Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 04:45 PM EDT

PDB ID	:	3CWW
Title	:	Crystal Structure of IDE-bradykinin complex
Authors	:	Malito, E.; Tang, W.J.
Deposited on	:	2008-04-23
Resolution	:	1.96 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

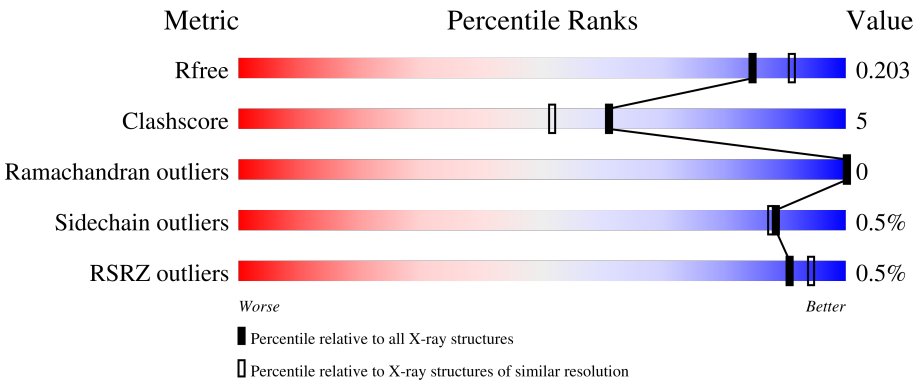
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.96 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	990	87% 9% ·
1	B	990	% 87% 9% ·
2	D	4	50% 50%
2	E	4	50% 25% 50% 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17281 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	953	7753	4999	1304	1428	22	0	0	0
1	B	953	7741	4993	1303	1423	22	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	78	ILE	MET	engineered mutation	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	365	ALA	GLU	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	508	ALA	GLU	engineered mutation	UNP P14735
A	511	ALA	LYS	engineered mutation	UNP P14735
A	517	ALA	ASP	engineered mutation	UNP P14735
A	542	ALA	LYS	engineered mutation	UNP P14735
A	543	ALA	GLU	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	555	ALA	VAL	engineered mutation	UNP P14735
A	567	PHE	LYS	engineered mutation	UNP P14735
A	568	PHE	LYS	engineered mutation	UNP P14735
A	569	LEU	LYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	657	ALA	LYS	engineered mutation	UNP P14735
A	705	ALA	ASP	engineered mutation	UNP P14735
A	764	ALA	VAL	engineered mutation	UNP P14735
A	765	ALA	ARG	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	845	GLY	SER	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	934	ALA	GLU	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
A	997	ALA	GLU	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	78	ILE	MET	engineered mutation	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	365	ALA	GLU	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	508	ALA	GLU	engineered mutation	UNP P14735
B	511	ALA	LYS	engineered mutation	UNP P14735
B	517	ALA	ASP	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	542	ALA	LYS	engineered mutation	UNP P14735
B	543	ALA	GLU	engineered mutation	UNP P14735
B	555	ALA	VAL	engineered mutation	UNP P14735
B	567	PHE	LYS	engineered mutation	UNP P14735
B	568	PHE	LYS	engineered mutation	UNP P14735
B	569	LEU	LYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	657	ALA	LYS	engineered mutation	UNP P14735
B	705	ALA	ASP	engineered mutation	UNP P14735
B	764	ALA	VAL	engineered mutation	UNP P14735
B	765	ALA	ARG	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	845	GLY	SER	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	934	ALA	GLU	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735
B	997	ALA	GLU	engineered mutation	UNP P14735

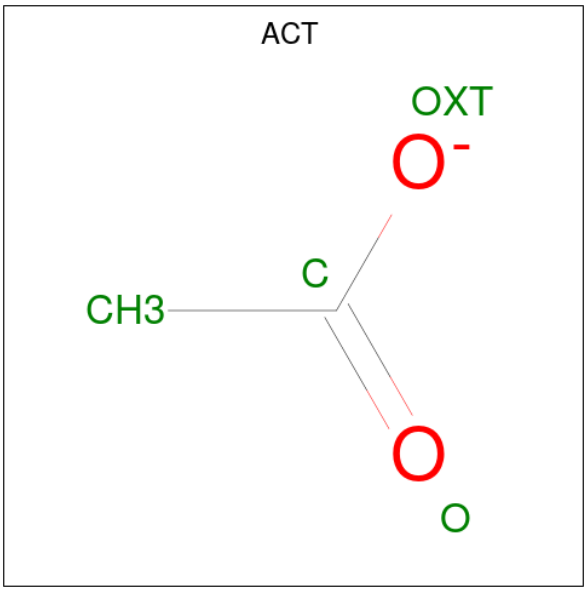
- Molecule 2 is a protein called bradykinin N-terminal tetrapeptide analogue.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	4	21	14	4	3	0	0	1
			Total	C	N	O			
2	E	3	19	13	3	3	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

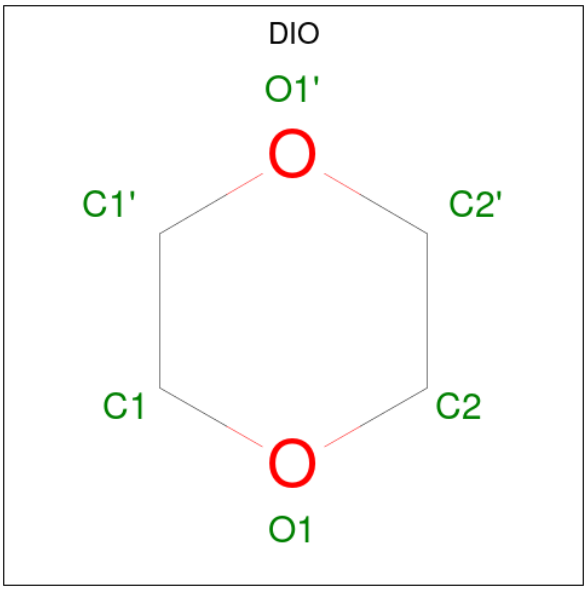
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
			Total	Zn		
3	B	1	1	1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	4	2	0	0
			Total	C	O		
5	A	1	6	4	2	0	0
			Total	C	O		
5	B	1	6	4	2	0	0
			Total	C	O		
5	B	1	6	4	2	0	0
			Total	C	O		
5	B	1	6	4	2	0	0

- Molecule 6 is water.

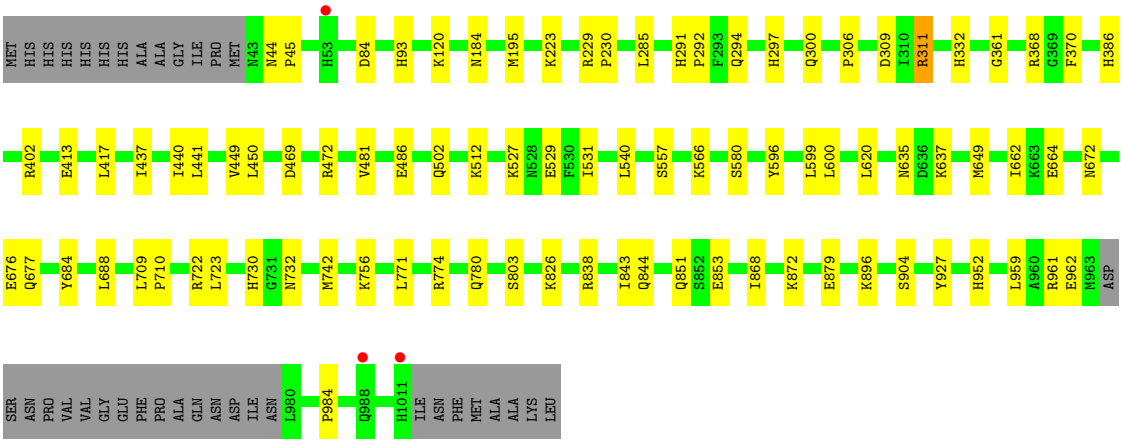
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	887	887	887	0	0
			Total	O		
6	B	812	812	812	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

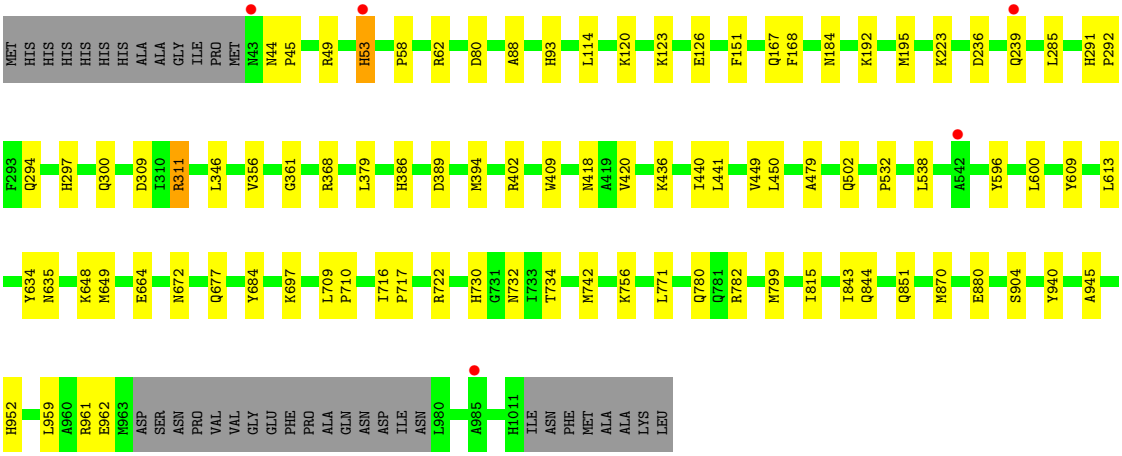
• Molecule 1: Insulin-degrading enzyme

Chain A:



• Molecule 1: Insulin-degrading enzyme

Chain B:

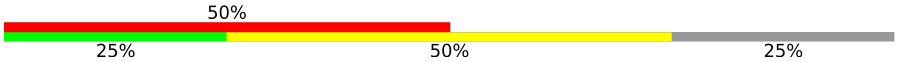


• Molecule 2: bradykinin N-terminal tetrapeptide analogue

Chain D:

• Molecule 2: bradykinin N-terminal tetrapeptide analogue

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	262.45Å 262.45Å 90.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.77 – 1.96 49.60 – 1.96	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.77-1.96) 97.6 (49.60-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 1.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.208 0.177 , 0.203	Depositor DCC
R_{free} test set	12504 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17281	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, ACT, DIO

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	0.48	0/7948	0.57	2/10758 (0.0%)
1	B	0.46	0/7936	0.56	1/10743 (0.0%)
2	D	0.41	0/22	0.75	0/31
2	E	0.41	0/20	0.74	0/28
All	All	0.47	0/15926	0.57	3/21560 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	311	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	838	ARG	NE-CZ-NH2	-5.14	117.73	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	7753	0	7706	69	0
1	B	7741	0	7692	72	0
2	D	21	0	22	3	0
2	E	19	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	6	0	0
4	B	8	0	6	1	0
5	A	12	0	16	1	0
5	B	18	0	24	1	0
6	A	887	0	0	11	0
6	B	812	0	0	10	0
All	All	17281	0	15493	141	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 5.

All (141) 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:B:239:GLN:NE2	6:B:4175:HOH:O	2.11	0.83
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.62	0.82
1:A:677:GLN:HE21	1:A:851:GLN:HE22	1.28	0.82
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.28	0.81
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.63	0.81
1:B:361:GLY:O	2:D:3:PRO:HD3	1.81	0.81
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.31	0.79
1:A:361:GLY:O	2:E:3:PRO:HD3	1.85	0.77
1:B:309:ASP:H	1:B:672:ASN:HD21	1.31	0.77
1:B:880:GLU:OE2	6:B:4293:HOH:O	2.03	0.77
1:A:557:SER:HB2	1:A:742:MET:CE	2.16	0.76
1:A:300:GLN:NE2	1:A:502:GLN:HE21	1.84	0.75
1:A:300:GLN:HE21	1:A:502:GLN:HE21	1.32	0.75
1:A:294:GLN:H	1:A:297:HIS:HD2	1.34	0.74
1:B:418:ASN:HD21	4:B:3003:ACT:H1	1.52	0.73
1:B:239:GLN:HA	1:B:239:GLN:OE1	1.88	0.72
1:A:309:ASP:H	1:A:672:ASN:HD21	1.40	0.70
1:B:479:ALA:HB2	5:B:4001:DIO:H21	1.72	0.70
1:A:332:HIS:HD2	6:A:4893:HOH:O	1.74	0.68
1:A:557:SER:HB2	1:A:742:MET:HE2	1.75	0.68
1:A:229:ARG:HD3	6:A:4823:HOH:O	1.95	0.66
1:B:294:GLN:H	1:B:297:HIS:HD2	1.42	0.66
1:B:309:ASP:H	1:B:672:ASN:ND2	1.93	0.66
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.27	0.66
1:B:53:HIS:ND1	1:B:53:HIS:N	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.78	0.65
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.95	0.65
1:A:600:LEU:HD23	1:A:620:LEU:HD21	1.80	0.63
1:A:120:LYS:NZ	6:A:4707:HOH:O	2.33	0.62
1:A:868:ILE:HD11	1:A:984:PRO:HG3	1.82	0.61
1:A:402:ARG:NH2	6:A:4553:HOH:O	2.33	0.61
1:A:93:HIS:CE1	1:A:368:ARG:HE	2.18	0.61
1:B:677:GLN:HE21	1:B:851:GLN:HE22	1.47	0.61
1:B:192:LYS:HD2	6:B:4784:HOH:O	2.02	0.60
1:A:417:LEU:HD21	1:A:531:ILE:HG12	1.81	0.60
1:B:195:MET:HE2	6:B:4745:HOH:O	2.01	0.59
1:A:780:GLN:HE21	1:A:959:LEU:HD21	1.67	0.59
1:A:961:ARG:HD2	1:A:962:GLU:OE2	2.03	0.59
1:B:780:GLN:HE21	1:B:959:LEU:HD11	1.69	0.58
1:A:361:GLY:O	2:E:2:PRO:HA	2.02	0.58
1:B:291:HIS:ND1	1:B:292:PRO:HD2	2.17	0.58
1:A:557:SER:HB2	1:A:742:MET:HE3	1.85	0.57
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.05	0.57
1:B:49:ARG:HD2	6:B:4755:HOH:O	2.04	0.57
1:B:635:ASN:HD21	1:B:732:ASN:HD22	1.52	0.57
1:B:114:LEU:HD13	1:B:168:PHE:HB3	1.87	0.56
1:A:93:HIS:HE1	1:A:368:ARG:NH2	2.01	0.55
1:B:961:ARG:HD2	1:B:962:GLU:OE2	2.06	0.55
1:A:309:ASP:H	1:A:672:ASN:ND2	2.03	0.55
1:A:635:ASN:HD21	1:A:732:ASN:HD22	1.54	0.55
6:B:4817:HOH:O	2:D:2:PRO:HB3	2.06	0.55
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.16	0.55
1:B:635:ASN:ND2	1:B:732:ASN:HD22	2.05	0.55
1:A:774:ARG:HD3	6:A:4824:HOH:O	2.07	0.55
1:B:386:HIS:HE1	6:B:4610:HOH:O	1.90	0.54
1:B:300:GLN:NE2	1:B:502:GLN:HE21	2.05	0.54
1:A:184:ASN:HD21	1:A:223:LYS:NZ	2.06	0.54
1:B:402:ARG:NH2	6:B:4454:HOH:O	2.40	0.54
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.88	0.53
1:B:93:HIS:CE1	1:B:368:ARG:HE	2.25	0.53
1:A:386:HIS:HE1	6:A:4432:HOH:O	1.92	0.53
1:A:730:HIS:HD2	1:A:904:SER:OG	1.90	0.53
1:B:609:TYR:CE2	1:B:613:LEU:HD11	2.44	0.52
1:B:780:GLN:HE21	1:B:959:LEU:HD21	1.74	0.52
1:A:677:GLN:NE2	1:A:851:GLN:HE22	2.03	0.52
1:B:780:GLN:NE2	1:B:959:LEU:HD11	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.45	0.51
1:B:294:GLN:H	1:B:297:HIS:CD2	2.27	0.51
1:B:309:ASP:N	1:B:672:ASN:HD21	2.06	0.51
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.20	0.51
1:A:512:LYS:NZ	6:A:4340:HOH:O	2.44	0.50
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.93	0.50
1:A:676:GLU:HA	1:A:676:GLU:OE1	2.10	0.50
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.39	0.50
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.93	0.49
1:B:93:HIS:HE1	1:B:368:ARG:NH2	2.05	0.49
1:A:635:ASN:ND2	1:A:732:ASN:HD22	2.10	0.49
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.94	0.49
1:A:294:GLN:H	1:A:297:HIS:CD2	2.22	0.49
1:B:236:ASP:CG	1:B:239:GLN:HG2	2.32	0.49
1:B:285:LEU:HD21	1:B:368:ARG:NE	2.28	0.49
1:B:730:HIS:HD2	1:B:904:SER:OG	1.96	0.49
1:A:722:ARG:HA	1:A:756:LYS:O	2.13	0.48
1:A:803:SER:HA	1:A:927:TYR:CE2	2.49	0.48
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.49	0.48
1:B:538:LEU:HD13	1:B:734:THR:HG23	1.95	0.48
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.39	0.47
1:A:600:LEU:HD23	1:A:620:LEU:CD2	2.45	0.47
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.49	0.47
1:A:868:ILE:CD1	1:A:984:PRO:HG3	2.45	0.47
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.95	0.47
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.97	0.46
1:B:815:ILE:HG22	1:B:870:MET:HG3	1.98	0.46
1:A:879:GLU:HG2	6:B:4598:HOH:O	2.16	0.46
1:B:771:LEU:HB2	1:B:952:HIS:HB3	1.98	0.45
1:B:600:LEU:HD11	1:B:648:LYS:CG	2.46	0.45
1:A:306:PRO:HG3	1:A:481:VAL:HG12	1.99	0.45
1:B:722:ARG:HA	1:B:756:LYS:O	2.17	0.44
1:A:843:ILE:HG22	1:A:844:GLN:N	2.32	0.44
1:B:236:ASP:OD2	1:B:239:GLN:HG2	2.18	0.44
1:B:596:TYR:OH	1:B:649:MET:HG3	2.17	0.44
1:A:566:LYS:HD3	6:A:4868:HOH:O	2.18	0.44
1:B:677:GLN:NE2	1:B:851:GLN:HE22	2.14	0.44
1:B:843:ILE:HG22	1:B:844:GLN:N	2.33	0.44
1:B:120:LYS:HD3	1:B:167:GLN:CD	2.37	0.44
1:A:580:SER:HB2	1:A:723:LEU:HD23	1.99	0.43
1:A:826:LYS:NZ	6:A:4753:HOH:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:VAL:HG12	1:B:634:TYR:OH	2.19	0.43
1:A:441:LEU:CD2	1:A:449:VAL:HG11	2.39	0.43
1:A:872:LYS:HZ1	1:B:58:PRO:HA	1.84	0.43
1:A:229:ARG:HB3	1:A:230:PRO:HD3	2.00	0.43
1:A:184:ASN:HD21	1:A:223:LYS:HZ1	1.67	0.43
1:A:285:LEU:HD21	1:A:368:ARG:NE	2.33	0.43
1:A:44:ASN:HA	1:A:45:PRO:HD3	1.81	0.43
1:B:799:MET:HE3	1:B:799:MET:HB3	1.83	0.43
1:A:843:ILE:HG22	1:A:844:GLN:H	1.83	0.43
1:B:361:GLY:O	2:D:2:PRO:HA	2.19	0.43
1:A:195:MET:HE2	6:A:4848:HOH:O	2.19	0.42
1:A:437:ILE:HA	1:A:440:ILE:HG12	2.02	0.42
1:B:62:ARG:HG2	1:B:80:ASP:HB2	2.02	0.42
1:A:730:HIS:CD2	1:A:904:SER:OG	2.72	0.42
1:A:413:GLU:OE2	1:A:527:LYS:HD2	2.20	0.42
1:A:596:TYR:OH	1:A:649:MET:HG3	2.19	0.42
1:B:436:LYS:HE3	1:B:440:ILE:HD13	2.01	0.42
1:B:600:LEU:CD1	1:B:648:LYS:HG3	2.50	0.42
1:A:469:ASP:OD1	1:A:472:ARG:NH2	2.46	0.42
1:B:44:ASN:HA	1:B:45:PRO:HD3	1.78	0.42
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.55	0.41
1:B:184:ASN:HD21	1:B:223:LYS:HZ1	1.67	0.41
1:A:84:ASP:OD2	1:A:896:LYS:HG3	2.20	0.41
1:A:677:GLN:HE21	1:A:851:GLN:NE2	2.07	0.41
1:B:300:GLN:HE21	1:B:502:GLN:HE21	1.66	0.41
1:B:123:LYS:HB3	1:B:126:GLU:HB2	2.01	0.41
5:A:4002:DIO:O1'	6:A:4694:HOH:O	2.21	0.41
1:B:600:LEU:CD1	1:B:648:LYS:CG	2.99	0.41
1:B:346:LEU:HD21	1:B:394:MET:HG2	2.03	0.41
1:A:120:LYS:HE3	1:B:409:TRP:HB3	2.04	0.40
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.57	0.40
1:A:291:HIS:ND1	1:A:292:PRO:HD2	2.36	0.40
1:A:529:GLU:O	1:A:637:LYS:HE2	2.21	0.40
1:B:782:ARG:HD3	6:B:4747:HOH:O	2.22	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	949/990 (96%)	933 (98%)	16 (2%)	0	100	100
1	B	949/990 (96%)	929 (98%)	20 (2%)	0	100	100
2	D	2/4 (50%)	2 (100%)	0	0	100	100
2	E	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1901/1988 (96%)	1865 (98%)	36 (2%)	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	837/867 (96%)	833 (100%)	4 (0%)	88	88
1	B	834/867 (96%)	830 (100%)	4 (0%)	88	88
2	D	2/2 (100%)	2 (100%)	0	100	100
2	E	2/2 (100%)	2 (100%)	0	100	100
All	All	1675/1738 (96%)	1667 (100%)	8 (0%)	88	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	LEU
1	A	486	GLU

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Mol	Chain	Res	Type
1	A	540	LEU
1	A	853	GLU
1	B	53	HIS
1	B	356	VAL
1	B	450	LEU
1	B	742	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	93	HIS
1	A	184	ASN
1	A	231	ASN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	407	GLN
1	A	635	ASN
1	A	672	ASN
1	A	677	GLN
1	A	730	HIS
1	A	780	GLN
1	A	821	ASN
1	A	922	ASN
1	B	52	ASN
1	B	93	HIS
1	B	184	ASN
1	B	231	ASN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	376	ASN
1	B	386	HIS
1	B	407	GLN
1	B	418	ASN
1	B	499	GLN
1	B	635	ASN
1	B	672	ASN
1	B	677	GLN
1	B	730	HIS
1	B	780	GLN

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Mol	Chain	Res	Type
1	B	841	ASN
1	B	922	ASN
1	B	993	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	DIO	B	4003	-	6,6,6	0.98	0	6,6,6	0.32	0
5	DIO	A	4006	-	6,6,6	0.71	0	6,6,6	0.42	0
4	ACT	B	3003	-	3,3,3	1.48	1 (33%)	3,3,3	0.67	0
4	ACT	A	3002	-	3,3,3	1.54	1 (33%)	3,3,3	0.80	0
5	DIO	B	4001	-	6,6,6	0.55	0	6,6,6	0.38	0
4	ACT	A	3001	-	3,3,3	1.54	1 (33%)	3,3,3	0.39	0
4	ACT	B	3004	-	3,3,3	1.65	1 (33%)	3,3,3	0.80	0
5	DIO	A	4002	-	6,6,6	1.08	0	6,6,6	0.33	0
5	DIO	B	4005	-	6,6,6	0.63	0	6,6,6	0.27	0

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
5	DIO	B	4003	-	-	-	0/1/1/1
5	DIO	A	4006	-	-	-	0/1/1/1
5	DIO	B	4001	-	-	-	0/1/1/1
5	DIO	A	4002	-	-	-	0/1/1/1
5	DIO	B	4005	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3004	ACT	OXT-C	2.47	1.42	1.30
4	A	3002	ACT	OXT-C	2.29	1.41	1.30
4	A	3001	ACT	OXT-C	2.24	1.41	1.30
4	B	3003	ACT	OXT-C	2.16	1.41	1.30

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3003	ACT	1	0
5	B	4001	DIO	1	0
5	A	4002	DIO	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 (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	953/990 (96%)	-0.33	3 (0%) 94 96	17, 27, 40, 63	0
1	B	953/990 (96%)	-0.32	5 (0%) 91 94	20, 29, 42, 78	0
2	D	4/4 (100%)	1.19	0 100 100	24, 32, 34, 43	4 (100%)
2	E	3/4 (75%)	2.15	2 (66%) 0 0	25, 25, 32, 37	3 (100%)
All	All	1913/1988 (96%)	-0.32	10 (0%) 91 94	17, 28, 41, 78	7 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	ASN	7.9
1	A	53	HIS	2.9
2	E	3	PRO	2.7
2	E	1	ALA	2.6
1	B	542	ALA	2.6
1	B	239	GLN	2.6
1	B	53	HIS	2.5
1	A	1011	HIS	2.4
1	B	985	ALA	2.1
1	A	988	GLN	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
5	DIO	A	4002	6/6	0.72	0.15	37,40,43,43	0
4	ACT	B	3003	4/4	0.82	0.19	44,48,52,58	0
4	ACT	A	3001	4/4	0.83	0.18	39,42,49,49	0
5	DIO	B	4003	6/6	0.83	0.11	37,45,46,46	0
5	DIO	B	4005	6/6	0.85	0.25	46,54,56,58	0
4	ACT	B	3004	4/4	0.87	0.12	36,41,46,48	0
5	DIO	A	4006	6/6	0.90	0.10	31,34,40,41	0
4	ACT	A	3002	4/4	0.93	0.15	41,42,49,54	0
5	DIO	B	4001	6/6	0.95	0.08	29,33,35,37	0
3	ZN	B	2001	1/1	0.98	0.13	25,25,25,25	0
3	ZN	A	2002	1/1	0.98	0.11	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.