2.56	0.53
1:B:187:LEU:O	1:B:189:PRO:CD	2.56	0.53
1:B:338:ILE:HD11	1:B:417:LYS:HG3	1.89	0.53
1:B:177:PRO:HB2	1:B:179:TYR:HD1	1.74	0.52
1:A:139:TYR:CE2	1:A:287:VAL:HG11	2.44	0.52
1:B:134:ASP:O	1:B:137:VAL:HG23	2.09	0.52
1:A:228:THR:HG21	1:A:290:THR:HA	1.90	0.52
1:B:228:THR:HG21	1:B:290:THR:HA	1.92	0.52
1:B:99:MET:HG3	1:B:259:LYS:HG2	1.92	0.52
1:A:48:GLY:O	1:A:378:SER:OG	2.22	0.52
1:A:407:TYR:HB2	1:A:411:TRP:HB2	1.92	0.52
1:A:107:LEU:CD2	1:A:108:ASP:O	2.59	0.51
1:A:252:VAL:O	1:A:255:THR:HG22	2.11	0.51
1:B:84:GLN:HB3	1:B:203:ARG:HB3	1.93	0.51
1:A:325:ASP:HB3	1:A:328:ARG:HG3	1.93	0.51
1:A:413:GLN:HA	1:A:416:LYS:HD2	1.92	0.51
1:A:28:LEU:HD23	1:A:182:PHE:HZ	1.76	0.51
1:A:423:VAL:HG21	1:A:427:TYR:N	2.26	0.50
1:B:40:TRP:CE3	1:B:142:LEU:HD22	2.47	0.50
1:A:370:TRP:O	1:A:373:PRO:HD2	2.11	0.50
1:A:285:TYR:CE2	1:A:378:SER:HB3	2.46	0.50
1:A:88:GLN:HA	1:A:203:ARG:HH12	1.77	0.50
1:B:347:LEU:HD22	1:B:349:SER:H	1.76	0.50
1:A:179:TYR:O	1:A:182:PHE:N	2.38	0.50
1:B:101:LEU:HD22	1:B:106:ARG:HH22	1.76	0.50
1:A:321:HIS:CE1	1:B:226:THR:HG22	2.48	0.49
1:A:84:GLN:HB3	1:A:203:ARG:HB3	1.93	0.49
1:A:275:LEU:HD12	1:A:279:TYR:CZ	2.47	0.49
1:B:36:VAL:HG12	1:B:146:LEU:HD21	1.94	0.49
1:A:254:THR:O	1:A:259:LYS:HE2	2.12	0.49
1:B:99:MET:HG3	1:B:259:LYS:CG	2.42	0.49
1:A:318:GLN:OE1	1:A:350:GLY:HA3	2.12	0.49
1:B:309:TYR:HA	1:B:366:ILE:HD11	1.94	0.49
1:B:368:LEU:HD13	1:B:385:ILE:HG13	1.94	0.49
1:B:91:ALA:HB1	1:B:112:ASN:HB3	1.94	0.48
1:A:100:LYS:HB3	1:A:105:SER:OG	2.12	0.48
1:A:423:VAL:HG21	1:A:427:TYR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:HG2	1:A:253:LEU:O	2.14	0.48
1:B:40:TRP:CZ3	1:B:142:LEU:HD22	2.49	0.48
2:A:501:NDP:H8A	2:A:501:NDP:H3B	1.96	0.48
1:A:103:ASP:CB	1:A:105:SER:HB2	2.42	0.48
1:B:161:TYR:CE1	1:B:180:ASP:HB2	2.48	0.48
1:B:385:ILE:HA	1:B:385:ILE:HD13	1.59	0.47
1:B:107:LEU:HD22	1:B:190:ARG:NH2	2.29	0.47
1:B:298:ILE:O	1:B:302:VAL:HG22	2.15	0.47
1:B:275:LEU:O	1:B:279:TYR:HB2	2.14	0.47
1:A:213:ASN:HB3	1:A:235:VAL:HG23	1.96	0.47
1:B:356:ARG:NH1	1:B:415:ARG:HG2	2.30	0.47
1:B:400:ASP:OD1	1:B:415:ARG:NH2	2.48	0.47
1:B:101:LEU:HB2	1:B:102:PRO:HD3	1.97	0.47
1:A:99:MET:HG3	1:A:259:LYS:CG	2.43	0.47
1:A:322:PHE:CG	1:A:347:LEU:HD13	2.50	0.47
1:B:87:LEU:O	1:B:91:ALA:N	2.47	0.46
1:B:206:MET:O	1:B:209:TRP:HB3	2.15	0.46
1:A:224:HIS:CG	1:A:290:THR:HG21	2.50	0.46
1:A:413:GLN:O	1:A:416:LYS:HB2	2.15	0.46
1:B:190:ARG:HG2	1:B:195:ASP:HA	1.98	0.46
1:A:347:LEU:N	2:A:501:NDP:N1A	2.60	0.46
1:B:121:LEU:HA	1:B:121:LEU:HD13	1.69	0.46
1:B:333:LYS:HG2	1:B:334:PRO:CD	2.44	0.46
1:B:354:ILE:HG22	1:B:424:PRO:HG3	1.98	0.46
1:A:231:MET:O	1:A:235:VAL:HG12	2.16	0.46
1:B:100:LYS:HD2	1:B:105:SER:O	2.14	0.46
1:A:99:MET:SD	1:A:259:LYS:HD3	2.55	0.46
1:B:138:LEU:HB3	1:B:212:MET:HG2	1.96	0.46
1:B:99:MET:HB3	1:B:100:LYS:H	1.62	0.45
1:B:115:PHE:CD1	1:B:115:PHE:C	2.88	0.45
1:B:313:ARG:O	1:B:317:ILE:HG23	2.17	0.45
1:B:99:MET:CG	1:B:259:LYS:HD3	2.40	0.45
1:B:388:PHE:CE2	1:B:392:LEU:HD11	2.51	0.45
1:B:333:LYS:CB	1:B:334:PRO:CD	2.93	0.45
1:A:412:LEU:O	1:A:416:LYS:HG3	2.15	0.45
1:B:302:VAL:O	1:B:306:LEU:HG	2.17	0.45
1:A:393:LEU:HD23	1:A:393:LEU:HA	1.82	0.45
1:A:107:LEU:HD13	1:A:188:ASN:ND2	2.32	0.45
1:A:102:PRO:O	1:A:103:ASP:CB	2.65	0.45
1:B:70:THR:HG23	1:B:73:ALA:H	1.82	0.45
1:B:98:GLY:HA3	1:B:109:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:TRP:HH2	1:B:370:TRP:CH2	2.35	0.44
1:B:248:HIS:CE1	1:B:313:ARG:NH1	2.86	0.44
1:A:87:LEU:HD21	1:A:119:PHE:CD2	2.52	0.44
1:A:216:MET:HE3	1:A:283:ALA:HB3	2.00	0.44
1:A:115:PHE:CD1	1:A:115:PHE:C	2.91	0.43
1:A:191:ILE:O	1:A:194:LEU:HB3	2.18	0.43
1:A:45:TYR:N	1:A:45:TYR:CD1	2.85	0.43
1:A:102:PRO:O	1:A:103:ASP:HB3	2.16	0.43
1:B:347:LEU:N	2:B:501:NDP:N1A	2.55	0.43
1:B:206:MET:HG3	1:B:275:LEU:CD2	2.48	0.43
1:A:230:PRO:HG3	1:A:293:LEU:CD2	2.48	0.43
1:A:339:LYS:HE3	1:A:339:LYS:HB2	1.72	0.43
1:B:323:ARG:NH2	1:B:345:LEU:O	2.47	0.43
1:A:188:ASN:OD1	1:A:188:ASN:N	2.50	0.43
1:B:53:THR:HB	1:B:55:ASP:H	1.84	0.43
1:A:107:LEU:CD1	1:A:190:ARG:HH21	2.32	0.43
1:A:203:ARG:HB2	1:A:204:PRO:HD3	2.01	0.43
1:B:243:ILE:HD12	1:B:243:ILE:HG23	1.76	0.43
1:A:99:MET:HG3	1:A:259:LYS:HD3	2.00	0.43
1:A:423:VAL:CG2	1:A:427:TYR:N	2.82	0.42
1:B:59:TRP:CE3	1:B:59:TRP:HA	2.54	0.42
1:B:141:GLN:O	1:B:145:LEU:HG	2.20	0.42
1:A:190:ARG:HG2	1:A:195:ASP:HA	2.01	0.42
1:A:196:LEU:CB	1:A:263:PHE:HE2	2.33	0.42
1:B:212:MET:HE3	1:B:280:THR:HG21	2.00	0.42
1:B:91:ALA:CB	1:B:112:ASN:HB3	2.49	0.42
1:A:99:MET:HG3	1:A:259:LYS:CD	2.50	0.42
1:A:121:LEU:HA	1:A:121:LEU:HD12	1.45	0.42
1:A:124:VAL:HG11	1:A:211:LEU:HD22	2.01	0.42
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.92	0.42
1:B:339:LYS:HE3	1:B:339:LYS:HB2	1.76	0.41
1:A:216:MET:HB2	1:A:216:MET:HE2	1.80	0.41
1:B:333:LYS:CG	1:B:334:PRO:CD	2.86	0.41
1:B:197:LYS:NZ	1:B:261:GLU:O	2.35	0.41
1:A:91:ALA:O	1:A:110:ARG:NH2	2.53	0.41
1:A:347:LEU:HD23	1:A:352:TRP:CD1	2.55	0.41
1:B:242:LEU:O	1:B:245:TYR:HB3	2.20	0.41
1:B:87:LEU:O	1:B:91:ALA:HB2	2.20	0.41
1:B:203:ARG:HB2	1:B:204:PRO:HD3	2.02	0.41
1:A:213:ASN:ND2	1:A:238:GLN:OE1	2.53	0.41
1:B:95:THR:HA	1:B:110:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:TRP:CE2	1:B:398:ARG:HD2	2.55	0.41
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.84	0.41
1:B:423:VAL:HB	1:B:427:TYR:H	1.85	0.41
1:B:380:ILE:HB	1:B:381:PRO:HD3	2.01	0.41
1:B:151:ILE:O	1:B:155:VAL:HG12	2.20	0.41
1:B:134:ASP:OD1	1:B:134:ASP:N	2.54	0.41
1:B:204:PRO:O	1:B:208:PHE:HB2	2.20	0.41
1:A:357:HIS:N	1:A:421:ARG:O	2.54	0.41
1:B:45:TYR:CD2	1:B:65:HIS:CD2	3.08	0.41
1:A:317:ILE:HG22	1:A:321:HIS:CD2	2.56	0.41
1:A:252:VAL:O	1:A:258:ILE:HG13	2.20	0.41
1:B:423:VAL:H	1:B:427:TYR:C	2.25	0.41
1:A:145:LEU:HD13	1:A:208:PHE:HZ	1.86	0.41
1:A:329:ILE:HG13	1:A:329:ILE:H	1.58	0.41
1:B:234:VAL:HG23	1:B:373:PRO:HG2	2.02	0.41
1:A:344:SER:HB2	1:A:407:TYR:HE1	1.86	0.40
1:A:275:LEU:HD12	1:A:279:TYR:CE2	2.56	0.40
1:A:321:HIS:NE2	1:B:226:THR:CG2	2.79	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	389/427 (91%)	353 (91%)	36 (9%)	0	100	100
1	B	385/427 (90%)	349 (91%)	36 (9%)	0	100	100
All	All	774/854 (91%)	702 (91%)	72 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	331/358 (92%)	305 (92%)	26 (8%)	15 33
1	B	327/358 (91%)	299 (91%)	28 (9%)	13 28
All	All	658/716 (92%)	604 (92%)	54 (8%)	14 30

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	CYS
1	A	92	PRO
1	A	100	LYS
1	A	110	ARG
1	A	112	ASN
1	A	120	THR
1	A	121	LEU
1	A	127	LEU
1	A	129	THR
1	A	134	ASP
1	A	146	LEU
1	A	156	PHE
1	A	163	TRP
1	A	179	TYR
1	A	187	LEU
1	A	196	LEU
1	A	219	LYS
1	A	227	VAL
1	A	229	VAL
1	A	263	PHE
1	A	267	LEU
1	A	281	LEU
1	A	282	GLN
1	A	293	LEU
1	A	295	VAL
1	A	337	TYR
1	B	42	CYS

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Mol	Chain	Res	Type
1	B	120	THR
1	B	121	LEU
1	B	127	LEU
1	B	134	ASP
1	B	151	ILE
1	B	179	TYR
1	B	183	MET
1	B	187	LEU
1	B	201	GLU
1	B	206	MET
1	B	216	MET
1	B	229	VAL
1	B	250	GLU
1	B	263	PHE
1	B	267	LEU
1	B	280	THR
1	B	281	LEU
1	B	288	HIS
1	B	306	LEU
1	B	317	ILE
1	B	329	ILE
1	B	333	LYS
1	B	337	TYR
1	B	347	LEU
1	B	385	ILE
1	B	416	LYS
1	B	421	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN

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	$\#\|Z\| > 2$
2	NDP	A	501	-	26,33,52	1.19	2 (7%)	34,52,80	1.67	5 (14%)
2	NDP	B	501	-	26,33,52	1.15	2 (7%)	34,52,80	1.80	5 (14%)

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
2	NDP	A	501	-	-	0/17/37/77	0/3/3/5
2	NDP	B	501	-	-	0/17/37/77	0/3/3/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NDP	C2A-N3A	2.09	1.35	1.32
2	A	501	NDP	C2A-N3A	2.14	1.36	1.32
2	B	501	NDP	C5A-C4A	3.56	1.48	1.40
2	A	501	NDP	C5A-C4A	3.86	1.49	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NDP	N3A-C2A-N1A	-7.47	123.17	128.89
2	A	501	NDP	N3A-C2A-N1A	-5.85	124.41	128.89
2	B	501	NDP	PA-O3-PN	-3.41	121.23	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NDP	PA-O3-PN	-3.04	122.47	132.67
2	A	501	NDP	O2B-C2B-C3B	-2.41	102.15	111.51
2	B	501	NDP	C4A-C5A-N7A	-2.07	107.57	109.48
2	A	501	NDP	O4B-C1B-C2B	-2.04	102.91	106.60
2	B	501	NDP	P2B-O2B-C2B	2.36	127.22	121.56
2	A	501	NDP	O2N-PN-O1N	3.19	120.84	110.58
2	B	501	NDP	O2N-PN-O1N	3.19	120.85	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDP	2	0
2	B	501	NDP	1	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	393/427 (92%)	0.43	31 (7%)	15	14	47, 86, 148, 227	0
1	B	389/427 (91%)	0.25	23 (5%)	26	26	42, 82, 139, 239	0
All	All	782/854 (91%)	0.34	54 (6%)	20	19	42, 84, 145, 239	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	PHE	10.6
1	A	186	ALA	7.2
1	A	177	PRO	7.0
1	B	102	PRO	6.3
1	B	105	SER	5.6
1	A	162	PHE	4.8
1	A	185	THR	4.8
1	A	328	ARG	4.7
1	A	327	ASN	4.5
1	B	332	GLY	4.2
1	B	52	PHE	4.2
1	A	23	PHE	4.0
1	B	327	ASN	3.9
1	A	187	LEU	3.9
1	A	424	PRO	3.9
1	B	193	SER	3.7
1	A	426	ILE	3.4
1	A	59	TRP	3.4
1	B	101	LEU	3.4
1	A	102	PRO	3.4
1	A	54	SER	3.4
1	B	71	TRP	3.1
1	A	26	LEU	3.1
1	A	324	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	333	LYS	3.1
1	B	328	ARG	3.0
1	A	99	MET	3.0
1	B	103	ASP	2.9
1	A	160	LEU	2.9
1	B	90	TRP	2.8
1	A	262	LYS	2.8
1	A	180	ASP	2.6
1	A	179	TYR	2.6
1	B	341	LYS	2.4
1	B	334	PRO	2.4
1	A	333	LYS	2.4
1	B	182	PHE	2.4
1	A	61	ARG	2.4
1	B	185	THR	2.4
1	A	423	VAL	2.3
1	A	263	PHE	2.3
1	B	261	GLU	2.3
1	B	330	VAL	2.3
1	B	92	PRO	2.3
1	B	263	PHE	2.3
1	A	101	LEU	2.2
1	B	260	HIS	2.2
1	A	329	ILE	2.2
1	A	325	ASP	2.2
1	B	94	PRO	2.1
1	A	72	HIS	2.1
1	A	66	VAL	2.1
1	B	100	LYS	2.0
1	A	90	TRP	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

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
2	NDP	B	501	31/48	0.92	0.16	-0.51	46,89,114,364	0
2	NDP	A	501	31/48	0.89	0.17	-0.58	41,77,119,301	0

6.5 Other polymers

There are no such residues in this entry.