Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:40 AM GMT

PDB ID	:	3BR9
Title	:	Crystal Structure of HCV NS5B Polymerase with a Novel Pyridazinone Inhibitor
Authors	:	Zhao, Q.; Showalter, R.E.; Han, Q.; Kissinger, C.R.
Deposited on	:	2007-12-21
Resolution	:	2.30 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:

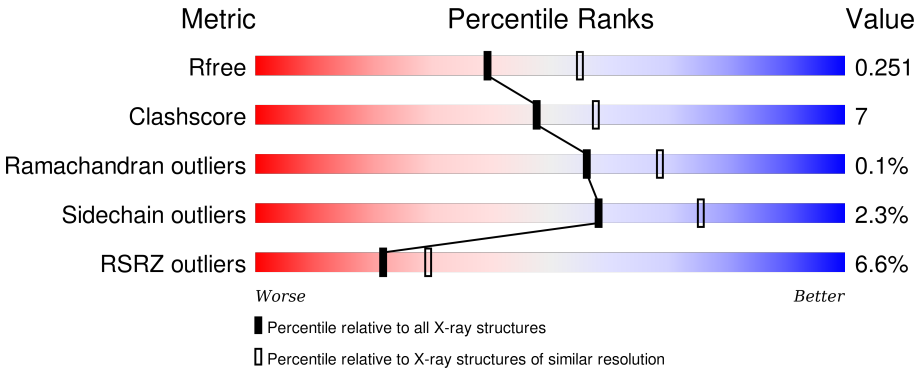
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	578	5% 78% 18%
1	B	578	8% 79% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9162 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.

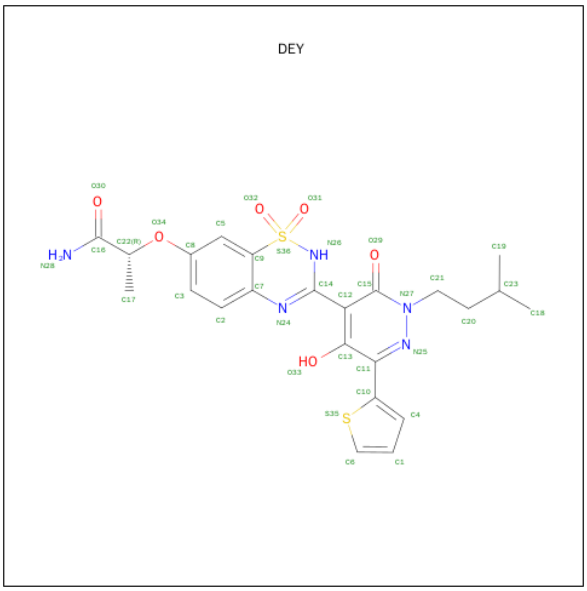
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4334	2735	764	804	31			
1	B	557	Total	C	N	O	S	0	0	0
			4334	2735	764	804	31			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLN	ARG	ENGINEERED	UNP P26663
A	571	LEU	-	EXPRESSION TAG	UNP P26663
A	572	GLU	-	EXPRESSION TAG	UNP P26663
A	573	HIS	-	EXPRESSION TAG	UNP P26663
A	574	HIS	-	EXPRESSION TAG	UNP P26663
A	575	HIS	-	EXPRESSION TAG	UNP P26663
A	576	HIS	-	EXPRESSION TAG	UNP P26663
A	577	HIS	-	EXPRESSION TAG	UNP P26663
A	578	HIS	-	EXPRESSION TAG	UNP P26663
B	544	GLN	ARG	ENGINEERED	UNP P26663
B	571	LEU	-	EXPRESSION TAG	UNP P26663
B	572	GLU	-	EXPRESSION TAG	UNP P26663
B	573	HIS	-	EXPRESSION TAG	UNP P26663
B	574	HIS	-	EXPRESSION TAG	UNP P26663
B	575	HIS	-	EXPRESSION TAG	UNP P26663
B	576	HIS	-	EXPRESSION TAG	UNP P26663
B	577	HIS	-	EXPRESSION TAG	UNP P26663
B	578	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is (2R)-2-({3-[5-HYDROXY-2-(3-METHYLBUTYL)-3-OXO-6-THIOPHEN-2-YL-2,3-DIHYDROPYRIDAZIN-4-YL]-1,1-DIOXIDO-2H-1,2,4-BENZOTHIADIAZIN-7-YL}OXY)PROPANAMIDE (three-letter code: DEY) (formula: $C_{23}H_{25}N_5O_6S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 36 23 5 6 2	0	0
2	B	1	Total C N O S 36 23 5 6 2	0	0

- Molecule 3 is water.

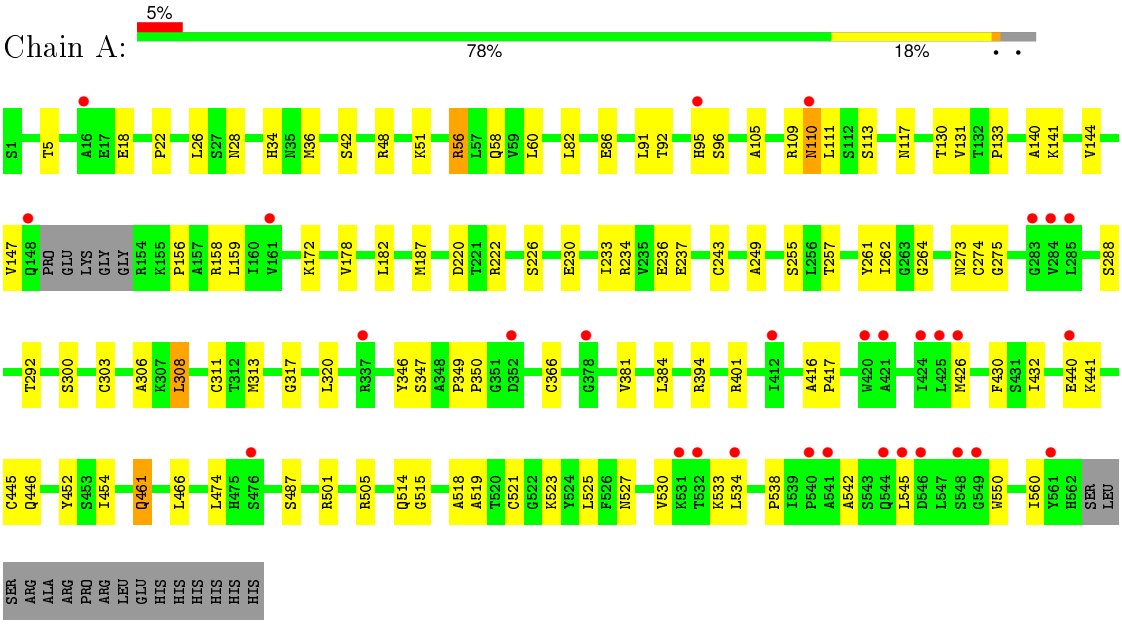
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	209	Total O 209 209	0	0
3	B	213	Total O 213 213	0	0

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.

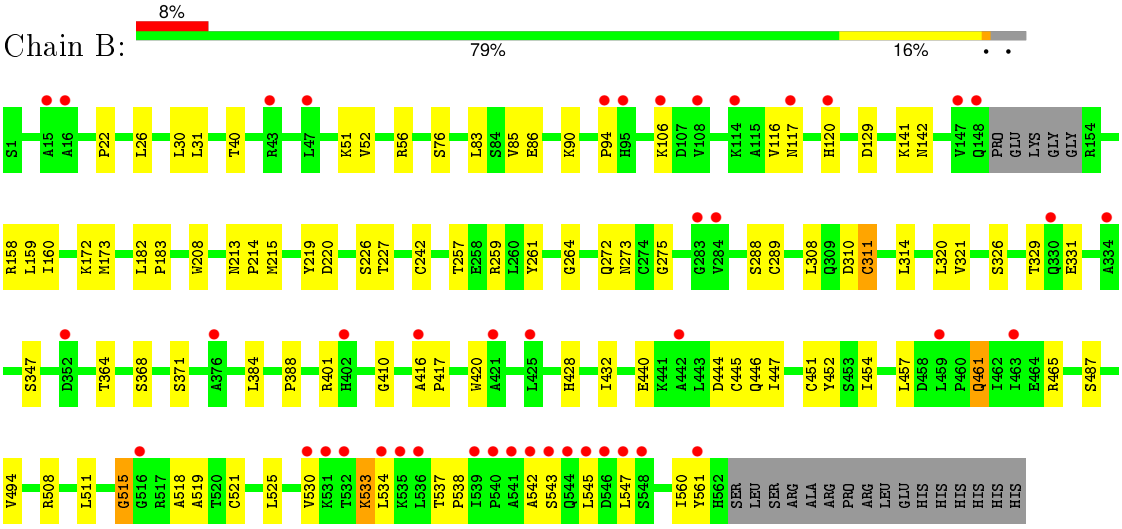
- Molecule 1: RNA-directed RNA polymerase

Chain A:



- Molecule 1: RNA-directed RNA polymerase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.50Å 104.31Å 125.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.60 – 2.30 28.63 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (28.60-2.30) 90.5 (28.63-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.251 0.195 , 0.251	Depositor DCC
R_{free} test set	2286 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	5 of 45268 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9162	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.50 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.8202e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: DEY

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	0.63	2/4428 (0.0%)	0.68	1/6009 (0.0%)
1	B	0.63	1/4428 (0.0%)	0.69	0/6009
All	All	0.63	3/8856 (0.0%)	0.69	1/12018 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	CYS	CB-SG	-8.16	1.68	1.82
1	A	311	CYS	CB-SG	-6.56	1.71	1.82
1	A	274	CYS	CB-SG	-5.22	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466	LEU	CA-CB-CG	5.20	127.27	115.30

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	4334	0	4354	67	0
1	B	4334	0	4354	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	25	9	0
2	B	36	0	25	8	0
3	A	209	0	0	3	0
3	B	213	0	0	5	0
All	All	9162	0	8758	129	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 7.

All (129) 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:446:GLN:O	2:A:579:DEY:H1	1.78	0.83
1:A:313:MET:HG2	1:A:320:LEU:HD11	1.63	0.79
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.24	0.78
1:B:446:GLN:O	2:B:579:DEY:H1	1.85	0.76
1:A:461:GLN:HB3	1:A:542:ALA:HA	1.70	0.73
1:A:384:LEU:HD23	2:A:579:DEY:H18B	1.72	0.72
1:A:95:HIS:CD2	1:A:95:HIS:H	2.06	0.70
1:B:141:LYS:HE2	1:B:158:ARG:HH21	1.57	0.69
1:A:92:THR:O	1:A:109:ARG:HD2	1.97	0.64
1:A:441:LYS:HE3	3:A:784:HOH:O	1.98	0.63
2:A:579:DEY:H4	2:A:579:DEY:O33	1.99	0.63
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.82	0.60
1:B:508:ARG:HH22	1:B:534:LEU:HD13	1.65	0.60
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.84	0.60
1:B:85:VAL:HG11	1:B:116:VAL:HG13	1.84	0.60
1:A:130:THR:HG22	1:A:255:SER:HB2	1.85	0.59
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.33	0.58
1:A:22:PRO:HG2	1:A:401:ARG:HG3	1.86	0.57
1:B:451:CYS:HB2	3:B:792:HOH:O	2.03	0.57
1:A:538:PRO:HG2	1:B:272:GLN:HG3	1.86	0.57
1:A:521:CYS:O	1:A:525:LEU:HB2	2.05	0.56
1:B:511:LEU:HB3	1:B:518:ALA:O	2.06	0.56
1:A:381:VAL:HG11	1:A:474:LEU:HD22	1.86	0.56
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.45	0.56
1:A:273:ASN:ND2	1:A:275:GLY:H	2.03	0.55
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.88	0.55
1:A:288:SER:HA	2:A:579:DEY:H17	1.89	0.55
1:B:26:LEU:HD13	1:B:432:ILE:HG12	1.88	0.55
1:A:42:SER:HA	1:A:140:ALA:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:SER:HA	1:B:242:CYS:O	2.07	0.54
1:A:264:GLY:HA3	3:A:614:HOH:O	2.07	0.54
1:A:445:CYS:SG	1:A:454:ILE:HG13	2.48	0.54
1:B:86:GLU:O	1:B:90:LYS:HG2	2.07	0.54
1:B:30:LEU:HB2	1:B:428:HIS:CE1	2.43	0.53
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.89	0.53
1:B:40:THR:O	1:B:142:ASN:HA	2.08	0.53
1:B:521:CYS:O	1:B:525:LEU:HB2	2.08	0.53
1:A:234:ARG:CG	1:A:262:ILE:HD11	2.39	0.53
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.90	0.53
1:B:310:ASP:HB2	3:B:755:HOH:O	2.10	0.52
1:A:306:ALA:CB	1:A:308:LEU:HD13	2.40	0.52
1:A:141:LYS:NZ	1:A:158:ARG:HH21	2.08	0.52
2:A:579:DEY:O33	2:A:579:DEY:C4	2.58	0.51
1:A:306:ALA:HB3	1:A:308:LEU:HD13	1.93	0.51
1:B:30:LEU:O	1:B:494:VAL:HG13	2.11	0.51
1:A:317:GLY:HA3	2:A:579:DEY:H17B	1.91	0.50
1:A:514:GLN:HB2	1:A:518:ALA:HB3	1.93	0.50
1:A:257:THR:HA	1:A:261:TYR:HB2	1.93	0.50
1:B:273:ASN:ND2	1:B:275:GLY:H	2.10	0.50
1:B:141:LYS:HE2	1:B:158:ARG:NH2	2.24	0.50
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.52	0.50
1:B:461:GLN:HB3	1:B:542:ALA:HA	1.93	0.49
2:B:579:DEY:H4	2:B:579:DEY:O33	2.12	0.49
1:A:523:LYS:HG3	1:A:534:LEU:HD22	1.95	0.49
2:B:579:DEY:N24	2:B:579:DEY:O29	2.43	0.49
1:B:530:VAL:O	1:B:533:LYS:HE3	2.13	0.49
1:B:465:ARG:HH12	1:B:545:LEU:H	1.61	0.48
1:B:264:GLY:HA3	3:B:597:HOH:O	2.13	0.48
1:A:178:VAL:HG23	3:A:783:HOH:O	2.14	0.48
2:B:579:DEY:O33	2:B:579:DEY:N26	2.46	0.47
1:A:36:MET:O	1:A:147:VAL:HG13	2.14	0.47
1:B:257:THR:HA	1:B:261:TYR:HB2	1.96	0.47
1:B:384:LEU:HD23	2:B:579:DEY:H18B	1.96	0.47
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.97	0.47
1:B:208:TRP:CE2	1:B:214:PRO:HB2	2.50	0.47
1:B:331:GLU:HG2	3:B:753:HOH:O	2.15	0.47
1:B:141:LYS:HD3	1:B:160:ILE:HB	1.96	0.47
2:B:579:DEY:C4	2:B:579:DEY:O33	2.63	0.47
1:A:501:ARG:O	1:A:505:ARG:HG3	2.15	0.47
1:A:51:LYS:HE2	1:A:156:PRO:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ASN:O	1:A:533:LYS:HE2	2.15	0.47
1:A:220:ASP:O	1:A:350:PRO:HA	2.15	0.46
1:B:129:ASP:O	1:B:259:ARG:HD2	2.15	0.46
1:A:58:GLN:HG2	1:A:60:LEU:HD21	1.96	0.46
1:B:215:MET:HB2	1:B:326:SER:HB2	1.98	0.46
1:B:22:PRO:HG2	1:B:401:ARG:HG3	1.98	0.45
1:B:416:ALA:N	1:B:417:PRO:CD	2.80	0.45
1:A:5:THR:O	1:A:275:GLY:HA3	2.16	0.44
1:A:346:TYR:O	1:A:347:SER:HB3	2.17	0.44
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.98	0.44
1:A:530:VAL:O	1:A:533:LYS:HE3	2.17	0.44
1:B:308:LEU:CB	1:B:311:CYS:SG	3.02	0.44
1:A:426:MET:O	1:A:430:PHE:HB2	2.18	0.44
1:B:182:LEU:C	1:B:182:LEU:HD23	2.38	0.44
1:B:447:ILE:HA	2:B:579:DEY:H4	2.00	0.44
1:B:227:THR:HB	1:B:347:SER:O	2.18	0.43
1:A:28:ASN:OD1	1:A:34:HIS:CE1	2.71	0.43
1:B:213:ASN:HA	1:B:214:PRO:HD2	1.83	0.43
1:A:234:ARG:HG2	1:A:262:ILE:HD11	2.01	0.43
1:A:26:LEU:HD13	1:A:432:ILE:HG12	2.00	0.43
1:B:83:LEU:HB2	1:B:173:MET:HA	2.01	0.43
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.53	0.43
1:B:444:ASP:HA	1:B:452:TYR:O	2.19	0.43
1:B:94:PRO:HD3	1:B:561:TYR:CD1	2.53	0.43
1:B:129:ASP:HB3	1:B:259:ARG:NH1	2.33	0.43
1:A:48:ARG:HG2	1:A:159:LEU:HG	2.00	0.43
1:A:113:SER:O	1:A:117:ASN:CG	2.57	0.43
1:A:18:GLU:OE2	1:A:401:ARG:NH2	2.46	0.43
1:A:222:ARG:HH21	1:A:349:PRO:CG	2.32	0.43
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.58	0.43
1:B:410:GLY:HA3	3:B:758:HOH:O	2.18	0.43
1:B:440:GLU:HG2	1:B:457:LEU:HD11	2.01	0.43
1:B:364:THR:HA	1:B:368:SER:O	2.19	0.43
1:A:86:GLU:HA	1:A:111:LEU:HD21	2.01	0.43
1:A:131:VAL:O	1:A:133:PRO:HD3	2.19	0.42
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.50	0.42
1:A:187:MET:HE1	1:A:292:THR:HG22	2.00	0.42
2:A:579:DEY:O29	2:A:579:DEY:N24	2.50	0.42
1:A:96:SER:HB3	1:A:105:ALA:HB2	2.02	0.42
1:A:303:CYS:HA	1:A:308:LEU:HD22	2.01	0.42
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD2	1:A:226:SER:O	2.20	0.42
1:A:366:CYS:HB3	2:A:579:DEY:O29	2.18	0.42
1:A:313:MET:HG2	1:A:320:LEU:CD1	2.42	0.41
1:A:234:ARG:HG3	1:A:262:ILE:HD11	2.01	0.41
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.50	0.41
1:A:95:HIS:CD2	1:A:95:HIS:N	2.81	0.41
1:A:416:ALA:N	1:A:417:PRO:CD	2.83	0.41
1:A:233:ILE:O	1:A:236:GLU:HG2	2.21	0.41
1:B:288:SER:HA	2:B:579:DEY:H17	2.03	0.41
1:B:85:VAL:HG21	1:B:120:HIS:CE1	2.56	0.41
1:B:537:THR:O	1:B:538:PRO:C	2.57	0.41
1:A:452:TYR:CE1	1:A:550:TRP:CD1	3.09	0.41
1:A:230:GLU:HG3	1:A:262:ILE:HD13	2.03	0.41
1:B:52:VAL:HB	1:B:226:SER:OG	2.20	0.41
1:A:91:LEU:HB2	1:A:172:LYS:HD3	2.04	0.40
2:A:579:DEY:N26	2:A:579:DEY:O33	2.52	0.40
1:A:461:GLN:HB2	1:A:545:LEU:HD11	2.04	0.40
1:A:110:ASN:C	1:A:110:ASN:HD22	2.25	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	553/578 (96%)	538 (97%)	15 (3%)	0	100	100
1	B	553/578 (96%)	535 (97%)	17 (3%)	1 (0%)	52	64
All	All	1106/1156 (96%)	1073 (97%)	32 (3%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	515	GLY

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	475/493 (96%)	467 (98%)	8 (2%)	68 83
1	B	475/493 (96%)	461 (97%)	14 (3%)	50 66
All	All	950/986 (96%)	928 (98%)	22 (2%)	58 75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	110	ASN
1	A	237	GLU
1	A	300	SER
1	A	308	LEU
1	A	440	GLU
1	A	461	GLN
1	A	487	SER
1	B	31	LEU
1	B	51	LYS
1	B	56	ARG
1	B	106	LYS
1	B	117	ASN
1	B	159	LEU
1	B	220	ASP
1	B	329	THR
1	B	371	SER
1	B	461	GLN
1	B	487	SER
1	B	533	LYS
1	B	543	SER
1	B	547	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	110	ASN
1	A	117	ASN
1	A	273	ASN
1	A	330	GLN
1	A	374	HIS
1	B	117	ASN
1	B	273	ASN
1	B	406	ASN

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

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	DEY	A	579	-	32,39,39	1.23	2 (6%)	36,58,58	1.97	10 (27%)
2	DEY	B	579	-	32,39,39	1.13	3 (9%)	36,58,58	2.15	7 (19%)

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	DEY	A	579	-	-	0/15/36/36	0/3/4/4
2	DEY	B	579	-	-	0/15/36/36	0/3/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	DEY	C11-N25	-3.74	1.30	1.33
2	B	579	DEY	C11-N25	-3.14	1.30	1.33
2	B	579	DEY	C12-C14	-2.22	1.45	1.49
2	B	579	DEY	C16-N28	2.51	1.37	1.32
2	A	579	DEY	C9-S36	3.09	1.78	1.76

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	579	DEY	C12-C14-N26	-3.42	113.28	118.46
2	B	579	DEY	C1-C6-S35	-3.42	109.45	113.23
2	B	579	DEY	C12-C14-N26	-2.91	114.05	118.46
2	A	579	DEY	C20-C21-N27	-2.55	106.02	111.58
2	B	579	DEY	O32-S36-C9	-2.52	106.03	109.19
2	A	579	DEY	C1-C6-S35	-2.50	110.47	113.23
2	A	579	DEY	C22-C16-N28	-2.48	113.25	116.92
2	A	579	DEY	C12-C13-C11	-2.36	117.25	121.06
2	A	579	DEY	O32-S36-N26	-2.34	106.59	108.21
2	B	579	DEY	C12-C13-C11	-2.29	117.37	121.06
2	A	579	DEY	C7-N24-C14	2.36	120.99	117.40
2	A	579	DEY	O31-S36-C9	2.52	112.36	109.19
2	B	579	DEY	O31-S36-C9	2.57	112.42	109.19
2	A	579	DEY	O30-C16-C22	3.34	123.68	118.99
2	B	579	DEY	O30-C16-C22	3.35	123.70	118.99
2	A	579	DEY	C10-C11-N25	7.44	120.92	113.81
2	B	579	DEY	C10-C11-N25	9.54	122.93	113.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	579	DEY	9	0
2	B	579	DEY	8	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	557/578 (96%)	0.33	30 (5%)	29 38	28, 41, 59, 86	0
1	B	557/578 (96%)	0.45	44 (7%)	15 22	29, 43, 61, 91	0
All	All	1114/1156 (96%)	0.39	74 (6%)	22 29	28, 42, 60, 91	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	LEU	6.7
1	A	546	ASP	6.5
1	A	548	SER	5.7
1	B	16	ALA	5.4
1	A	544	GLN	5.3
1	B	532	THR	5.1
1	B	540	PRO	4.9
1	B	546	ASP	4.9
1	B	548	SER	4.7
1	B	545	LEU	4.5
1	B	542	ALA	4.2
1	B	535	LYS	4.1
1	A	421	ALA	4.0
1	B	352	ASP	4.0
1	A	412	ILE	4.0
1	B	531	LYS	3.9
1	B	534	LEU	3.9
1	A	148	GLN	3.8
1	A	531	LYS	3.7
1	A	534	LEU	3.7
1	B	43	ARG	3.6
1	A	425	LEU	3.6
1	A	16	ALA	3.5
1	B	402	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	352	ASP	3.3
1	A	532	THR	3.3
1	B	425	LEU	3.2
1	B	94	PRO	3.2
1	B	541	ALA	3.1
1	B	516	GLY	3.1
1	A	540	PRO	3.1
1	B	117	ASN	3.1
1	B	95	HIS	3.1
1	B	544	GLN	3.0
1	B	148	GLN	3.0
1	B	547	LEU	2.9
1	B	376	ALA	2.9
1	A	549	GLY	2.8
1	B	530	VAL	2.8
1	A	95	HIS	2.8
1	A	161	VAL	2.7
1	A	110	ASN	2.6
1	B	416	ALA	2.6
1	B	120	HIS	2.6
1	B	463	ILE	2.5
1	B	334	ALA	2.5
1	A	476	SER	2.5
1	B	330	GLN	2.5
1	B	539	ILE	2.4
1	A	541	ALA	2.4
1	B	106	LYS	2.4
1	A	378	GLY	2.3
1	B	459	LEU	2.3
1	A	284	VAL	2.3
1	A	424	ILE	2.3
1	B	284	VAL	2.3
1	A	426	MET	2.3
1	B	108	VAL	2.2
1	A	420	TRP	2.2
1	B	114	LYS	2.2
1	B	421	ALA	2.2
1	A	440	GLU	2.2
1	B	283	GLY	2.2
1	B	536	LEU	2.2
1	A	561	TYR	2.1
1	B	15	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	442	ALA	2.1
1	A	285	LEU	2.1
1	B	47	LEU	2.1
1	B	561	TYR	2.1
1	B	543	SER	2.1
1	A	283	GLY	2.0
1	B	147	VAL	2.0
1	A	337	ARG	2.0

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

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	DEY	B	579	36/36	0.93	0.16	0.35	38,43,46,52	0
2	DEY	A	579	36/36	0.94	0.14	-0.08	37,41,45,52	0

6.5 Other polymers

There are no such residues in this entry.