



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:38 PM GMT

PDB ID : 4CY8
Title : 2-hydroxybiphenyl 3-monooxygenase (HbpA) in complex with FAD
Authors : Jensen, C.N.; Farrugia, J.E.; Frank, A.; Man, H.; Hart, S.; Turkenburg, J.P.; Grogan, G.
Deposited on : 2014-04-10
Resolution : 2.03 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

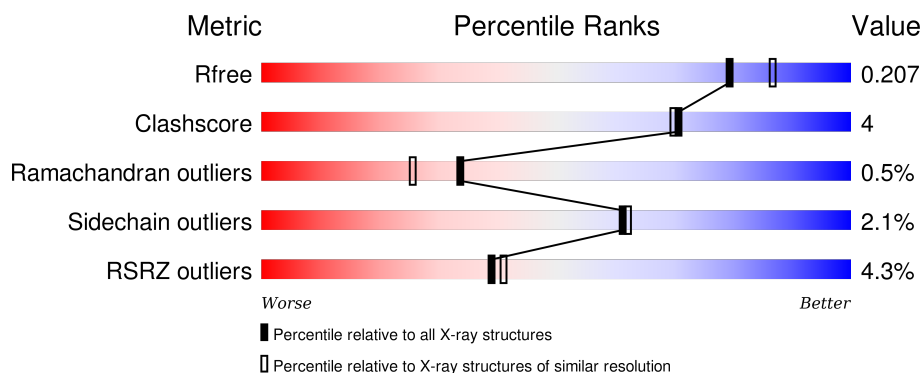
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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 $\leq 5\%$. 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	586	<div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
1	B	586	<div> <div>82%</div> <div>7%</div> <div>9%</div> </div>
1	C	586	<div> <div>83%</div> <div>6%</div> <div>10%</div> </div>
1	D	586	<div> <div>85%</div> <div>5%</div> <div>8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17641 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.

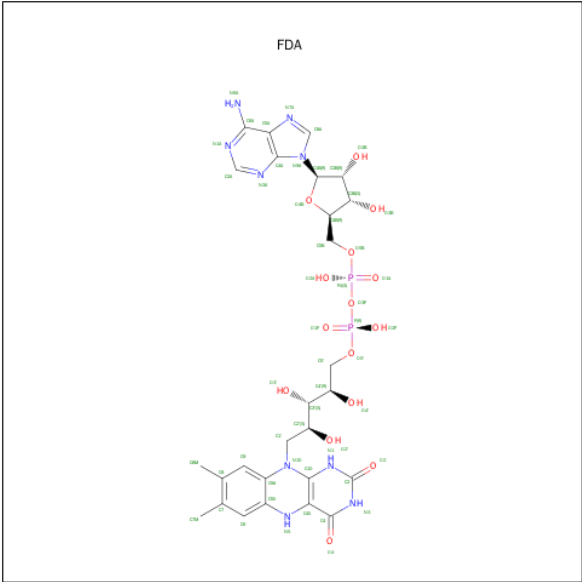
- Molecule 1 is a protein called 2-HYDROXYBIPHENYL 3-MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			3999	2533	700	748	18			
1	B	535	Total	C	N	O	S	0	0	0
			3939	2491	696	734	18			
1	C	530	Total	C	N	O	S	0	0	0
			3916	2472	693	734	17			
1	D	537	Total	C	N	O	S	0	0	0
			3968	2514	694	742	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	GLN	THR	ENGINEERED MUTATION	UNP O06647
B	347	GLN	THR	ENGINEERED MUTATION	UNP O06647
C	347	GLN	THR	ENGINEERED MUTATION	UNP O06647
D	347	GLN	THR	ENGINEERED MUTATION	UNP O06647

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

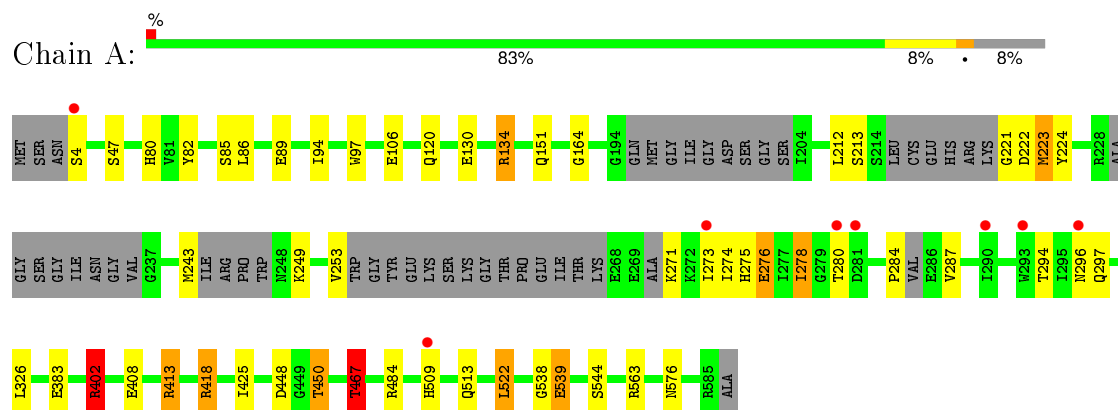
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	417	Total	O	0	0
			417	417		
3	B	417	Total	O	0	0
			417	417		
3	C	404	Total	O	0	0
			404	404		
3	D	369	Total	O	0	0
			369	369		

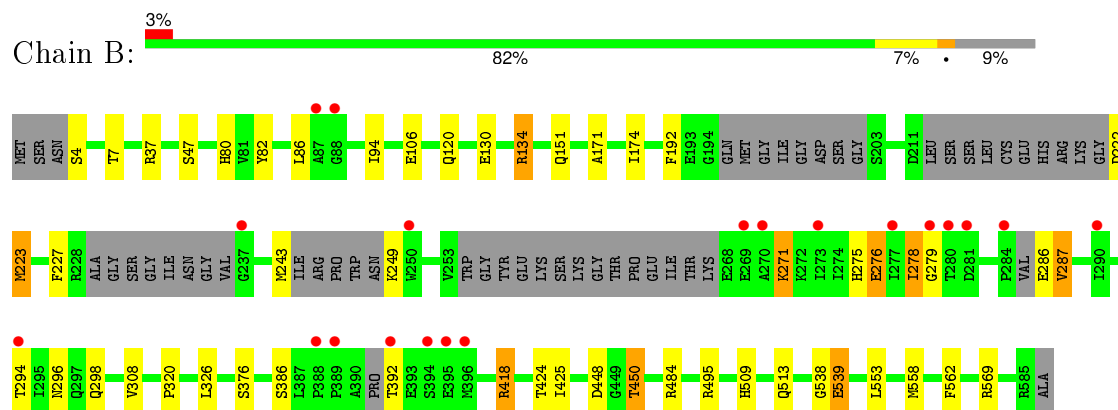
3 Residue-property plots [i](#)

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.

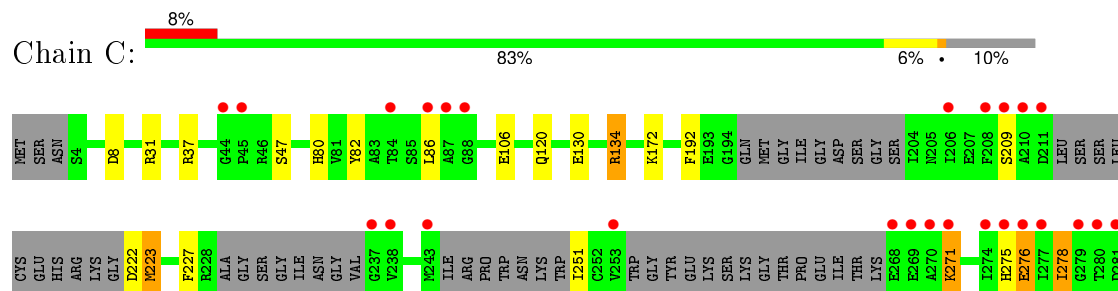
• Molecule 1: 2-HYDROXYBIPHENYL 3-MONOOXYGENASE

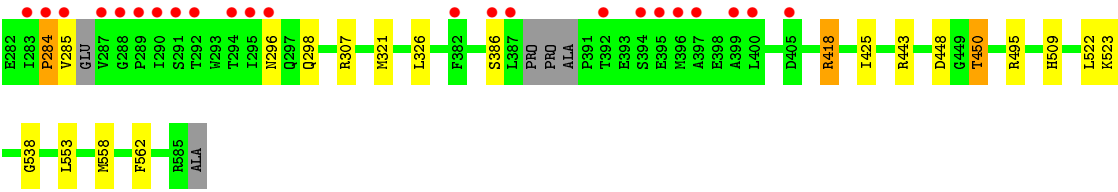


• Molecule 1: 2-HYDROXYBIPHENYL 3-MONOOXYGENASE

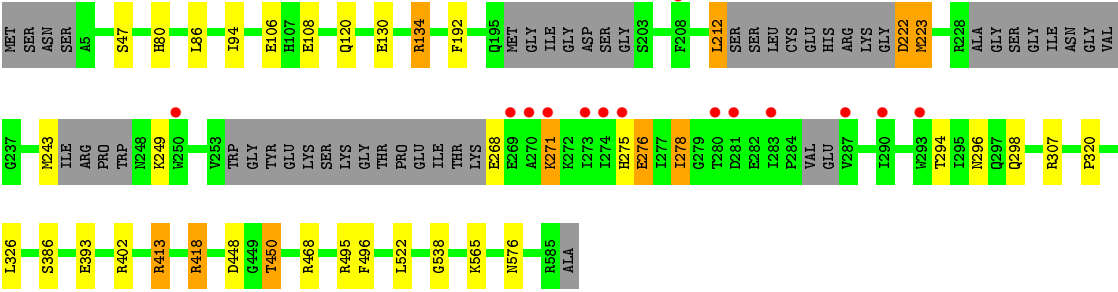
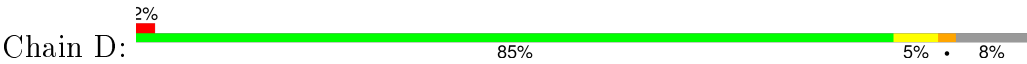


• Molecule 1: 2-HYDROXYBIPHENYL 3-MONOOXYGENASE





● Molecule 1: 2-HYDROXYBIPHENYL 3-MONOOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.00 Å 96.18 Å 102.16 Å 114.09° 95.80° 109.31°	Depositor
Resolution (Å)	59.53 – 2.03 59.53 – 2.03	Depositor EDS
% Data completeness (in resolution range)	90.0 (59.53-2.03) 74.2 (59.53-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.03 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.169 , 0.202 0.176 , 0.207	Depositor DCC
R_{free} test set	7349 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 146665 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17641	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FDA

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	0.85	7/4080 (0.2%)	0.93	8/5541 (0.1%)
1	B	0.84	4/4017 (0.1%)	0.88	7/5454 (0.1%)
1	C	0.83	2/3990 (0.1%)	0.91	9/5415 (0.2%)
1	D	0.84	4/4048 (0.1%)	0.87	7/5500 (0.1%)
All	All	0.84	17/16135 (0.1%)	0.90	31/21910 (0.1%)

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	2
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	9

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	GLU	CD-OE1	7.02	1.33	1.25
1	B	539	GLU	CG-CD	7.00	1.62	1.51
1	A	106	GLU	CD-OE1	6.89	1.33	1.25
1	D	106	GLU	CD-OE2	6.64	1.32	1.25
1	D	418	ARG	CD-NE	-6.59	1.35	1.46
1	C	106	GLU	CD-OE2	6.32	1.32	1.25
1	A	539	GLU	CG-CD	6.26	1.61	1.51
1	A	418	ARG	CD-NE	-6.11	1.36	1.46
1	A	97	TRP	CB-CG	5.80	1.60	1.50
1	A	539	GLU	CD-OE1	5.67	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	539	GLU	CD-OE2	5.56	1.31	1.25
1	A	82	TYR	CG-CD2	-5.50	1.32	1.39
1	D	106	GLU	CG-CD	5.44	1.60	1.51
1	D	106	GLU	CD-OE1	5.34	1.31	1.25
1	B	539	GLU	CD-OE1	5.32	1.31	1.25
1	C	106	GLU	CD-OE1	5.26	1.31	1.25
1	B	539	GLU	CD-OE2	5.03	1.31	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ARG	NE-CZ-NH2	-17.34	111.63	120.30
1	C	418	ARG	NE-CZ-NH2	-15.49	112.55	120.30
1	D	418	ARG	NE-CZ-NH2	-14.79	112.90	120.30
1	B	418	ARG	NE-CZ-NH2	-14.34	113.13	120.30
1	A	418	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	C	418	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	D	418	ARG	NE-CZ-NH1	11.90	126.25	120.30
1	B	418	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	C	134	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	B	134	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	134	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	D	134	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	A	402	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	C	134	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	134	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	522	LEU	CB-CG-CD2	-6.95	99.19	111.00
1	A	402	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	37	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	467	THR	N-CA-CB	-6.37	98.19	110.30
1	A	134	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	37	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	134	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	307	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	D	222	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	569	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	37	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	307	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	212	LEU	CA-CB-CG	5.39	127.70	115.30
1	B	558	MET	CG-SD-CE	5.23	108.57	100.20
1	C	558	MET	CG-SD-CE	5.19	108.51	100.20
1	C	443	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	LYS	Peptide
1	A	278	ILE	Peptide
1	B	271	LYS	Peptide
1	B	278	ILE	Peptide
1	C	271	LYS	Peptide
1	C	278	ILE	Peptide
1	C	284	PRO	Peptide
1	D	271	LYS	Peptide
1	D	278	ILE	Peptide

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	3999	0	3847	45	4
1	B	3939	0	3758	37	0
1	C	3916	0	3748	33	0
1	D	3968	0	3805	28	0
2	A	53	0	33	2	0
2	B	53	0	33	3	0
2	C	53	0	33	3	0
2	D	53	0	33	3	0
3	A	417	0	0	20	0
3	B	417	0	0	18	1
3	C	404	0	0	13	3
3	D	369	0	0	8	0
All	All	17641	0	15290	139	4

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 4.

All (139) 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:308:VAL:HG22	3:B:2169:HOH:O	1.49	1.10
1:B:174:ILE:HB	3:B:2169:HOH:O	1.51	1.10
1:A:296:ASN:HB2	3:A:2209:HOH:O	1.53	1.07
1:C:425:ILE:HG22	3:C:2257:HOH:O	1.56	1.01
1:D:576:ASN:HB3	3:D:2364:HOH:O	1.67	0.93
1:B:539:GLU:HG2	3:B:2189:HOH:O	1.72	0.89
1:A:284:PRO:N	3:A:2206:HOH:O	2.06	0.87
1:A:4:SER:CB	3:A:2002:HOH:O	2.23	0.87
1:D:320:PRO:O	3:D:2179:HOH:O	1.93	0.84
1:A:539:GLU:HG2	3:A:2196:HOH:O	1.78	0.82
1:A:425:ILE:HG22	3:A:2303:HOH:O	1.79	0.81
1:A:467:THR:HG21	1:A:544:SER:O	1.79	0.81
1:B:425:ILE:HG22	3:B:2272:HOH:O	1.81	0.81
1:A:164:GLY:O	3:A:2174:HOH:O	1.98	0.81
1:A:275:HIS:O	1:A:276:GLU:CB	2.29	0.79
1:A:326:LEU:H	2:A:1586:FDA:HN1	1.31	0.79
1:C:275:HIS:O	1:C:276:GLU:CB	2.33	0.77
1:B:278:ILE:CB	3:B:2194:HOH:O	2.34	0.76
1:C:8:ASP:OD2	3:C:2005:HOH:O	2.03	0.75
1:A:576:ASN:HB3	3:A:2411:HOH:O	1.85	0.75
1:C:82:TYR:HD1	1:C:227:PHE:HE1	1.31	0.74
1:D:275:HIS:O	1:D:276:GLU:CB	2.36	0.73
1:B:275:HIS:O	1:B:276:GLU:CB	2.39	0.70
1:D:418:ARG:HD2	3:D:2243:HOH:O	1.90	0.70
1:D:108:GLU:CD	3:D:2087:HOH:O	2.32	0.68
1:A:576:ASN:OD1	3:A:2369:HOH:O	2.12	0.67
1:D:268:GLU:N	3:D:2159:HOH:O	2.27	0.67
1:A:418:ARG:HD2	3:A:2297:HOH:O	1.94	0.67
1:D:418:ARG:CD	3:D:2243:HOH:O	2.43	0.67
1:B:279:GLY:HA2	3:B:2194:HOH:O	1.94	0.66
1:C:425:ILE:HB	3:C:2256:HOH:O	1.95	0.66
1:B:418:ARG:CD	3:B:2267:HOH:O	2.42	0.66
1:B:418:ARG:HD2	3:B:2267:HOH:O	1.96	0.66
1:B:326:LEU:H	2:B:1586:FDA:HN1	1.43	0.65
1:C:209:SER:O	1:C:285:VAL:CB	2.45	0.64
1:C:326:LEU:H	2:C:1586:FDA:HN1	1.44	0.64
1:A:85:SER:OG	3:A:2080:HOH:O	2.15	0.64
1:C:82:TYR:HD1	1:C:227:PHE:CE1	2.15	0.63
1:A:418:ARG:CD	3:A:2297:HOH:O	2.48	0.61
3:A:2382:HOH:O	1:C:418:ARG:HD2	2.01	0.61
1:B:275:HIS:CB	3:B:2195:HOH:O	2.49	0.61
1:A:467:THR:CG2	1:A:563:ARG:HH11	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:O	1:A:278:ILE:HG22	2.02	0.60
1:B:275:HIS:HA	3:B:2194:HOH:O	2.02	0.59
1:A:243:MET:HG2	1:A:249:LYS:O	2.03	0.59
1:B:320:PRO:O	3:B:2214:HOH:O	2.16	0.58
1:B:243:MET:HG2	1:B:249:LYS:O	2.03	0.58
1:C:523:LYS:CB	3:C:2331:HOH:O	2.51	0.58
1:D:243:MET:HG2	1:D:249:LYS:O	2.03	0.58
1:A:212:LEU:HD22	1:A:278:ILE:HD11	1.85	0.58
1:C:31:ARG:HD2	3:C:2016:HOH:O	2.04	0.58
1:B:495:ARG:NE	3:B:2341:HOH:O	2.21	0.57
1:C:222:ASP:CB	3:C:2077:HOH:O	2.53	0.56
3:A:2382:HOH:O	1:C:418:ARG:CD	2.53	0.56
1:B:130:GLU:OE2	1:B:134:ARG:HD2	2.05	0.56
1:A:130:GLU:OE2	1:A:134:ARG:HD2	2.05	0.56
1:C:130:GLU:OE2	1:C:134:ARG:HD2	2.05	0.55
1:D:130:GLU:OE2	1:D:134:ARG:HD2	2.06	0.55
1:B:418:ARG:HD3	3:B:2267:HOH:O	2.05	0.55
1:A:418:ARG:HD3	1:C:538:GLY:HA3	1.88	0.55
1:C:284:PRO:HA	3:C:2181:HOH:O	2.07	0.54
1:D:326:LEU:H	2:D:1586:FDA:HN1	1.55	0.54
1:B:80:HIS:CD2	1:B:223:MET:HB3	2.43	0.54
1:C:80:HIS:CD2	1:C:223:MET:HB3	2.43	0.54
1:B:392:THR:CB	3:B:2259:HOH:O	2.56	0.53
1:D:393:GLU:CB	3:D:2226:HOH:O	2.57	0.53
1:A:538:GLY:HA3	1:C:418:ARG:HD3	1.91	0.53
1:A:222:ASP:CB	3:A:2078:HOH:O	2.57	0.52
1:B:538:GLY:HA3	1:D:418:ARG:HD3	1.92	0.52
1:A:425:ILE:CG2	3:A:2303:HOH:O	2.48	0.52
1:C:425:ILE:CG2	3:C:2257:HOH:O	2.33	0.52
1:D:402:ARG:NE	1:D:413:ARG:NH2	2.58	0.51
1:D:402:ARG:CD	1:D:413:ARG:HH21	2.23	0.51
1:A:467:THR:HG22	1:A:563:ARG:HH11	1.76	0.50
1:A:221:GLY:N	1:A:224:TYR:HH	2.09	0.50
1:A:278:ILE:HG23	1:A:280:THR:H	1.76	0.50
1:C:509:HIS:ND1	3:C:2339:HOH:O	2.35	0.50
1:B:222:ASP:CB	3:B:2080:HOH:O	2.60	0.49
1:B:286:GLU:O	1:B:287:VAL:CB	2.60	0.49
1:D:86:LEU:HB3	1:D:278:ILE:O	2.13	0.49
1:B:484:ARG:NH1	3:B:2336:HOH:O	2.28	0.48
1:D:192:PHE:HB3	1:D:298:GLN:HG2	1.94	0.48
1:B:47:SER:HA	2:B:1586:FDA:C4X	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LEU:HB3	1:C:278:ILE:O	2.12	0.48
1:B:86:LEU:HB3	1:B:278:ILE:O	2.13	0.48
1:B:47:SER:HA	2:B:1586:FDA:N5	2.29	0.47
1:A:86:LEU:HB3	1:A:278:ILE:O	2.13	0.47
1:D:402:ARG:HG2	3:D:2231:HOH:O	2.13	0.47
1:C:192:PHE:HB3	1:C:298:GLN:HG2	1.97	0.47
1:C:448:ASP:OD1	1:C:450:THR:HG22	2.14	0.47
1:C:495:ARG:NE	3:C:2325:HOH:O	2.19	0.47
1:A:80:HIS:CD2	1:A:223:MET:HB3	2.49	0.47
1:D:80:HIS:CD2	1:D:223:MET:HB3	2.49	0.47
1:C:82:TYR:CD1	1:C:227:PHE:CE1	3.01	0.47
1:B:47:SER:OG	1:B:120:GLN:HB2	2.14	0.47
1:D:402:ARG:HD2	1:D:413:ARG:NH2	2.31	0.46
1:B:82:TYR:OH	1:B:424:THR:OG1	2.26	0.46
1:C:172:LYS:HE2	3:C:2134:HOH:O	2.14	0.46
1:D:448:ASP:OD1	1:D:450:THR:HG22	2.16	0.46
1:B:192:PHE:HB3	1:B:298:GLN:HG2	1.98	0.46
1:D:402:ARG:CD	1:D:413:ARG:NH2	2.80	0.45
1:A:448:ASP:OD1	1:A:450:THR:HG22	2.16	0.45
1:B:448:ASP:OD1	1:B:450:THR:HG22	2.17	0.45
1:B:4:SER:C	3:B:2002:HOH:O	2.55	0.45
1:A:47:SER:OG	1:A:120:GLN:HB2	2.17	0.45
1:C:425:ILE:HD12	3:C:2256:HOH:O	2.17	0.45
1:C:284:PRO:O	1:C:285:VAL:CB	2.65	0.44
1:D:47:SER:HA	2:D:1586:FDA:C4X	2.47	0.44
1:B:418:ARG:HD3	1:D:538:GLY:HA3	1.99	0.44
1:C:47:SER:HA	2:C:1586:FDA:N5	2.32	0.44
1:A:275:HIS:HA	1:A:278:ILE:HG22	1.99	0.44
1:D:47:SER:HA	2:D:1586:FDA:N5	2.32	0.44
1:D:47:SER:OG	1:D:120:GLN:HB2	2.18	0.44
1:A:278:ILE:HG21	1:A:278:ILE:HD13	1.82	0.44
1:A:484:ARG:HD2	3:A:2181:HOH:O	2.17	0.44
1:A:509:HIS:NE2	1:A:513:GLN:OE1	2.51	0.43
1:A:326:LEU:C	1:A:326:LEU:HD23	2.38	0.43
1:C:47:SER:OG	1:C:120:GLN:HB2	2.19	0.43
1:A:297:GLN:HG2	3:A:2210:HOH:O	2.17	0.43
1:D:326:LEU:HD23	1:D:326:LEU:C	2.39	0.43
1:A:89:GLU:CB	3:A:2278:HOH:O	2.67	0.43
1:B:82:TYR:HD2	1:B:227:PHE:CE1	2.37	0.43
1:D:496:PHE:HB2	1:D:522:LEU:HD12	2.01	0.42
1:A:402:ARG:HD3	1:A:402:ARG:HA	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:SER:HA	2:C:1586:FDA:C4X	2.50	0.42
1:B:7:THR:O	1:B:171:ALA:HA	2.19	0.42
1:D:450:THR:HG23	1:D:468:ARG:HE	1.84	0.42
1:A:467:THR:HG22	1:A:563:ARG:NH1	2.34	0.41
1:A:273:ILE:O	1:A:275:HIS:O	2.38	0.41
1:C:553:LEU:HB3	1:C:562:PHE:HB3	2.02	0.41
1:A:253:VAL:HG23	3:A:2202:HOH:O	2.18	0.41
1:A:151:GLN:HG3	3:A:2160:HOH:O	2.20	0.41
1:A:47:SER:HA	2:A:1586:FDA:N5	2.35	0.41
1:B:376:SER:HB3	3:B:2256:HOH:O	2.21	0.41
1:A:467:THR:HG23	1:A:563:ARG:HH11	1.82	0.41
1:A:413:ARG:H	1:A:413:ARG:HG2	1.75	0.40
1:B:509:HIS:NE2	1:B:513:GLN:OE1	2.54	0.40
1:C:321:MET:HE2	3:C:2199:HOH:O	2.20	0.40
1:B:553:LEU:HB3	1:B:562:PHE:HB3	2.04	0.40

All (4) 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:402:ARG:NH2	3:C:2248:HOH:O[1_455]	0.87	1.33
1:A:383:GLU:OE2	3:B:2330:HOH:O[1_565]	1.54	0.66
1:A:402:ARG:CZ	3:C:2248:HOH:O[1_455]	1.62	0.58
1:A:402:ARG:NE	3:C:2248:HOH:O[1_455]	2.07	0.13

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	523/586 (89%)	507 (97%)	13 (2%)	3 (1%)	30 21
1	B	519/586 (89%)	505 (97%)	11 (2%)	3 (1%)	30 21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	514/586 (88%)	500 (97%)	12 (2%)	2 (0%)	39	32
1	D	523/586 (89%)	508 (97%)	13 (2%)	2 (0%)	39	32
All	All	2079/2344 (89%)	2020 (97%)	49 (2%)	10 (0%)	34	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	VAL
1	B	287	VAL
1	A	276	GLU
1	B	276	GLU
1	C	276	GLU
1	D	276	GLU
1	B	271	LYS
1	C	271	LYS
1	D	271	LYS
1	A	213	SER

5.3.2 Protein sidechains ⓘ

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	395/467 (85%)	386 (98%)	9 (2%)	58	58
1	B	380/467 (81%)	373 (98%)	7 (2%)	66	68
1	C	382/467 (82%)	376 (98%)	6 (2%)	70	72
1	D	388/467 (83%)	377 (97%)	11 (3%)	51	49
All	All	1545/1868 (83%)	1512 (98%)	33 (2%)	61	62

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	223	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	294	THR
1	A	402	ARG
1	A	408	GLU
1	A	413	ARG
1	A	450	THR
1	A	467	THR
1	A	522	LEU
1	B	94	ILE
1	B	151	GLN
1	B	223	MET
1	B	294	THR
1	B	296	ASN
1	B	386	SER
1	B	450	THR
1	C	223	MET
1	C	251	ILE
1	C	296	ASN
1	C	386	SER
1	C	450	THR
1	C	522	LEU
1	D	94	ILE
1	D	212	LEU
1	D	222	ASP
1	D	223	MET
1	D	294	THR
1	D	296	ASN
1	D	386	SER
1	D	413	ARG
1	D	450	THR
1	D	495	ARG
1	D	565	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	297	GLN

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 ⓘ

4 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	FDA	A	1586	-	48,58,58	1.40	8 (16%)	54,89,89	2.37	10 (18%)
2	FDA	B	1586	-	48,58,58	1.58	8 (16%)	54,89,89	2.56	15 (27%)
2	FDA	C	1586	-	48,58,58	1.80	8 (16%)	54,89,89	2.31	13 (24%)
2	FDA	D	1586	-	48,58,58	1.59	9 (18%)	54,89,89	2.50	14 (25%)

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	FDA	A	1586	-	-	0/30/50/50	0/6/6/6
2	FDA	B	1586	-	-	0/30/50/50	0/6/6/6
2	FDA	C	1586	-	-	0/30/50/50	0/6/6/6
2	FDA	D	1586	-	-	0/30/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1586	FDA	C9A-N10	2.01	1.41	1.38
2	A	1586	FDA	C5A-C4A	2.08	1.45	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1586	FDA	C9A-N10	2.14	1.41	1.38
2	D	1586	FDA	C10-N10	2.14	1.41	1.39
2	C	1586	FDA	C1'-N10	2.16	1.50	1.48
2	C	1586	FDA	C5A-C4A	2.30	1.45	1.40
2	B	1586	FDA	C2A-N3A	2.30	1.36	1.32
2	C	1586	FDA	C10-N10	2.33	1.41	1.39
2	A	1586	FDA	C8-C7	2.51	1.47	1.41
2	A	1586	FDA	C4-N3	2.63	1.38	1.33
2	D	1586	FDA	C5A-C4A	2.66	1.46	1.40
2	A	1586	FDA	C10-N10	2.69	1.42	1.39
2	D	1586	FDA	C1'-N10	2.71	1.51	1.48
2	B	1586	FDA	C10-N10	2.84	1.42	1.39
2	D	1586	FDA	C4-N3	2.93	1.38	1.33
2	B	1586	FDA	C8-C7	2.99	1.49	1.41
2	D	1586	FDA	C5'-C4'	3.08	1.56	1.51
2	B	1586	FDA	C9A-C5X	3.17	1.49	1.42
2	D	1586	FDA	C9A-C5X	3.26	1.49	1.42
2	D	1586	FDA	C8-C7	3.26	1.49	1.41
2	B	1586	FDA	C4-N3	3.35	1.39	1.33
2	A	1586	FDA	C9A-C5X	3.47	1.49	1.42
2	C	1586	FDA	C8-C7	3.58	1.50	1.41
2	A	1586	FDA	C4-C4X	3.69	1.48	1.41
2	D	1586	FDA	C4X-C10	3.72	1.48	1.41
2	C	1586	FDA	C9A-C5X	3.74	1.50	1.42
2	A	1586	FDA	C4X-C10	3.96	1.48	1.41
2	C	1586	FDA	C9A-N10	4.03	1.44	1.38
2	B	1586	FDA	C4X-C10	4.22	1.48	1.41
2	B	1586	FDA	C4-C4X	4.32	1.49	1.41
2	D	1586	FDA	C4-C4X	4.48	1.50	1.41
2	C	1586	FDA	C4X-C10	4.78	1.50	1.41
2	C	1586	FDA	C4-C4X	5.97	1.53	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1586	FDA	N3A-C2A-N1A	-9.67	121.49	128.89
2	B	1586	FDA	N3A-C2A-N1A	-8.89	122.08	128.89
2	A	1586	FDA	C4X-C10-N10	-6.51	116.68	120.52
2	A	1586	FDA	C4-C4X-C10	-6.38	115.86	119.94
2	A	1586	FDA	N3A-C2A-N1A	-6.02	124.28	128.89
2	B	1586	FDA	C4-C4X-C10	-5.78	116.24	119.94
2	C	1586	FDA	C4X-C4-N3	-5.15	116.55	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1586	FDA	N3A-C2A-N1A	-5.07	125.02	128.89
2	D	1586	FDA	C4X-C4-N3	-5.05	116.68	123.59
2	B	1586	FDA	C1B-N9A-C4A	-4.92	119.52	126.94
2	D	1586	FDA	C1B-N9A-C4A	-4.47	120.20	126.94
2	C	1586	FDA	C4-C4X-C10	-4.11	117.31	119.94
2	D	1586	FDA	C4-C4X-C10	-3.95	117.42	119.94
2	B	1586	FDA	C4X-C4-N3	-3.84	118.34	123.59
2	A	1586	FDA	C4X-C4-N3	-3.81	118.38	123.59
2	B	1586	FDA	C4X-C10-N10	-3.53	118.44	120.52
2	C	1586	FDA	C1B-N9A-C4A	-3.39	121.83	126.94
2	C	1586	FDA	C4A-C5A-N7A	-3.28	106.46	109.48
2	D	1586	FDA	O3B-C3B-C4B	-2.98	102.11	111.05
2	B	1586	FDA	C4B-O4B-C1B	-2.67	106.79	109.72
2	D	1586	FDA	C4X-C10-N10	-2.16	119.25	120.52
2	D	1586	FDA	O4B-C1B-N9A	-2.08	103.75	108.10
2	A	1586	FDA	N6A-C6A-N1A	2.10	123.72	119.20
2	A	1586	FDA	O2'-C2'-C1'	2.25	115.47	109.94
2	C	1586	FDA	O4'-C4'-C3'	2.34	114.91	109.02
2	D	1586	FDA	N6A-C6A-N1A	2.36	124.28	119.20
2	C	1586	FDA	C6-C5X-C9A	2.45	122.20	118.98
2	B	1586	FDA	C5X-C9A-N10	2.46	119.49	117.62
2	C	1586	FDA	O3P-P-O5'	2.55	109.69	102.94
2	B	1586	FDA	O5B-PA-O1A	2.68	120.03	109.62
2	D	1586	FDA	O3P-PA-O5B	2.71	110.13	102.94
2	B	1586	FDA	O2'-C2'-C1'	2.84	116.94	109.94
2	D	1586	FDA	C4-C4X-N5	2.91	122.25	118.72
2	D	1586	FDA	O2'-C2'-C1'	2.94	117.16	109.94
2	C	1586	FDA	C1'-N10-C9A	3.06	122.30	118.86
2	A	1586	FDA	C4-C4X-N5	3.12	122.51	118.72
2	B	1586	FDA	C2B-C1B-N9A	3.13	119.08	114.29
2	B	1586	FDA	O3P-P-O5'	3.17	111.33	102.94
2	A	1586	FDA	C2B-C1B-N9A	3.18	119.15	114.29
2	C	1586	FDA	C4-C4X-N5	3.21	122.61	118.72
2	B	1586	FDA	N6A-C6A-N1A	3.34	126.37	119.20
2	B	1586	FDA	C4-C4X-N5	3.40	122.85	118.72
2	D	1586	FDA	C2B-C1B-N9A	3.78	120.07	114.29
2	C	1586	FDA	C2B-C1B-N9A	4.55	121.25	114.29
2	D	1586	FDA	C4X-N5-C5X	5.04	122.56	116.76
2	B	1586	FDA	C4X-N5-C5X	5.07	122.59	116.76
2	A	1586	FDA	C4X-N5-C5X	5.16	122.69	116.76
2	C	1586	FDA	C4X-N5-C5X	5.94	123.60	116.76
2	B	1586	FDA	C4-N3-C2	8.18	122.32	115.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1586	FDA	C4-N3-C2	8.25	122.38	115.25
2	C	1586	FDA	C4-N3-C2	8.28	122.41	115.25
2	A	1586	FDA	C4-N3-C2	8.39	122.50	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1586	FDA	2	0
2	B	1586	FDA	3	0
2	C	1586	FDA	3	0
2	D	1586	FDA	3	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, 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	539/586 (91%)	-0.28	8 (1%) 76 77	19, 32, 66, 93	0
1	B	535/586 (91%)	-0.21	20 (3%) 45 47	19, 31, 73, 113	0
1	C	530/586 (90%)	0.08	49 (9%) 11 12	18, 30, 75, 93	0
1	D	537/586 (91%)	-0.29	14 (2%) 59 61	19, 33, 71, 99	0
All	All	2141/2344 (91%)	-0.18	91 (4%) 39 41	18, 31, 71, 113	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	396	MET	7.6
1	C	210	ALA	5.1
1	C	277	ILE	4.6
1	B	389	PRO	4.6
1	C	87	ALA	4.5
1	C	280	THR	4.5
1	C	283	ILE	4.4
1	D	270	ALA	4.3
1	B	280	THR	4.3
1	C	394	SER	4.1
1	D	274	ILE	4.0
1	C	206	ILE	3.9
1	C	292	THR	3.8
1	C	392	THR	3.7
1	C	285	VAL	3.7
1	C	279	GLY	3.7
1	D	269	GLU	3.6
1	D	275	HIS	3.6
1	C	276	GLU	3.4
1	D	280	THR	3.4
1	C	290	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	274	ILE	3.3
1	C	209	SER	3.3
1	B	392	THR	3.3
1	C	296	ASN	3.1
1	C	400	LEU	3.1
1	D	293	TRP	3.1
1	B	396	MET	3.0
1	C	387	LEU	3.0
1	C	397	ALA	3.0
1	B	284	PRO	3.0
1	D	208	PHE	2.9
1	C	269	GLU	2.9
1	C	382	PHE	2.9
1	B	88	GLY	2.9
1	A	290	ILE	2.8
1	A	296	ASN	2.8
1	C	208	PHE	2.8
1	D	281	ASP	2.8
1	B	87	ALA	2.8
1	B	279	GLY	2.8
1	C	270	ALA	2.8
1	C	291	SER	2.7
1	C	237	GLY	2.7
1	D	290	ILE	2.6
1	C	275	HIS	2.6
1	C	405	ASP	2.6
1	D	283	ILE	2.6
1	D	250	TRP	2.6
1	C	238	VAL	2.6
1	D	273	ILE	2.6
1	C	281	ASP	2.6
1	C	268	GLU	2.5
1	B	270	ALA	2.5
1	C	395	GLU	2.5
1	B	237	GLY	2.5
1	C	243	MET	2.5
1	B	395	GLU	2.5
1	C	289	PRO	2.5
1	A	280	THR	2.4
1	B	294	THR	2.4
1	A	509	HIS	2.4
1	C	288	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	84	THR	2.3
1	A	281	ASP	2.3
1	D	287	VAL	2.3
1	A	4	SER	2.3
1	B	273	ILE	2.3
1	B	277	ILE	2.3
1	B	394	SER	2.3
1	C	44	GLY	2.3
1	C	88	GLY	2.3
1	C	86	LEU	2.3
1	A	273	ILE	2.2
1	C	295	ILE	2.2
1	C	399	ALA	2.2
1	C	253	VAL	2.2
1	C	271	LYS	2.2
1	B	250	TRP	2.2
1	B	281	ASP	2.2
1	B	290	ILE	2.2
1	C	211	ASP	2.1
1	C	294	THR	2.1
1	C	287	VAL	2.1
1	C	284	PRO	2.1
1	D	271	LYS	2.1
1	B	388	PRO	2.1
1	A	293	TRP	2.0
1	C	45	PRO	2.0
1	C	386	SER	2.0
1	B	269	GLU	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
2	FDA	B	1586	53/53	0.97	0.10	0.45	23,30,42,51	0
2	FDA	A	1586	53/53	0.98	0.10	0.18	21,29,34,40	0
2	FDA	D	1586	53/53	0.97	0.10	0.02	25,33,40,45	0
2	FDA	C	1586	53/53	0.97	0.10	-0.05	23,30,42,48	0

6.5 Other polymers

There are no such residues in this entry.