Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:53 PM GMT

PDB ID	:	1VKG
Title	:	Crystal Structure of Human HDAC8 complexed with CRA-19156
Authors	:	Somoza, J.R.; Skene, R.J.; Katz, B.A.; Mol, C.; Ho, J.D.; Jennings, A.J.; Luong, C.; Arvai, A.; Buggy, J.J.; Chi, E.; Tang, J.; Sang, B.-C.; Verner, E.; Wynands, R.; Leahy, E.M.; Dougan, D.R.; Snell, G.; Navre, M.; Knuth, M.W.; Swanson, R.V.; McRee, D.E.; Tari, L.W.
Deposited on	:	2004-05-13
Resolution	:	2.20 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:

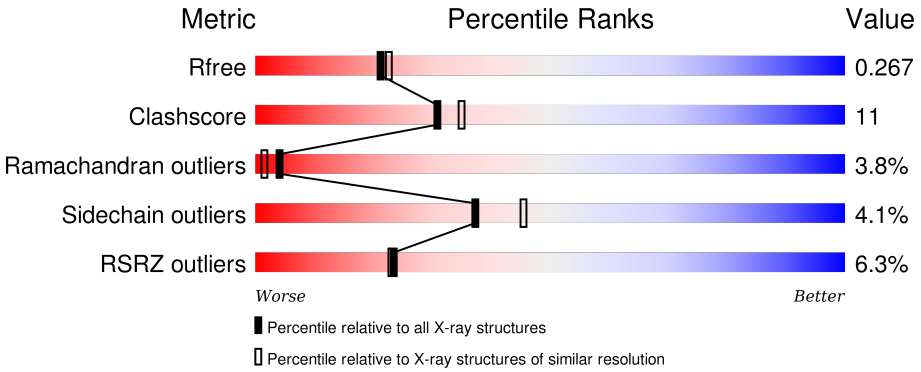
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	377	6% 63% 24% 5% • 8%
1	B	377	6% 65% 24% • 8%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	401	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11640 atoms, of which 5898 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 Histone deacetylase 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	H	N	O	S	0	3	0
			5401	1742	2684	454	503	18			
1	B	348	Total	C	H	N	O	S	0	0	0
			5397	1740	2682	454	503	18			

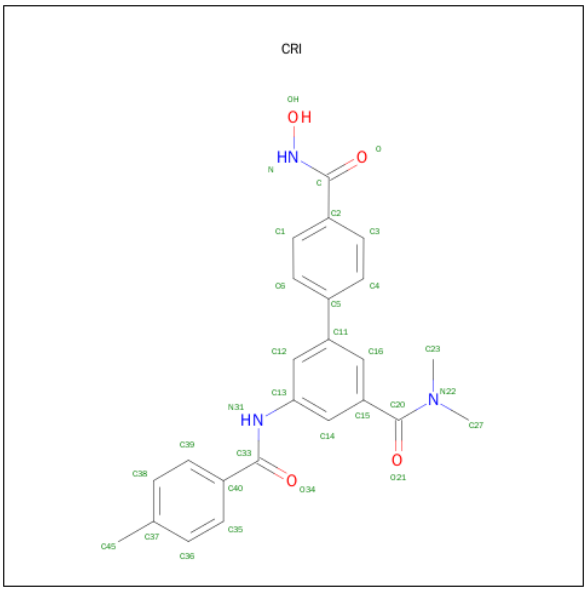
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 5-(4-METHYL-BENZOYLAMINO)-BIPHENYL-3,4'-DICARBOXYLIC ACID 3-DIMETHYLAMIDE-4'-HYDROXYAMIDE (three-letter code: CRI) (formula: $C_{24}H_{23}N_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			53	24	22	3	4		
4	B	1	Total	C	H	N	O	0	0
			53	24	22	3	4		

- Molecule 5 is water.

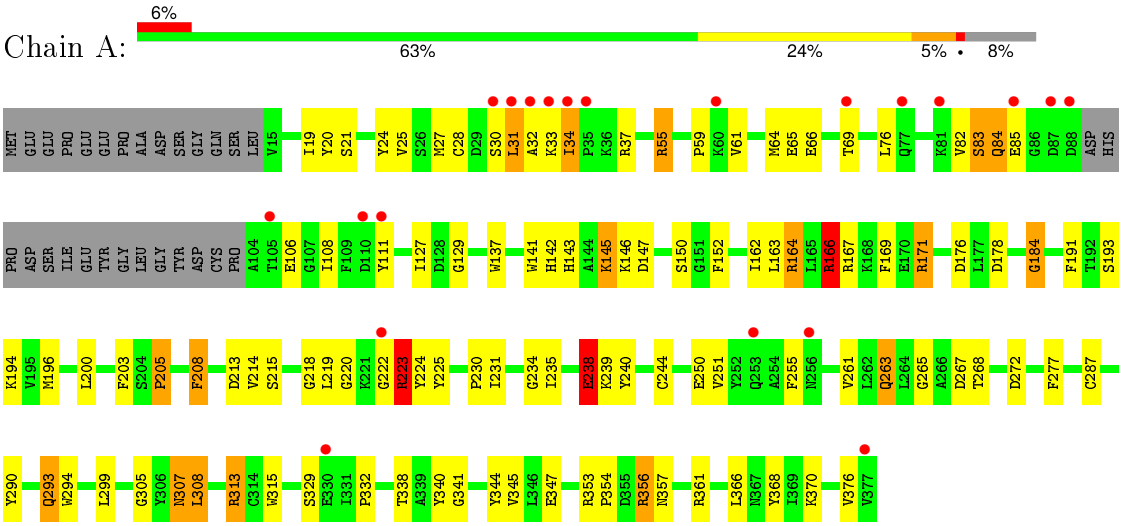
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	129	Total	H	O	0	0
			387	258	129		
5	B	115	Total	H	O	0	0
			345	230	115		

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.

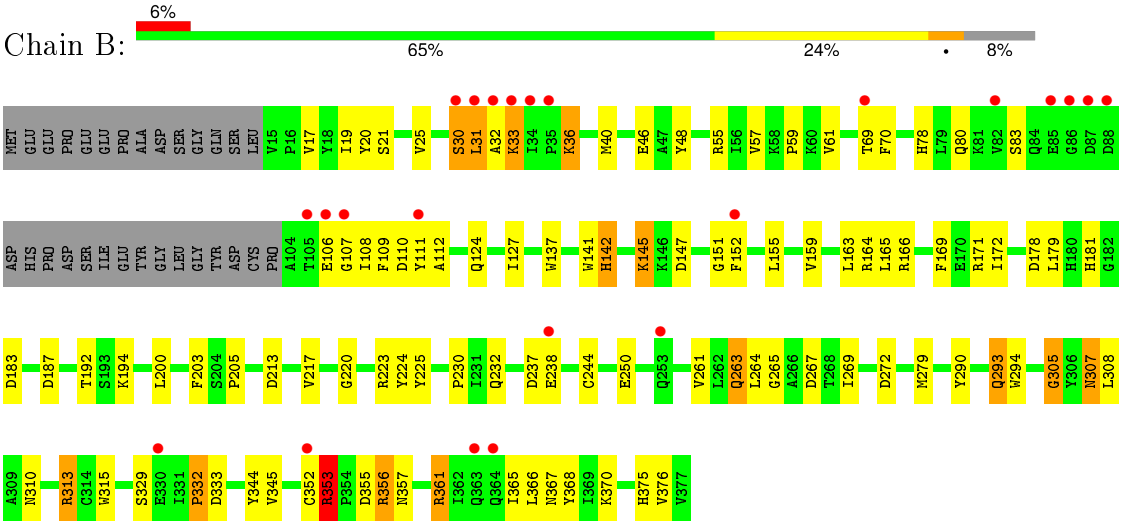
- Molecule 1: Histone deacetylase 8

Chain A:



- Molecule 1: Histone deacetylase 8

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	82.63Å 92.71Å 98.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 7.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.5 (7.00-2.20) 96.3 (7.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.65 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.237 , 0.304 0.256 , 0.267	Depositor DCC
R_{free} test set	1866 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 99.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 36638 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11640	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: NA, ZN, CRI

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	1.35	2/2807 (0.1%)	1.43	32/3802 (0.8%)
1	B	1.37	4/2780 (0.1%)	1.47	35/3767 (0.9%)
All	All	1.36	6/5587 (0.1%)	1.45	67/7569 (0.9%)

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	0	11
1	B	0	7
All	All	0	18

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	GLU	CD-OE2	10.06	1.36	1.25
1	A	238	GLU	CD-OE2	9.99	1.36	1.25
1	B	141	TRP	CG-CD2	-5.46	1.34	1.43
1	B	315	TRP	CB-CG	5.35	1.59	1.50
1	B	46	GLU	CG-CD	5.25	1.59	1.51
1	A	315	TRP	CG-CD2	-5.18	1.34	1.43

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	294	TRP	CD1-NE1-CE2	9.78	117.80	109.00
1	A	141	TRP	CD1-NE1-CE2	9.59	117.63	109.00
1	B	294	TRP	CD1-NE1-CE2	9.33	117.39	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	141	TRP	CD1-NE1-CE2	9.20	117.28	109.00
1	A	137	TRP	CD1-NE1-CE2	8.82	116.94	109.00
1	A	164	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	B	137	TRP	CD1-NE1-CE2	8.50	116.65	109.00
1	A	315	TRP	CD1-NE1-CE2	8.46	116.61	109.00
1	B	141	TRP	NE1-CE2-CZ2	8.15	139.36	130.40
1	B	315	TRP	CD1-NE1-CE2	8.00	116.20	109.00
1	A	137	TRP	NE1-CE2-CZ2	7.81	139.00	130.40
1	B	294	TRP	NE1-CE2-CZ2	7.63	138.79	130.40
1	A	315	TRP	NE1-CE2-CZ2	7.57	138.73	130.40
1	A	141	TRP	NE1-CE2-CZ2	7.41	138.55	130.40
1	A	353	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	137	TRP	CG-CD1-NE1	-7.24	102.86	110.10
1	B	307	ASN	N-CA-C	-7.07	91.91	111.00
1	B	141	TRP	CG-CD1-NE1	-6.91	103.19	110.10
1	B	294	TRP	CG-CD1-NE1	-6.83	103.27	110.10
1	A	294	TRP	NE1-CE2-CZ2	6.82	137.90	130.40
1	A	200	LEU	N-CA-C	-6.80	92.63	111.00
1	B	137	TRP	NE1-CE2-CZ2	6.72	137.79	130.40
1	B	244	CYS	CA-CB-SG	6.72	126.09	114.00
1	B	315	TRP	NE1-CE2-CZ2	6.67	137.74	130.40
1	A	223	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	267	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	B	137	TRP	CG-CD1-NE1	-6.58	103.53	110.10
1	B	353	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	294	TRP	CG-CD1-NE1	-6.50	103.60	110.10
1	B	313	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	30	SER	N-CA-C	6.41	128.30	111.00
1	A	294	TRP	NE1-CE2-CD2	-6.37	100.93	107.30
1	A	244	CYS	CA-CB-SG	6.33	125.39	114.00
1	B	141	TRP	NE1-CE2-CD2	-6.24	101.06	107.30
1	A	313	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	141	TRP	NE1-CE2-CD2	-6.21	101.08	107.30
1	B	333	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	141	TRP	CG-CD1-NE1	-6.15	103.95	110.10
1	B	294	TRP	NE1-CE2-CD2	-6.06	101.24	107.30
1	A	315	TRP	NE1-CE2-CD2	-6.06	101.24	107.30
1	A	213	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	61	VAL	N-CA-C	-5.98	94.85	111.00
1	A	315	TRP	CG-CD1-NE1	-5.97	104.12	110.10
1	A	356	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	B	200	LEU	N-CA-C	-5.72	95.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	TRP	NE1-CE2-CD2	-5.70	101.60	107.30
1	A	261	VAL	N-CA-C	-5.54	96.05	111.00
1	B	78	HIS	CA-CB-CG	-5.53	104.20	113.60
1	B	261	VAL	N-CA-C	-5.48	96.19	111.00
1	B	315	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	B	137	TRP	NE1-CE2-CD2	-5.31	101.99	107.30
1	B	36	LYS	N-CA-C	5.27	125.24	111.00
1	A	299	LEU	N-CA-C	-5.24	96.85	111.00
1	A	176	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	315	TRP	NE1-CE2-CD2	-5.20	102.10	107.30
1	B	213	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	272	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	A	315	TRP	CG-CD2-CE3	-5.17	129.25	133.90
1	B	356	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	141	TRP	CG-CD2-CE3	-5.13	129.28	133.90
1	B	61	VAL	N-CA-C	-5.11	97.20	111.00
1	B	357	ASN	CA-CB-CG	-5.11	102.17	113.40
1	B	147	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	B	305	GLY	N-CA-C	-5.08	100.41	113.10
1	A	55	ARG	N-CA-C	-5.05	97.36	111.00
1	B	355	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	287	CYS	CA-CB-SG	5.03	123.05	114.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	167	ARG	Sidechain
1	A	171	ARG	Sidechain
1	A	208	PHE	Peptide
1	A	223	ARG	Sidechain
1	A	313	ARG	Sidechain
1	A	356	ARG	Sidechain
1	A	361	ARG	Sidechain
1	A	37	ARG	Sidechain
1	A	55	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	223	ARG	Sidechain
1	B	313	ARG	Sidechain
1	B	353	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	356	ARG	Sidechain
1	B	361	ARG	Sidechain
1	B	55	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2717	2684	2656	70	1
1	B	2715	2682	2679	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	22	23	1	0
4	B	31	22	22	0	0
5	A	129	258	0	1	0
5	B	115	230	0	0	1
All	All	5742	5898	5380	114	1

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 11.

All (114) 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:33:LYS:CB	1:B:33:LYS:HG3	1.66	1.24
1:A:33:LYS:HB3	1:B:33:LYS:CG	1.70	1.20
1:A:33:LYS:HB3	1:B:33:LYS:HG3	0.88	0.86
1:A:69:THR:HG22	1:A:163:LEU:HD13	1.61	0.83
1:B:366:LEU:O	1:B:370:LYS:HG3	1.90	0.71
1:A:263:GLN:HE21	1:A:263:GLN:C	1.95	0.70
1:A:178:ASP:HB2	1:A:263:GLN:HE22	1.57	0.69
1:A:193:SER:HB2	1:A:225:TYR:CE2	2.31	0.65
1:B:194:LYS:HE2	1:B:194:LYS:HA	1.77	0.65
1:A:33:LYS:HB3	1:B:33:LYS:CB	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HE3	5:A:471:HOH:O	1.96	0.64
1:B:124:GLN:NE2	1:B:164:ARG:HE	1.96	0.62
1:A:366:LEU:O	1:A:370[A]:LYS:HG3	1.99	0.61
1:A:366:LEU:O	1:A:370[B]:LYS:HG3	1.99	0.60
1:A:64:MET:SD	1:A:76:LEU:HB3	2.42	0.59
1:B:112:ALA:HB1	1:B:155:LEU:HB2	1.85	0.57
1:B:31:LEU:HG	1:B:111:TYR:CD2	2.40	0.56
1:A:31:LEU:O	1:A:33:LYS:N	2.39	0.56
1:B:70:PHE:CD1	1:B:159:VAL:HG11	2.41	0.55
1:B:69:THR:HG22	1:B:163:LEU:HD13	1.89	0.55
1:A:329:SER:O	1:A:345:VAL:HA	2.06	0.54
1:A:30:SER:N	1:A:34:ILE:HG21	2.22	0.54
1:B:31:LEU:O	1:B:33:LYS:N	2.41	0.53
1:A:145:LYS:CE	1:A:184:GLY:HA2	2.38	0.53
1:A:290:TYR:O	1:A:293:GLN:HG3	2.07	0.53
1:B:203:PHE:CB	1:B:230:PRO:HB3	2.40	0.52
1:A:203:PHE:HB3	1:A:230:PRO:HB3	1.91	0.51
1:A:203:PHE:CB	1:A:230:PRO:HB3	2.41	0.51
1:A:20:TYR:CD1	1:A:21:SER:N	2.79	0.51
1:B:178:ASP:HB2	1:B:263:GLN:OE1	2.11	0.51
1:A:250:GLU:HG3	1:A:370[A]:LYS:HG2	1.94	0.50
1:A:250:GLU:HG3	1:A:370[B]:LYS:HG2	1.94	0.50
1:A:143:HIS:O	1:A:150:SER:HB3	2.12	0.50
1:A:191:PHE:CE2	1:A:219:LEU:HB2	2.47	0.50
1:A:225:TYR:CE2	1:A:376:VAL:HG13	2.46	0.49
1:A:145:LYS:NZ	1:A:145:LYS:HA	2.27	0.49
1:B:69:THR:HG22	1:B:163:LEU:CD1	2.43	0.49
1:B:107:GLY:O	1:B:110:ASP:N	2.46	0.49
1:B:290:TYR:O	1:B:293:GLN:HG3	2.13	0.49
1:B:290:TYR:O	1:B:293:GLN:CG	2.61	0.48
1:A:31:LEU:HG	1:A:111:TYR:CD2	2.49	0.48
1:B:181:HIS:CD2	1:B:183:ASP:HB3	2.49	0.48
1:A:263:GLN:NE2	1:A:265:GLY:H	2.12	0.48
1:B:17:VAL:HG13	1:B:57:VAL:CG2	2.43	0.48
1:B:48:TYR:CE2	1:B:332:PRO:HD2	2.48	0.48
1:A:178:ASP:HB2	1:A:263:GLN:NE2	2.27	0.48
1:A:205:PRO:O	1:B:353:ARG:HD2	2.14	0.48
1:B:33:LYS:HB3	1:B:33:LYS:NZ	2.29	0.47
1:A:208:PHE:CE1	4:A:402:CRI:H26	2.50	0.47
1:B:263:GLN:C	1:B:263:GLN:HE21	2.18	0.47
1:A:225:TYR:CZ	1:A:376:VAL:HG13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:HG3	1:A:66:GLU:N	2.30	0.47
1:A:196:MET:SD	1:A:251:VAL:HG13	2.55	0.47
1:A:33:LYS:HB2	1:B:33:LYS:HG3	1.81	0.46
1:A:205:PRO:HG2	1:B:352:CYS:O	2.16	0.46
1:B:106:GLU:CD	1:B:106:GLU:N	2.69	0.46
1:A:84:GLN:HG2	1:A:85:GLU:H	1.81	0.46
1:A:193:SER:HB2	1:A:225:TYR:CZ	2.50	0.46
1:A:223:ARG:HG2	1:A:224:TYR:CE1	2.51	0.46
1:B:127:ILE:HD11	1:B:165:LEU:HA	1.97	0.46
1:B:124:GLN:NE2	1:B:164:ARG:HH21	2.14	0.46
1:A:293:GLN:C	1:A:293:GLN:HE21	2.18	0.45
1:A:341:GLY:HA2	1:A:344:TYR:CE1	2.51	0.45
1:B:361:ARG:HE	1:B:365:ILE:HD11	1.81	0.45
1:A:83:SER:O	1:A:106:GLU:HA	2.16	0.45
1:B:40:MET:SD	1:B:308:LEU:HB3	2.55	0.45
1:B:375:HIS:N	1:B:375:HIS:CD2	2.84	0.45
1:A:231:ILE:CG2	1:A:357:ASN:HD21	2.28	0.45
1:A:205:PRO:O	1:B:353:ARG:CD	2.65	0.45
1:A:24:TYR:CE1	1:A:28:CYS:SG	3.10	0.45
1:A:218:GLY:HA3	1:A:222:GLY:O	2.17	0.45
1:B:225:TYR:CZ	1:B:376:VAL:HG13	2.52	0.45
1:A:166:ARG:HA	1:A:169:PHE:O	2.17	0.44
1:B:106:GLU:H	1:B:106:GLU:CD	2.21	0.44
1:A:146:LYS:HG3	1:A:147:ASP:N	2.32	0.44
1:A:82:VAL:O	1:A:84:GLN:N	2.50	0.44
1:A:19:ILE:CG2	1:A:59:PRO:HB3	2.48	0.44
1:A:340:TYR:CD1	1:A:340:TYR:N	2.86	0.44
1:B:48:TYR:CZ	1:B:332:PRO:HD3	2.53	0.44
1:B:329:SER:O	1:B:345:VAL:HA	2.17	0.43
1:A:20:TYR:CG	1:A:21:SER:N	2.86	0.43
1:A:235:ILE:HD11	1:A:240:TYR:HA	2.00	0.43
1:A:20:TYR:CE1	1:A:25:VAL:HG21	2.53	0.43
1:A:214:VAL:HG22	1:A:368:TYR:CD2	2.53	0.43
1:A:347:GLU:CD	1:A:347:GLU:H	2.21	0.43
1:B:20:TYR:CE1	1:B:25:VAL:HG21	2.54	0.43
1:A:163:LEU:O	1:A:166:ARG:HB2	2.19	0.42
1:A:307:ASN:O	1:A:308:LEU:C	2.57	0.42
1:B:80:GLN:HA	1:B:109:PHE:CG	2.54	0.42
1:A:24:TYR:O	1:A:27:MET:HB3	2.20	0.42
1:A:171:ARG:HD2	1:A:255:PHE:O	2.19	0.42
1:B:352:CYS:O	1:B:352:CYS:SG	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HD13	1:A:169:PHE:CE1	2.55	0.42
1:B:30:SER:O	1:B:31:LEU:C	2.58	0.42
1:B:269:ILE:HA	1:B:279:MET:O	2.20	0.41
1:A:223:ARG:HG2	1:A:224:TYR:CD1	2.55	0.41
1:B:145:LYS:HZ2	1:B:145:LYS:HB3	1.84	0.41
1:A:231:ILE:HG22	1:A:357:ASN:HD21	1.86	0.41
1:A:234:GLY:HA3	1:A:354:PRO:O	2.20	0.41
1:A:162:ILE:O	1:A:163:LEU:C	2.57	0.41
1:B:217:VAL:O	1:B:224:TYR:N	2.50	0.41
1:A:145:LYS:NZ	1:A:184:GLY:HA2	2.35	0.41
1:B:151:GLY:O	1:B:152:PHE:HB2	2.21	0.41
1:B:264:LEU:O	1:B:265:GLY:C	2.59	0.41
1:B:250:GLU:HG3	1:B:370:LYS:HG2	2.03	0.41
1:B:367:ASN:O	1:B:368:TYR:C	2.58	0.40
1:B:169:PHE:HB2	1:B:172:ILE:HD11	2.03	0.40
1:A:178:ASP:CB	1:A:263:GLN:HE22	2.29	0.40
1:B:263:GLN:C	1:B:263:GLN:NE2	2.75	0.40
1:B:19:ILE:CG2	1:B:59:PRO:HB3	2.51	0.40
1:A:268:THR:HA	1:A:277:PHE:HB2	2.04	0.40
1:B:232:GLN:HE21	1:B:232:GLN:HA	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:O	5:B:472:HOH:H1[2_564]	1.50	0.10

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	347/377 (92%)	292 (84%)	43 (12%)	12 (4%)	4 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	344/377 (91%)	295 (86%)	35 (10%)	14 (4%)	3 1
All	All	691/754 (92%)	587 (85%)	78 (11%)	26 (4%)	4 1

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ALA
1	A	83	SER
1	B	31	LEU
1	B	32	ALA
1	B	36	LYS
1	B	237	ASP
1	B	272	ASP
1	B	344	TYR
1	A	31	LEU
1	A	108	ILE
1	A	129	GLY
1	A	220	GLY
1	B	108	ILE
1	B	179	LEU
1	A	308	LEU
1	B	142	HIS
1	A	152	PHE
1	A	305	GLY
1	A	205	PRO
1	B	83	SER
1	B	205	PRO
1	B	220	GLY
1	B	332	PRO
1	B	305	GLY
1	A	332	PRO
1	A	184	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	294/316 (93%)	280 (95%)	14 (5%)	31	37
1	B	291/316 (92%)	280 (96%)	11 (4%)	40	49
All	All	585/632 (93%)	560 (96%)	25 (4%)	37	43

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	84	GLN
1	A	142	HIS
1	A	145	LYS
1	A	166	ARG
1	A	215	SER
1	A	238	GLU
1	A	239[A]	LYS
1	A	239[B]	LYS
1	A	263	GLN
1	A	267	ASP
1	A	293	GLN
1	A	307	ASN
1	A	338	THR
1	B	21	SER
1	B	33	LYS
1	B	142	HIS
1	B	145	LYS
1	B	166	ARG
1	B	187	ASP
1	B	192	THR
1	B	263	GLN
1	B	293	GLN
1	B	307	ASN
1	B	310	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	124	GLN
1	A	181	HIS
1	A	232	GLN
1	A	256	ASN

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Mol	Chain	Res	Type
1	A	263	GLN
1	A	293	GLN
1	A	307	ASN
1	A	310	ASN
1	A	357	ASN
1	B	80	GLN
1	B	84	GLN
1	B	124	GLN
1	B	181	HIS
1	B	232	GLN
1	B	293	GLN
1	B	372	ASN
1	B	375	HIS

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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	CRI	A	402	2	33,33,33	2.35	6 (18%)	44,46,46	1.06	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CRI	B	402	2	33,33,33	2.23	6 (18%)	44,46,46	1.03	3 (6%)

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
4	CRI	A	402	2	-	0/26/26/26	0/3/3/3
4	CRI	B	402	2	-	0/26/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	CRI	C15-C20	-7.38	1.38	1.50
4	B	402	CRI	C15-C20	-6.08	1.40	1.50
4	A	402	CRI	C2-C	-5.31	1.38	1.50
4	A	402	CRI	C13-N31	-4.99	1.32	1.41
4	B	402	CRI	C40-C33	-4.75	1.40	1.50
4	B	402	CRI	C13-N31	-4.49	1.33	1.41
4	A	402	CRI	C40-C33	-4.39	1.40	1.50
4	B	402	CRI	C2-C	-4.33	1.41	1.50
4	B	402	CRI	C11-C5	-4.05	1.38	1.49
4	A	402	CRI	C11-C5	-4.04	1.38	1.49
4	A	402	CRI	C-N	5.03	1.39	1.32
4	B	402	CRI	C-N	5.24	1.39	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	402	CRI	C13-N31-C33	-3.05	119.58	126.78
4	A	402	CRI	C13-N31-C33	-2.95	119.81	126.78
4	A	402	CRI	O21-C20-C15	-2.29	115.84	120.17
4	B	402	CRI	O-C-N	-2.23	117.65	122.86
4	B	402	CRI	O34-C33-C40	-2.19	117.22	120.97
4	A	402	CRI	C11-C16-C15	2.06	123.21	121.19
4	A	402	CRI	C14-C15-C20	2.06	124.61	120.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	CRI	1	0

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	348/377 (92%)	0.12	21 (6%)	25	25	23, 46, 78, 100	0
1	B	348/377 (92%)	-0.01	23 (6%)	22	21	17, 42, 76, 100	0
All	All	696/754 (92%)	0.06	44 (6%)	23	23	17, 44, 78, 100	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	LEU	9.7
1	A	31	LEU	8.7
1	B	34	ILE	7.4
1	A	34	ILE	6.8
1	B	88	ASP	5.7
1	B	33	LYS	5.7
1	B	32	ALA	5.6
1	A	87	ASP	5.3
1	A	105	THR	5.2
1	B	105	THR	5.2
1	B	86	GLY	5.1
1	A	88	ASP	4.9
1	A	32	ALA	4.6
1	A	69	THR	4.5
1	B	352	CYS	4.4
1	A	85	GLU	3.7
1	B	87	ASP	3.7
1	A	33	LYS	3.6
1	A	81	LYS	3.6
1	B	69	THR	3.5
1	B	85	GLU	3.4
1	A	377	VAL	3.3
1	B	238	GLU	3.3
1	A	111	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	35	PRO	3.0
1	B	111	TYR	2.9
1	B	30	SER	2.9
1	A	222	GLY	2.8
1	B	253	GLN	2.7
1	B	330	GLU	2.5
1	B	106	GLU	2.5
1	B	82	VAL	2.5
1	A	330	GLU	2.4
1	B	152	PHE	2.4
1	B	35	PRO	2.4
1	A	253	GLN	2.3
1	A	110	ASP	2.3
1	A	60	LYS	2.1
1	B	363	GLN	2.1
1	B	364	GLN	2.1
1	A	30	SER	2.0
1	A	77	GLN	2.0
1	A	256	ASN	2.0
1	B	107	GLY	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	NA	A	401	1/1	0.78	0.23	9.30	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CRI	B	402	31/31	0.90	0.14	0.78	53,64,82,83	0
3	NA	B	401	1/1	0.94	0.10	0.07	30,30,30,30	0
4	CRI	A	402	31/31	0.92	0.14	-0.01	37,63,77,81	0
2	ZN	B	400	1/1	0.99	0.03	-3.44	44,44,44,44	0
2	ZN	A	400	1/1	0.99	0.03	-4.27	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.