



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:45 pm BST

PDB ID : 4WHR
Title : Anhydride reaction intermediate trapped in Protocatechuate 3,4-dioxygenase (pseudomonas putida) at pH 8.5
Authors : Knoot, C.J.; Lipscomb, J.D.
Deposited on : 2014-09-23
Resolution : 1.58 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

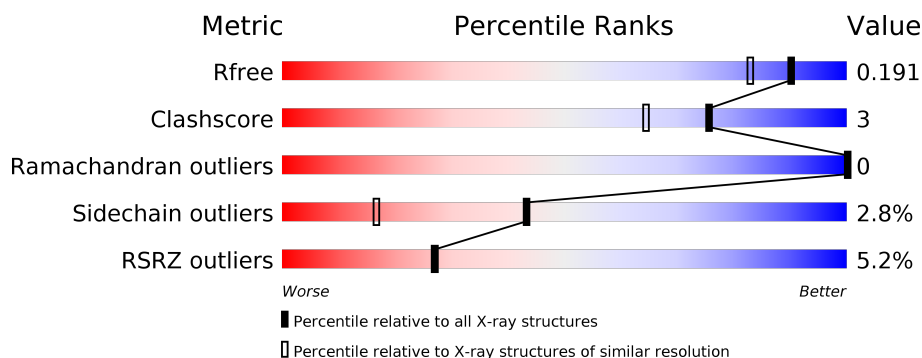
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 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 $\leq 5\%$. 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	200	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> <div>.</div> </div>
1	C	200	<div> <div>5%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>..</div> </div>
1	E	200	<div> <div>12%</div> <div> <div></div> <div>93%</div> <div>8%</div> </div> </div>
2	B	238	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> <div>.</div> </div>
2	D	238	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>
3	F	238	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> <div>.</div> </div>

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
7	TRS	B	604	-	X	-	-
8	3NJ	B	607	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11542 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 Protocatechuate 3,4-dioxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	4	0
			1606	1014	284	305	3			
1	E	200	Total	C	N	O	S	0	1	0
			1582	1000	278	301	3			
1	C	200	Total	C	N	O	S	0	2	0
			1589	1005	279	302	3			

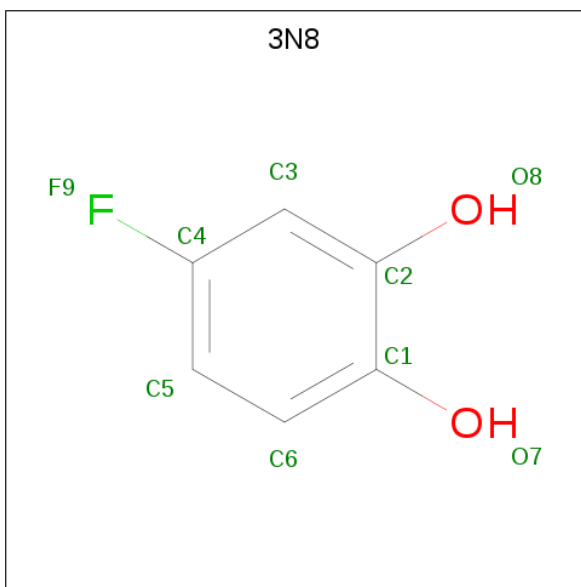
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	237	Total	C	N	O	S	0	2	0
			1893	1202	345	339	7			
2	B	238	Total	C	N	O	S	0	0	0
			1883	1193	344	338	8			

- Molecule 3 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

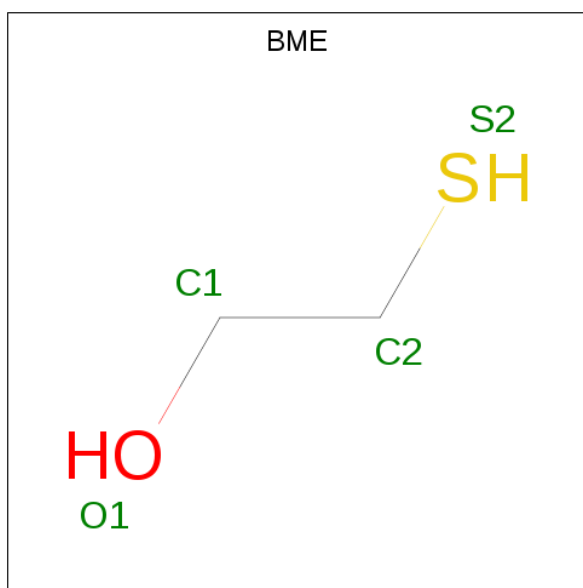
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	236	Total	C	N	O	S	0	1	0
			1876	1189	342	338	7			

- Molecule 4 is 4-fluorobenzene-1,2-diol (three-letter code: 3N8) (formula: C₆H₅FO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			9	6	1	2		
4	E	1	Total	C	F	O	0	0
			9	6	1	2		
4	C	1	Total	C	F	O	0	0
			9	6	1	2		
4	D	1	Total	C	F	O	0	0
			9	6	1	2		
4	D	1	Total	C	F	O	0	0
			9	6	1	2		
4	D	1	Total	C	F	O	0	0
			9	6	1	2		
4	D	1	Total	C	F	O	0	0
			9	6	1	2		
4	B	1	Total	C	F	O	0	0
			9	6	1	2		
4	B	1	Total	C	F	O	0	0
			9	6	1	2		
4	B	1	Total	C	F	O	0	0
			9	6	1	2		
4	F	1	Total	C	F	O	0	0
			9	6	1	2		
4	F	1	Total	C	F	O	0	0
			9	6	1	2		
4	F	1	Total	C	F	O	0	0
			9	6	1	2		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

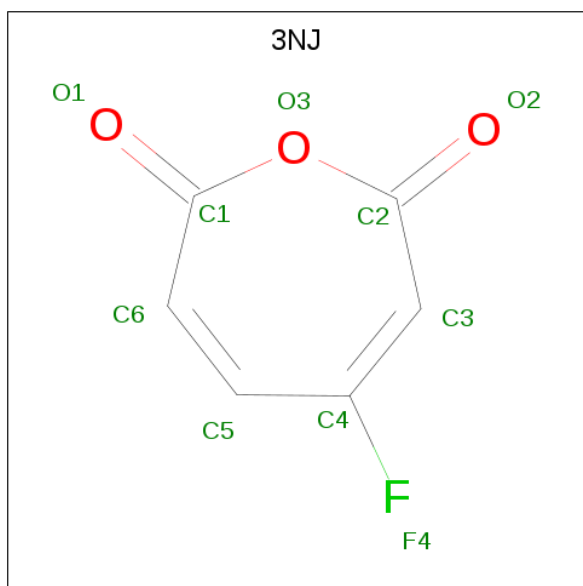
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe	0	0
			1	1		
6	D	1	Total	Fe	0	0
			1	1		
6	F	1	Total	Fe	0	0
			1	1		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is 4-fluorooxepine-2,7-dione (three-letter code: 3NJ) (formula: C₆H₃FO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	F	O	0	0
			10	6	1	3		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Cl 1 1	0	0

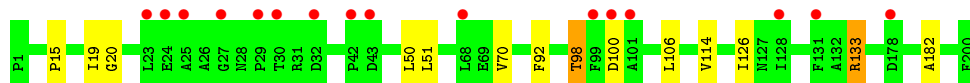
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	130	Total O 130 130	0	0
10	E	106	Total O 106 106	0	0
10	C	135	Total O 136 136	0	1
10	D	202	Total O 202 202	0	0
10	B	197	Total O 198 198	0	1
10	F	177	Total O 177 177	0	0

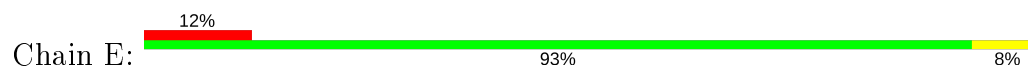
3 Residue-property plots [i](#)

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

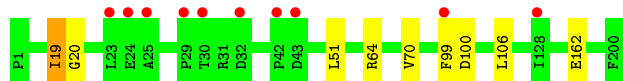
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



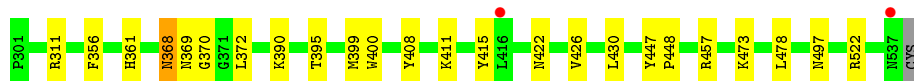
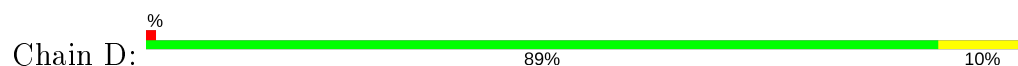
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



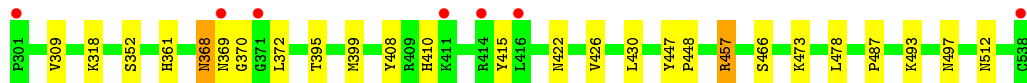
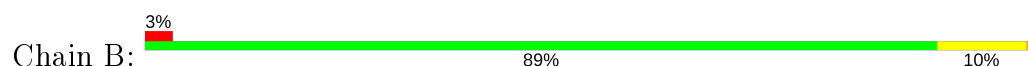
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



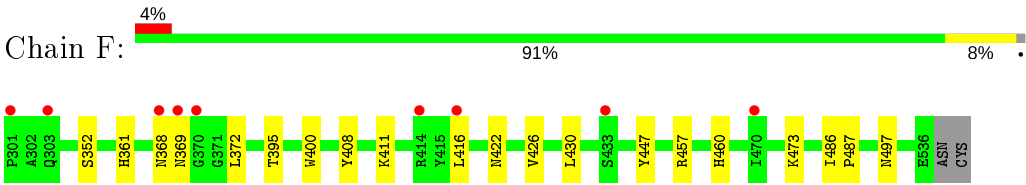
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- Molecule 3: Protocatechuate 3,4-dioxygenase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.44Å 140.64Å 168.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.47 – 1.58 31.47 – 1.58	Depositor EDS
% Data completeness (in resolution range)	91.3 (31.47-1.58) 91.3 (31.47-1.58)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.148 , 0.192 0.149 , 0.191	Depositor DCC
R_{free} test set	9462 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11542	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MHO, CSO, BME, CL, 3NJ, FE, TRS, 3N8

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	0.44	0/1646	0.67	0/2241
1	C	0.47	1/1629 (0.1%)	0.68	0/2218
1	E	0.43	0/1622	0.66	0/2209
2	B	0.47	0/1931	0.73	2/2627 (0.1%)
2	D	0.47	0/1941	0.74	3/2641 (0.1%)
3	F	0.46	0/1914	0.72	2/2603 (0.1%)
All	All	0.46	1/10683 (0.0%)	0.70	7/14539 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	GLU	CD-OE1	-5.18	1.20	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	457	ARG	NE-CZ-NH1	8.29	124.45	120.30
2	D	457	ARG	NE-CZ-NH1	7.46	124.03	120.30
2	B	457	ARG	NE-CZ-NH2	-7.12	116.74	120.30
3	F	457	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	D	311	ARG	NE-CZ-NH2	-5.97	117.31	120.30
3	F	457	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	D	457	ARG	NE-CZ-NH2	-5.60	117.50	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1606	0	1540	9	0
1	C	1589	0	1524	10	0
1	E	1582	0	1516	8	0
2	B	1883	0	1836	22	0
2	D	1893	0	1851	16	0
3	F	1876	0	1828	10	0
4	A	9	0	4	0	0
4	B	27	0	9	0	0
4	C	9	0	4	0	0
4	D	45	0	17	1	0
4	E	9	0	4	0	0
4	F	27	0	11	1	0
5	A	4	0	6	2	0
5	B	4	0	6	0	0
5	F	8	0	12	1	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	B	8	0	12	2	0
8	B	10	0	3	5	0
9	F	1	0	0	0	0
10	A	130	0	0	0	0
10	B	198	0	0	3	0
10	C	136	0	0	0	0
10	D	202	0	0	1	0
10	E	106	0	0	0	0
10	F	177	0	0	0	0
All	All	11542	0	10183	65	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 3.

All (65) 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)
2:B:447:TYR:OH	8:B:607:3NJ:H1	1.81	0.81
2:B:447:TYR:OH	8:B:607:3NJ:C3	2.31	0.78
1:C:19[B]:ILE:HG22	2:D:426:VAL:HG22	1.72	0.70
1:A:70:VAL:HG11	1:A:106:LEU:HD11	1.82	0.59
1:C:19[A]:ILE:HD11	2:D:400:TRP:HB2	1.87	0.57
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.34	0.57
1:C:19[A]:ILE:O	2:D:426:VAL:HG21	2.04	0.56
1:C:64:ARG:NE	1:C:99:PHE:O	2.38	0.56
2:D:369:ASN:H	2:D:422:ASN:HD22	1.53	0.56
1:C:19[A]:ILE:HD12	2:D:426:VAL:HG22	1.87	0.55
1:C:70:VAL:HG21	1:C:106:LEU:HD21	1.88	0.55
3:F:416:LEU:HB2	5:F:606:BME:H22	1.89	0.54
2:B:318:LYS:NZ	10:B:883:HOH:O	2.42	0.52
2:D:368:ASN:HD22	2:D:368:ASN:C	2.12	0.52
1:C:19[A]:ILE:O	2:D:426:VAL:CG2	2.57	0.52
3:F:369:ASN:H	3:F:422:ASN:HD22	1.58	0.52
7:B:604:TRS:H22	4:F:602:3N8:H3	1.92	0.51
2:B:368:ASN:HD22	2:B:368:ASN:C	2.13	0.51
2:B:415:TYR:HB2	10:B:890:HOH:O	2.10	0.51
2:D:361:HIS:H	2:D:361:HIS:CD2	2.29	0.51
2:D:415:TYR:HB2	10:D:901:HOH:O	2.11	0.51
2:B:369:ASN:H	2:B:422:ASN:HD22	1.57	0.50
2:D:478:LEU:C	2:D:478:LEU:HD23	2.32	0.50
2:B:478:LEU:HD23	2:B:478:LEU:C	2.32	0.49
2:B:361:HIS:CD2	2:B:361:HIS:H	2.30	0.49
2:D:356:PHE:CZ	2:D:430[B]:LEU:HG	2.47	0.49
1:E:15:PRO:HB3	1:E:133:ARG:HD3	1.94	0.49
1:C:51:LEU:HD12	1:C:106:LEU:HD23	1.94	0.48
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.43	0.48
2:B:368:ASN:HD22	2:B:369:ASN:N	2.12	0.48
1:E:19:ILE:HG13	3:F:400:TRP:HB2	1.97	0.46
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.51	0.46
1:A:19:ILE:HG23	2:B:410:HIS:HD2	1.80	0.45
1:C:19[A]:ILE:CD1	2:D:400:TRP:HB2	2.46	0.45
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.98	0.45
3:F:361:HIS:H	3:F:361:HIS:CD2	2.34	0.45
2:B:408:TYR:HE2	2:B:447:TYR:CZ	2.35	0.44
2:B:447:TYR:CZ	8:B:607:3NJ:H1	2.51	0.44
1:C:20:GLY:HA2	2:D:426:VAL:HG13	1.99	0.44
2:D:368:ASN:ND2	2:D:370:GLY:H	2.15	0.44
3:F:486:ILE:HB	3:F:487:PRO:HD3	1.99	0.44
1:A:19:ILE:O	2:B:426:VAL:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:ARG:NH1	8:B:607:3NJ:O2	2.49	0.44
2:B:447:TYR:CE1	8:B:607:3NJ:H1	2.52	0.44
3:F:447:TYR:CE2	3:F:460:HIS:HE1	2.36	0.43
4:D:605:3N8:H3	7:B:604:TRS:H12	1.99	0.43
1:E:20:GLY:HA2	3:F:426:VAL:HG13	1.99	0.43
1:A:98[A]:THR:OG1	1:A:100:ASP:OD1	2.30	0.43
2:B:368:ASN:ND2	2:B:370:GLY:H	2.16	0.43
1:A:92:PHE:CZ	5:A:302:BME:H11	2.54	0.43
2:D:408:TYR:HE2	2:D:447:TYR:CZ	2.36	0.43
2:D:447:TYR:HB2	2:D:448:PRO:HD2	2.00	0.43
1:A:20:GLY:HA2	2:B:426:VAL:HG13	2.01	0.42
1:A:15:PRO:HB3	1:A:133[B]:ARG:HD3	1.99	0.42
2:B:309:VAL:HG23	10:B:727:HOH:O	2.20	0.42
2:B:447:TYR:HB2	2:B:448:PRO:HD2	2.02	0.42
3:F:447:TYR:CE2	3:F:460:HIS:CE1	3.08	0.42
1:E:100:ASP:OD1	1:E:101:ALA:N	2.53	0.41
1:E:70:VAL:HG21	1:E:106:LEU:HD21	2.01	0.41
3:F:408:TYR:HE2	3:F:447:TYR:CZ	2.39	0.41
2:B:352:SER:HA	2:B:430:LEU:HD21	2.03	0.41
2:B:487:PRO:O	2:B:493:LYS:NZ	2.43	0.41
5:A:302:BME:H21	2:B:466:SER:CB	2.51	0.40
1:A:50:LEU:O	1:A:182:ALA:HA	2.22	0.40
3:F:352:SER:HA	3:F:430:LEU:HD21	2.03	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	202/200 (101%)	197 (98%)	5 (2%)	0	100	100
1	C	200/200 (100%)	196 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	199/200 (100%)	195 (98%)	4 (2%)	0	100	100
2	B	235/238 (99%)	229 (97%)	6 (3%)	0	100	100
2	D	236/238 (99%)	231 (98%)	5 (2%)	0	100	100
3	F	233/238 (98%)	229 (98%)	4 (2%)	0	100	100
All	All	1305/1314 (99%)	1277 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	167/163 (102%)	161 (96%)	6 (4%)	35	10
1	C	165/163 (101%)	162 (98%)	3 (2%)	59	34
1	E	164/163 (101%)	161 (98%)	3 (2%)	59	34
2	B	201/201 (100%)	194 (96%)	7 (4%)	36	11
2	D	202/201 (100%)	193 (96%)	9 (4%)	27	6
3	F	199/200 (100%)	193 (97%)	6 (3%)	41	15
All	All	1098/1091 (101%)	1064 (97%)	34 (3%)	43	14

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98[A]	THR
1	A	98[B]	THR
1	A	114[A]	VAL
1	A	114[B]	VAL
1	A	133[A]	ARG
1	A	133[B]	ARG
1	E	52	LEU
1	E	158	LEU
1	E	178	ASP

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Mol	Chain	Res	Type
1	C	19[A]	ILE
1	C	19[B]	ILE
1	C	100	ASP
2	D	368	ASN
2	D	372	LEU
2	D	390	LYS
2	D	395	THR
2	D	399	MET
2	D	411	LYS
2	D	473	LYS
2	D	497	ASN
2	D	522	ARG
2	B	368	ASN
2	B	372	LEU
2	B	395	THR
2	B	399	MET
2	B	473	LYS
2	B	497	ASN
2	B	512	ASN
3	F	368	ASN
3	F	372	LEU
3	F	395	THR
3	F	411	LYS
3	F	473	LYS
3	F	497	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	E	159	ASN
2	D	361	HIS
2	D	368	ASN
2	D	412	ASN
2	D	422	ASN
2	D	497	ASN
2	D	503	GLN
2	D	537	ASN
2	B	361	HIS
2	B	368	ASN
2	B	412	ASN
2	B	422	ASN

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Mol	Chain	Res	Type
2	B	497	ASN
2	B	503	GLN
2	B	534	HIS
3	F	361	HIS
3	F	368	ASN
3	F	369	ASN
3	F	412	ASN
3	F	422	ASN
3	F	497	ASN
3	F	503	GLN
3	F	534	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	CSO	F	429	3	3,6,7	1.13	0	0,6,8	0.00	-
2	CSO	D	429	2	3,6,7	1.55	0	0,6,8	0.00	-
2	CSO	B	429	2	3,6,7	1.46	0	0,6,8	0.00	-
3	MHO	F	488	3	7,8,9	0.92	0	4,9,11	2.43	2 (50%)

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	CSO	F	429	3	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	D	429	2	-	0/1/5/7	-
2	CSO	B	429	2	-	0/1/5/7	-
3	MHO	F	488	3	-	2/6/7/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	488	MHO	CE-SD-CG	3.94	106.68	97.71
3	F	488	MHO	OD1-SD-CE	2.57	111.45	106.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	488	MHO	CB-CG-SD-CE
3	F	488	MHO	CB-CG-SD-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	3N8	D	603	-	9,9,9	0.73	0	12,12,12	1.00	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	3N8	C	301	-	9,9,9	0.87	0	12,12,12	0.99	0
4	3N8	F	603	-	9,9,9	0.84	0	12,12,12	0.88	0
8	3NJ	B	607	-	2,10,10	1.91	0	2,13,13	4.62	1 (50%)
4	3N8	D	606	-	9,9,9	0.84	0	12,12,12	1.23	2 (16%)
4	3N8	B	602	-	9,9,9	0.90	0	12,12,12	1.01	1 (8%)
5	BME	A	302	-	3,3,3	0.26	0	1,2,2	0.10	0
4	3N8	D	602	-	9,9,9	0.80	0	12,12,12	1.41	3 (25%)
4	3N8	A	301	-	9,9,9	0.85	0	12,12,12	0.86	1 (8%)
4	3N8	D	605	-	9,9,9	0.88	0	12,12,12	1.11	1 (8%)
4	3N8	F	602	-	9,9,9	0.98	0	12,12,12	1.20	1 (8%)
4	3N8	F	601	-	9,9,9	0.68	0	12,12,12	1.10	1 (8%)
4	3N8	B	605	-	9,9,9	0.71	0	12,12,12	1.12	1 (8%)
4	3N8	B	603	-	9,9,9	0.78	0	12,12,12	0.96	0
7	TRS	B	604	-	7,7,7	0.79	0	9,9,9	3.43	8 (88%)
5	BME	F	606	-	3,3,3	0.27	0	1,2,2	0.93	0
4	3N8	D	604	-	9,9,9	0.83	0	12,12,12	0.91	1 (8%)
5	BME	B	606	-	3,3,3	0.35	0	1,2,2	0.06	0
5	BME	F	605	-	3,3,3	0.34	0	1,2,2	0.59	0
4	3N8	E	301	-	9,9,9	0.79	0	12,12,12	0.95	1 (8%)

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	3N8	D	603	-	-	-	0/1/1/1
4	3N8	F	601	-	-	-	0/1/1/1
4	3N8	A	301	-	-	-	0/1/1/1
4	3N8	D	604	-	-	-	0/1/1/1
8	3NJ	B	607	-	-	-	0/0/1/1
4	3N8	D	606	-	-	-	0/1/1/1
4	3N8	B	602	-	-	-	0/1/1/1
5	BME	A	302	-	-	0/1/1/1	-
4	3N8	D	602	-	-	-	0/1/1/1
4	3N8	F	602	-	-	-	0/1/1/1
4	3N8	D	605	-	-	-	0/1/1/1
4	3N8	B	605	-	-	-	0/1/1/1
4	3N8	C	301	-	-	-	0/1/1/1
4	3N8	B	603	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TRS	B	604	-	-	6/9/9/9	-
5	BME	F	606	-	-	0/1/1/1	-
4	3N8	F	603	-	-	-	0/1/1/1
5	BME	B	606	-	-	1/1/1/1	-
5	BME	F	605	-	-	1/1/1/1	-
4	3N8	E	301	-	-	-	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	607	3NJ	C6-C5-C4	-6.51	123.57	131.10
7	B	604	TRS	C2-C-N	-5.26	92.26	107.98
7	B	604	TRS	C1-C-N	-4.60	94.23	107.98
7	B	604	TRS	C3-C-N	-4.54	94.44	107.98
7	B	604	TRS	C2-C-C1	3.23	120.84	110.81
7	B	604	TRS	C3-C-C2	3.21	120.75	110.81
4	D	602	3N8	C5-C4-C3	-3.03	119.36	123.29
4	D	606	3N8	C5-C4-C3	-2.87	119.56	123.29
4	F	602	3N8	C5-C4-C3	-2.82	119.62	123.29
4	D	605	3N8	C5-C4-C3	-2.66	119.83	123.29
7	B	604	TRS	O1-C1-C	-2.46	103.19	111.00
4	D	603	3N8	C5-C4-C3	-2.44	120.12	123.29
4	D	602	3N8	F9-C4-C3	2.44	121.74	118.25
4	B	605	3N8	C5-C4-C3	-2.40	120.17	123.29
4	D	602	3N8	C6-C5-C4	2.36	120.81	118.36
4	F	601	3N8	C5-C4-C3	-2.36	120.23	123.29
4	B	602	3N8	C5-C4-C3	-2.30	120.30	123.29
4	D	606	3N8	F9-C4-C3	2.19	121.39	118.25
4	E	301	3N8	C5-C4-C3	-2.13	120.52	123.29
7	B	604	TRS	C3-C-C1	2.07	117.22	110.81
7	B	604	TRS	O2-C2-C	-2.04	104.52	111.00
4	D	604	3N8	C5-C4-C3	-2.04	120.64	123.29
4	A	301	3N8	C5-C4-C3	-2.04	120.64	123.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	605	BME	O1-C1-C2-S2
7	B	604	TRS	C2-C-C1-O1

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Mol	Chain	Res	Type	Atoms
7	B	604	TRS	C1-C-C3-O3
5	B	606	BME	O1-C1-C2-S2
7	B	604	TRS	N-C-C1-O1
7	B	604	TRS	C3-C-C2-O2
7	B	604	TRS	N-C-C3-O3
7	B	604	TRS	N-C-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	607	3NJ	5	0
5	A	302	BME	2	0
4	D	605	3N8	1	0
4	F	602	3N8	1	0
7	B	604	TRS	2	0
5	F	606	BME	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 ⓘ

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	200/200 (100%)	0.12	16 (8%)	12 12	15, 22, 43, 65	0
1	C	200/200 (100%)	-0.02	10 (5%)	28 29	15, 22, 38, 55	0
1	E	200/200 (100%)	0.44	24 (12%)	4 4	16, 29, 50, 69	0
2	B	237/238 (99%)	-0.16	7 (2%)	50 51	16, 19, 36, 56	0
2	D	236/238 (99%)	-0.24	2 (0%)	86 87	16, 19, 32, 51	0
3	F	234/238 (98%)	-0.14	9 (3%)	40 41	16, 21, 36, 61	1 (0%)
All	All	1307/1314 (99%)	-0.01	68 (5%)	27 27	15, 22, 40, 69	1 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	PHE	6.0
1	E	99	PHE	5.7
1	A	27	GLY	5.3
1	E	178	ASP	4.7
1	E	100	ASP	4.6
1	E	177	VAL	4.0
1	E	27	GLY	4.0
1	E	101	ALA	4.0
1	C	99	PHE	4.0
1	E	179	GLY	3.9
1	E	25	ALA	3.8
1	E	128	ILE	3.8
1	E	98[A]	THR	3.8
3	F	414	ARG	3.7
1	A	178	ASP	3.5
1	A	29	PRO	3.4
1	E	23	LEU	3.4
1	E	24	GLU	3.3
1	A	100	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	180	LYS	3.3
1	C	29	PRO	3.3
1	A	25	ALA	3.2
1	C	25	ALA	3.2
1	C	30	THR	3.1
1	A	101	ALA	3.1
1	E	29	PRO	3.0
2	B	301	PRO	2.9
3	F	301	PRO	2.9
1	E	126	ILE	2.8
1	E	30	THR	2.7
2	B	538	CYS	2.7
3	F	416	LEU	2.6
1	E	43	ASP	2.6
1	C	43	ASP	2.6
1	A	24	GLU	2.6
1	A	128	ILE	2.6
3	F	470	ILE	2.6
1	C	24	GLU	2.6
2	B	411	LYS	2.5
2	B	371	GLY	2.5
1	E	32	ASP	2.5
1	E	150	GLN	2.4
1	E	45	PRO	2.4
1	E	86	GLU	2.4
3	F	370	GLY	2.4
1	A	32	ASP	2.3
2	D	537	ASN	2.3
1	A	23	LEU	2.3
1	A	42	PRO	2.3
1	A	30	THR	2.3
1	A	43	ASP	2.3
1	C	32	ASP	2.3
1	C	42	PRO	2.2
1	A	68	LEU	2.2
1	E	102	GLY	2.2
1	E	42	PRO	2.2
3	F	369	ASN	2.2
3	F	433	SER	2.2
2	B	416	LEU	2.1
1	E	70	VAL	2.1
1	A	131	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	23	LEU	2.1
2	D	416	LEU	2.1
2	B	369	ASN	2.1
2	B	414	ARG	2.1
3	F	303	GLN	2.0
1	C	128	ILE	2.0
3	F	368	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSO	D	429	7/8	0.95	0.07	19,21,25,30	0
3	CSO	F	429	7/8	0.97	0.05	21,26,29,30	0
3	MHO	F	488	9/10	0.97	0.08	18,21,46,51	0
2	CSO	B	429	7/8	0.99	0.05	18,21,25,29	0

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. 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	BME	F	606	4/4	0.85	0.13	38,45,47,63	0
4	3N8	D	606	9/9	0.89	0.19	34,40,44,55	0
8	3NJ	B	607	10/10	0.90	0.19	15,27,36,40	10
7	TRS	B	604	8/8	0.91	0.10	40,44,49,54	0
4	3N8	D	603	9/9	0.91	0.17	30,34,46,48	0
4	3N8	B	603	9/9	0.92	0.11	29,33,42,53	0
4	3N8	D	605	9/9	0.93	0.07	29,32,36,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	3N8	F	603	9/9	0.93	0.08	31,35,39,45	0
5	BME	B	606	4/4	0.94	0.11	36,42,46,57	0
4	3N8	A	301	9/9	0.94	0.11	24,26,30,34	0
4	3N8	E	301	9/9	0.94	0.09	32,33,40,41	0
4	3N8	C	301	9/9	0.94	0.17	30,31,34,39	0
4	3N8	F	601	9/9	0.94	0.07	34,37,44,46	0
4	3N8	B	602	9/9	0.94	0.07	29,31,36,48	0
4	3N8	F	602	9/9	0.95	0.07	28,33,36,50	0
4	3N8	B	605	9/9	0.95	0.09	31,33,42,44	0
4	3N8	D	604	9/9	0.95	0.09	28,31,41,45	0
5	BME	F	605	4/4	0.96	0.15	41,44,52,53	0
5	BME	A	302	4/4	0.96	0.07	34,37,38,45	0
4	3N8	D	602	9/9	0.97	0.06	28,32,40,45	0
9	CL	F	604	1/1	0.98	0.06	54,54,54,54	0
6	FE	D	601	1/1	1.00	0.05	18,18,18,18	1
6	FE	F	607	1/1	1.00	0.05	18,18,18,18	1
6	FE	B	601	1/1	1.00	0.06	19,19,19,19	1

6.5 Other polymers ⓘ

There are no such residues in this entry.