Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:14 AM GMT

PDB ID	:	3DWB
Title	:	structure of human ECE-1 complexed with phosphoramidon
Authors	:	Oefner, C.
Deposited on	:	2008-07-22
Resolution	:	2.38 Å(reported)

The following versions of software and data (see references (i)) 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 2.38 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.
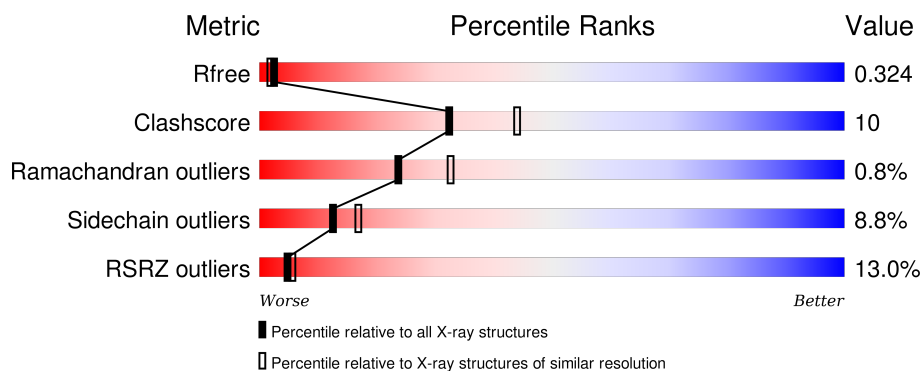
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	670	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5580 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 Endothelin-converting enzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			5305	3371	896	1011	27			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	SER	CYS	ENGINEERED	UNP P42892

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

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

- Molecule 3 is 5-(2-HYDROXYETHYL)NONANE-1,9-DIOL (three-letter code: 5HD) (formula: $C_{11}H_{24}O_3$).
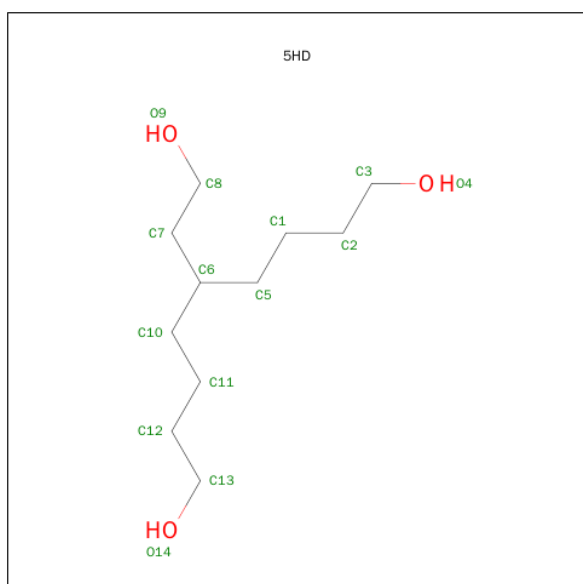
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 14	C 11	O 3	0	0

- Molecule 4 is N-ALPHA-L-RHAMNOPYRANOSYLOXY(HYDROXYPHOSPHINYL)-L-L EUCYL-L-TRYPTOPHAN (three-letter code: RDF) (formula: $C_{23}H_{34}N_3O_{10}P$).
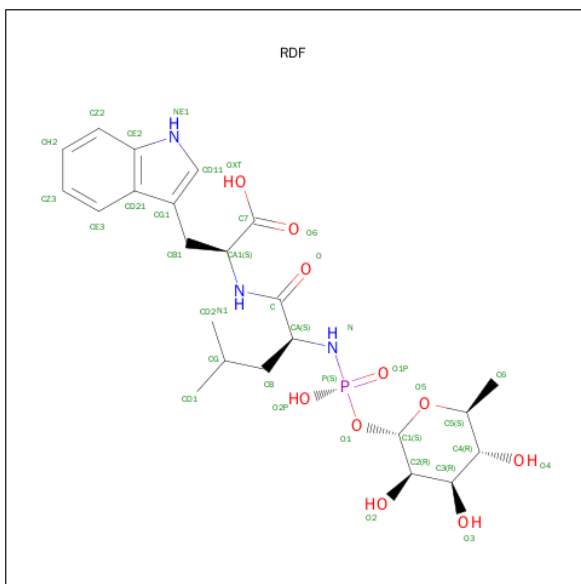
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 37	C 23	N 3	O 10	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total 223	O 223	0	0

3 Residue-property plots ⓘ

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: Endothelin-converting enzyme 1
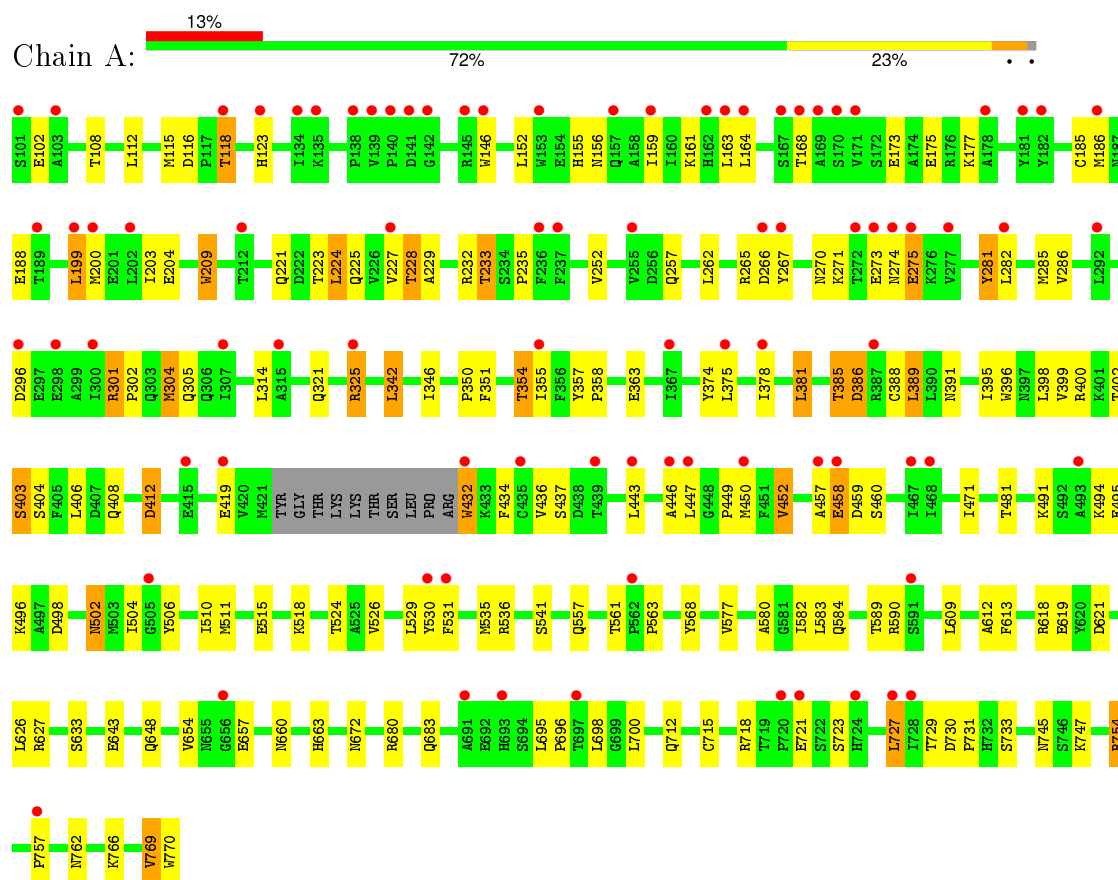
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.88Å 120.88Å 192.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.38 19.96 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.38) 99.1 (19.96-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	2.72 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.262 , 0.345 0.251 , 0.324	Depositor DCC
R_{free} test set	1705 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.0	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 33591 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5580	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5HD, RDF, ZN

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	0.91	12/5445 (0.2%)	0.78	8/7393 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	GLU	CD-OE2	33.18	1.62	1.25
1	A	275	GLU	CD-OE2	11.90	1.38	1.25
1	A	412	ASP	CG-OD1	10.97	1.50	1.25
1	A	419	GLU	CD-OE1	10.11	1.36	1.25
1	A	188	GLU	CG-CD	9.50	1.66	1.51
1	A	275	GLU	CD-OE1	9.03	1.35	1.25
1	A	458	GLU	CD-OE1	8.85	1.35	1.25
1	A	458	GLU	CD-OE2	6.29	1.32	1.25
1	A	419	GLU	CD-OE2	5.98	1.32	1.25
1	A	459	ASP	CG-OD2	5.93	1.39	1.25
1	A	281	TYR	C-O	5.83	1.34	1.23
1	A	408	GLN	C-O	5.11	1.33	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLU	OE1-CD-OE2	13.20	139.14	123.30
1	A	188	GLU	CG-CD-OE2	-11.89	94.53	118.30
1	A	412	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	754	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	621	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	342	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	769	VAL	CB-CA-C	5.08	121.06	111.40
1	A	680	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5305	0	5097	105	0
2	A	1	0	0	0	0
3	A	14	0	24	1	0
4	A	37	0	32	5	0
5	A	223	0	0	8	2
All	All	5580	0	5153	110	2

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 10.

All (110) 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)
4:A:817:RDF:CD11	4:A:817:RDF:HD1	0.97	1.10
4:A:817:RDF:CG1	4:A:817:RDF:HD1	2.10	0.82
1:A:648:GLN:HE22	1:A:745:ASN:HD21	1.28	0.81
1:A:363:GLU:HB2	5:A:987:HOH:O	1.80	0.81
1:A:580:ALA:HA	1:A:583:LEU:HD12	1.64	0.80
1:A:381:LEU:O	1:A:385:THR:HG23	1.82	0.79
4:A:817:RDF:CG1	4:A:817:RDF:CE3	2.52	0.77
1:A:391:ASN:O	1:A:395:ILE:HD12	1.86	0.76
1:A:526:VAL:HG11	1:A:529:LEU:HD12	1.67	0.75
1:A:209:TRP:HB3	1:A:395:ILE:HD13	1.70	0.73
4:A:817:RDF:CE2	4:A:817:RDF:CE3	2.41	0.72
1:A:458:GLU:OE2	1:A:506:TYR:OH	2.09	0.70
1:A:203:ILE:HD11	1:A:209:TRP:CD1	2.26	0.70
1:A:270:ASN:HB3	1:A:274:ASN:HD21	1.57	0.70
1:A:654:VAL:O	1:A:657:GLU:HG3	1.93	0.68
1:A:233:THR:HG22	1:A:235:PRO:HD3	1.73	0.68
1:A:524:THR:O	1:A:536:ARG:HD2	1.94	0.68
1:A:199:LEU:HB2	1:A:406:LEU:HD21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:817:RDF:NE1	4:A:817:RDF:HD1	2.08	0.68
1:A:123:HIS:ND1	5:A:874:HOH:O	2.26	0.67
1:A:164:LEU:HD21	1:A:447:LEU:HD21	1.79	0.65
1:A:285:MET:HB3	1:A:304:MET:HG3	1.76	0.65
1:A:672:ASN:HD21	1:A:745:ASN:HD22	1.46	0.64
1:A:285:MET:HB3	1:A:304:MET:CG	2.28	0.64
1:A:200:MET:O	1:A:203:ILE:HG22	1.98	0.62
1:A:654:VAL:O	1:A:657:GLU:CG	2.48	0.62
1:A:224:LEU:O	1:A:228:THR:HG23	1.99	0.62
1:A:199:LEU:HD12	1:A:406:LEU:HD11	1.82	0.62
1:A:116:ASP:OD1	1:A:118:THR:HG22	2.01	0.61
1:A:224:LEU:O	1:A:228:THR:CG2	2.49	0.60
1:A:502:ASN:ND2	1:A:504:ILE:HD11	2.17	0.59
1:A:185:CYS:HB3	1:A:530:TYR:CD1	2.38	0.58
1:A:399:VAL:O	1:A:403:SER:OG	2.21	0.58
1:A:173:GLU:O	1:A:177:LYS:HG3	2.05	0.57
1:A:386:ASP:OD1	1:A:389:LEU:HB2	2.05	0.57
1:A:281:TYR:O	1:A:285:MET:HG3	2.05	0.56
1:A:156:ASN:HA	1:A:159:ILE:HD12	1.86	0.56
1:A:449:PRO:HD3	1:A:510:ILE:HD12	1.86	0.56
1:A:203:ILE:HG23	1:A:204:GLU:N	2.20	0.56
1:A:161:LYS:HG3	1:A:436:VAL:HG21	1.87	0.55
1:A:648:GLN:NE2	1:A:745:ASN:HD21	2.01	0.55
1:A:229:ALA:HB2	1:A:355:ILE:HG22	1.89	0.55
1:A:203:ILE:CD1	1:A:209:TRP:CD1	2.90	0.55
1:A:515:GLU:OE1	1:A:518:LYS:NZ	2.35	0.54
1:A:510:ILE:HD11	1:A:511:MET:HE2	1.90	0.53
1:A:557:GLN:HE21	3:A:816:5HD:H11	1.74	0.52
1:A:762:ASN:OD1	1:A:766:LYS:NZ	2.42	0.52
1:A:185:CYS:HB3	1:A:530:TYR:CE1	2.45	0.52
1:A:396:TRP:O	1:A:399:VAL:HG22	2.09	0.52
1:A:350:PRO:O	1:A:354:THR:HG22	2.09	0.51
1:A:723:SER:O	1:A:727:LEU:HB2	2.10	0.51
1:A:443:LEU:O	1:A:446:ALA:HB3	2.10	0.51
1:A:496:LYS:HE2	1:A:612:ALA:HB1	1.91	0.51
1:A:325:ARG:NH2	5:A:846:HOH:O	2.43	0.51
1:A:155:HIS:NE2	1:A:159:ILE:HD11	2.27	0.50
1:A:186:MET:SD	1:A:432:TRP:HE3	2.35	0.50
1:A:257:GLN:HB3	1:A:374:TYR:CZ	2.47	0.50
1:A:729:THR:O	5:A:929:HOH:O	2.19	0.50
1:A:203:ILE:CG2	1:A:204:GLU:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:O	1:A:286:VAL:HG23	2.12	0.49
1:A:683:GLN:HG3	5:A:993:HOH:O	2.13	0.49
1:A:374:TYR:CZ	1:A:378:ILE:HD11	2.48	0.49
1:A:163:LEU:HD22	1:A:450:MET:HB3	1.94	0.49
1:A:452:VAL:HG21	1:A:511:MET:HE3	1.95	0.49
1:A:695:LEU:HB2	1:A:698:LEU:HD12	1.95	0.48
1:A:672:ASN:ND2	1:A:745:ASN:HD22	2.10	0.47
1:A:730:ASP:OD1	1:A:731:PRO:HD2	2.14	0.47
1:A:582:ILE:C	1:A:584:GLN:H	2.18	0.47
1:A:342:LEU:HD11	1:A:375:LEU:HB2	1.96	0.47
1:A:223:THR:O	1:A:227:VAL:HG22	2.13	0.47
1:A:357:TYR:CG	1:A:358:PRO:HA	2.49	0.47
1:A:267:TYR:O	1:A:271:LYS:HB2	2.14	0.47
1:A:618:ARG:HG3	1:A:619:GLU:N	2.29	0.47
1:A:164:LEU:HD21	1:A:447:LEU:CD2	2.44	0.47
1:A:203:ILE:HD11	1:A:209:TRP:CG	2.51	0.46
1:A:285:MET:HG2	1:A:396:TRP:CZ2	2.51	0.46
1:A:613:PHE:HB3	1:A:770:TRP:CZ2	2.51	0.46
1:A:712:GLN:HA	1:A:715:CYS:SG	2.56	0.45
1:A:747:LYS:HD2	5:A:1021:HOH:O	2.14	0.45
1:A:698:LEU:HD22	1:A:700:LEU:HD12	1.98	0.45
1:A:346:ILE:HD12	1:A:346:ILE:H	1.82	0.45
1:A:262:LEU:HD21	1:A:281:TYR:CD2	2.52	0.44
1:A:350:PRO:O	1:A:354:THR:CG2	2.66	0.44
1:A:449:PRO:CD	1:A:510:ILE:HD12	2.48	0.44
1:A:395:ILE:O	1:A:399:VAL:HG13	2.18	0.44
1:A:568:TYR:CE1	1:A:577:VAL:HB	2.52	0.44
1:A:657:GLU:HB3	5:A:902:HOH:O	2.18	0.43
1:A:357:TYR:HA	5:A:1014:HOH:O	2.18	0.43
1:A:502:ASN:ND2	1:A:504:ILE:CD1	2.82	0.43
1:A:273:GLU:HG2	1:A:274:ASN:OD1	2.19	0.42
1:A:457:ALA:O	1:A:460:SER:HB2	2.19	0.42
1:A:494:LYS:NZ	1:A:498:ASP:OD2	2.50	0.42
1:A:108:THR:HG23	1:A:698:LEU:HG	2.00	0.42
1:A:531:PHE:O	1:A:535:MET:HG2	2.19	0.42
1:A:221:GLN:HG2	1:A:225:GLN:NE2	2.33	0.42
1:A:225:GLN:HE21	1:A:351:PHE:HA	1.85	0.42
1:A:301:ARG:HB2	1:A:302:PRO:HD3	2.00	0.42
1:A:155:HIS:CE1	1:A:159:ILE:HD11	2.54	0.42
1:A:285:MET:HB3	1:A:304:MET:HG2	2.02	0.42
1:A:471:ILE:HG22	1:A:609:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:O	1:A:398:LEU:HB3	2.20	0.41
1:A:285:MET:HA	1:A:396:TRP:CH2	2.55	0.41
1:A:745:ASN:HA	1:A:766:LYS:HG2	2.01	0.41
1:A:561:THR:C	1:A:563:PRO:HD2	2.41	0.41
1:A:660:ASN:HB3	1:A:663:HIS:HB3	2.02	0.41
1:A:175:GLU:HB3	1:A:450:MET:HE2	2.03	0.41
1:A:402:THR:CG2	1:A:531:PHE:CE2	3.03	0.40
1:A:502:ASN:HD21	1:A:504:ILE:HD11	1.84	0.40
1:A:112:LEU:HD21	1:A:698:LEU:HD23	2.03	0.40
1:A:342:LEU:HD13	1:A:342:LEU:C	2.42	0.40

All (2) 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)
5:A:887:HOH:O	5:A:887:HOH:O[12_555]	1.84	0.36
5:A:821:HOH:O	5:A:987:HOH:O[7_655]	1.97	0.23

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	656/670 (98%)	621 (95%)	30 (5%)	5 (1%)	24	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	PHE
1	A	696	PRO
1	A	727	LEU
1	A	275	GLU
1	A	757	PRO

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	581/590 (98%)	530 (91%)	51 (9%)	12 17

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLU
1	A	115	MET
1	A	118	THR
1	A	146	TRP
1	A	152	LEU
1	A	168	THR
1	A	199	LEU
1	A	209	TRP
1	A	224	LEU
1	A	228	THR
1	A	232	ARG
1	A	233	THR
1	A	252	VAL
1	A	265	ARG
1	A	266	ASP
1	A	296	ASP
1	A	301	ARG
1	A	304	MET
1	A	305	GLN
1	A	314	LEU
1	A	321	GLN
1	A	325	ARG
1	A	354	THR
1	A	381	LEU
1	A	385	THR
1	A	386	ASP
1	A	388	CYS
1	A	389	LEU
1	A	400	ARG
1	A	403	SER

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Mol	Chain	Res	Type
1	A	404	SER
1	A	412	ASP
1	A	432	TRP
1	A	437	SER
1	A	452	VAL
1	A	481	THR
1	A	491	LYS
1	A	495	GLU
1	A	502	ASN
1	A	541	SER
1	A	589	THR
1	A	590	ARG
1	A	626	LEU
1	A	627	ARG
1	A	633	SER
1	A	643	GLU
1	A	718	ARG
1	A	721	GLU
1	A	733	SER
1	A	754	ARG
1	A	769	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	166	ASN
1	A	179	GLN
1	A	225	GLN
1	A	321	GLN
1	A	392	ASN
1	A	411	GLN
1	A	442	ASN
1	A	502	ASN
1	A	557	GLN
1	A	632	ASN
1	A	641	GLN
1	A	648	GLN
1	A	655	ASN
1	A	672	ASN

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)

Of 3 ligands modelled in this entry, 1 is 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	#$|Z| > 2$
3	5HD	A	816	-	13,13,13	0.35	0	12,13,13	0.52	0
4	RDF	A	817	2	34,39,39	1.32	3 (8%)	40,57,57	2.16	6 (15%)

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	5HD	A	816	-	-	0/13/13/13	0/0/0/0
4	RDF	A	817	2	-	0/22/50/50	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	817	RDF	CB1-CA1	2.11	1.56	1.53
4	A	817	RDF	P-O1P	2.29	1.48	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	817	RDF	P-N	5.07	1.66	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	817	RDF	O1-P-O1P	-9.55	98.10	115.51
4	A	817	RDF	O5-C1-O1	-3.81	106.34	111.36
4	A	817	RDF	C3-C4-C5	-2.31	105.82	109.72
4	A	817	RDF	CB-CA-N	-2.20	106.32	110.23
4	A	817	RDF	O5-C5-C6	2.55	112.22	106.64
4	A	817	RDF	O2P-P-O1P	5.60	121.69	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	816	5HD	1	0
4	A	817	RDF	5	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 (i)

6.1   Protein, DNA and RNA chains (i)

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, 95th 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	660/670 (98%)	0.73	86 (13%)	5	5	24, 47, 77, 86	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	ALA	8.1
1	A	275	GLU	7.7
1	A	141	ASP	5.9
1	A	170	SER	5.4
1	A	168	THR	5.3
1	A	273	GLU	5.1
1	A	447	LEU	4.5
1	A	162	HIS	4.5
1	A	142	GLY	4.4
1	A	135	LYS	4.2
1	A	103	ALA	4.2
1	A	167	SER	4.0
1	A	443	LEU	3.8
1	A	307	ILE	3.8
1	A	315	ALA	3.7
1	A	138	PRO	3.7
1	A	189	THR	3.6
1	A	272	THR	3.6
1	A	255	VAL	3.5
1	A	435	CYS	3.5
1	A	757	PRO	3.5
1	A	159	ILE	3.4
1	A	415	GLU	3.3
1	A	274	ASN	3.3
1	A	697	THR	3.3
1	A	171	VAL	3.2
1	A	153	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	458	GLU	3.2
1	A	375	LEU	3.2
1	A	446	ALA	3.2
1	A	164	LEU	3.1
1	A	146	TRP	3.1
1	A	419	GLU	3.0
1	A	468	ILE	3.0
1	A	432	TRP	2.9
1	A	266	ASP	2.9
1	A	505	GLY	2.9
1	A	212	THR	2.9
1	A	387	ARG	2.9
1	A	163	LEU	2.9
1	A	181	TYR	2.8
1	A	186	MET	2.8
1	A	145	ARG	2.7
1	A	325	ARG	2.7
1	A	367	ILE	2.7
1	A	355	ILE	2.6
1	A	728	ILE	2.6
1	A	236	PHE	2.6
1	A	237	PHE	2.6
1	A	298	GLU	2.6
1	A	134	ILE	2.6
1	A	282	LEU	2.6
1	A	378	ILE	2.6
1	A	140	PRO	2.5
1	A	200	MET	2.5
1	A	531	PHE	2.5
1	A	457	ALA	2.5
1	A	277	VAL	2.5
1	A	267	TYR	2.4
1	A	123	HIS	2.4
1	A	467	ILE	2.4
1	A	296	ASP	2.4
1	A	691	ALA	2.4
1	A	724	HIS	2.4
1	A	178	ALA	2.4
1	A	439	THR	2.4
1	A	562	PRO	2.4
1	A	493	ALA	2.3
1	A	727	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	118	THR	2.3
1	A	300	ILE	2.2
1	A	693	HIS	2.2
1	A	720	PRO	2.2
1	A	157	GLN	2.2
1	A	227	VAL	2.2
1	A	591	SER	2.1
1	A	530	TYR	2.1
1	A	721	GLU	2.1
1	A	292	LEU	2.1
1	A	199	LEU	2.1
1	A	450	MET	2.1
1	A	182	TYR	2.1
1	A	139	VAL	2.1
1	A	202	LEU	2.0
1	A	101	SER	2.0
1	A	656	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, 95th 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	5HD	A	816	14/14	0.72	0.21	1.51	50,55,56,56	0
4	RDF	A	817	37/37	0.93	0.14	-0.18	36,42,45,48	0
2	ZN	A	771	1/1	0.99	0.02	-2.75	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.