



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:00 AM UTC

PDB ID : 4WHR / pdb_00004whr
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

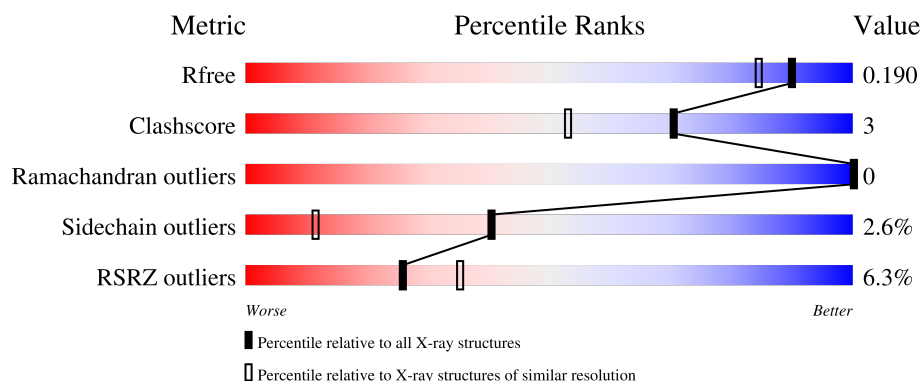
1 Overall quality at a glance

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}	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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 $\leq 5\%$. 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	8% 93% 6%
1	C	200	8% 96%
1	E	200	12% 92% 8%
2	B	238	3% 88% 11%
2	D	238	3% 91% 8%

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Mol	Chain	Length	Quality of chain
3	F	238	

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			

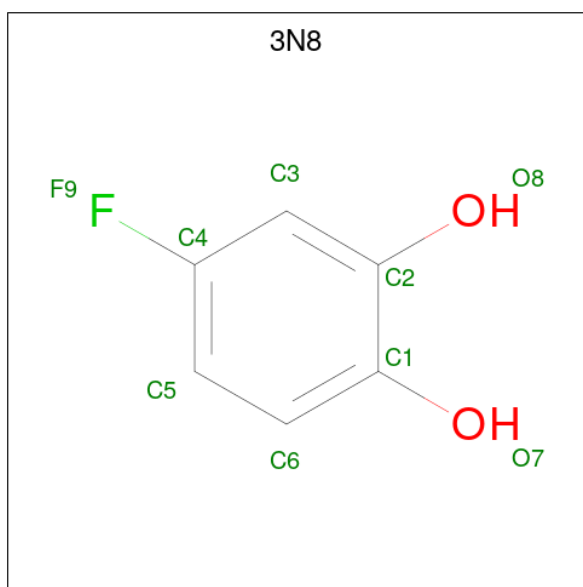
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

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.

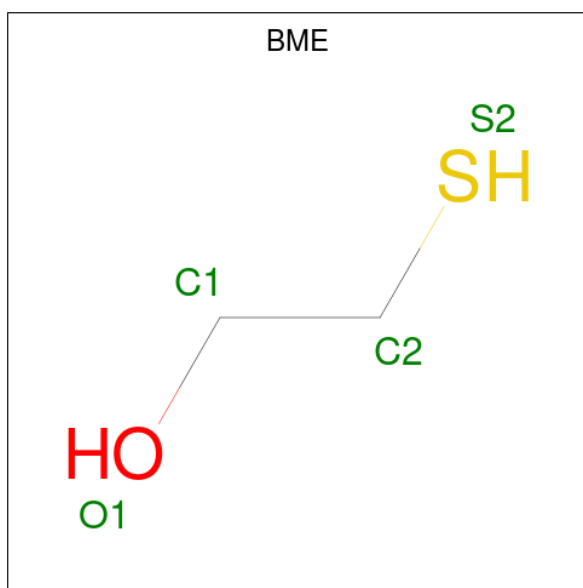
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	236	Total	C	N	O	S	0	1	0
			1876	1189	342	338	7			

- Molecule 4 is 4-fluorobenzene-1,2-diol (CCD ID: 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 (CCD ID: 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 (CCD ID: FE) (formula: Fe).

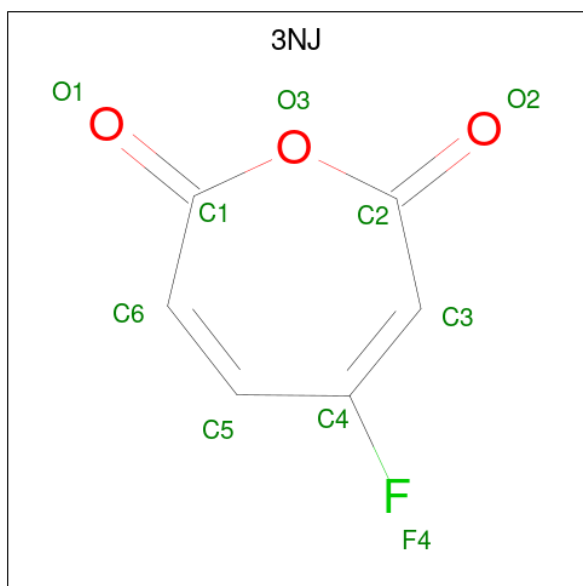
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Fe	0	0
			1	1		
6	B	1	Total	Fe	0	0
			1	1		
6	F	1	Total	Fe	0	0
			1	1		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: 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 (CCD ID: 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 (CCD ID: CL) (formula: Cl).

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

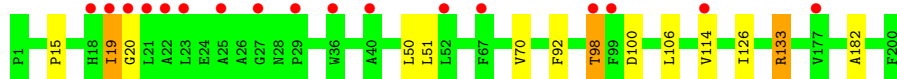
- Molecule 10 is water.

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

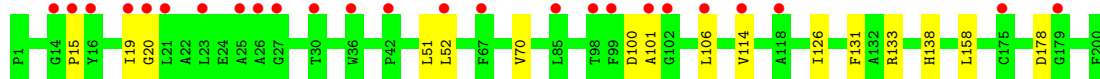
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: Protocatechuate 3,4-dioxygenase alpha chain



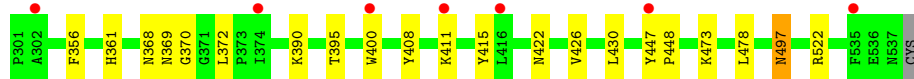
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



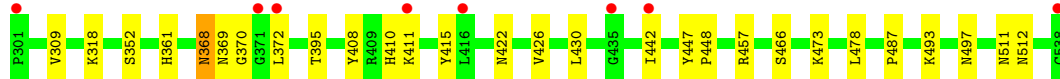
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



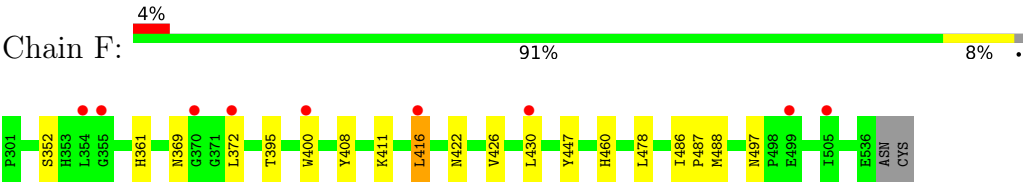
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- 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 0.148 , 0.190	Depositor DCC
R_{free} test set	9462 reflections (4.59%)	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)	0.41 , 58.1	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	0.95	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, TRS, MHO, 3N8, FE, BME, 3NJ, CSO

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	0.58	0/1646	0.74	0/2241
1	C	0.59	0/1629	0.75	0/2218
1	E	0.57	0/1622	0.71	0/2209
2	B	0.62	0/1931	0.80	0/2627
2	D	0.61	0/1941	0.79	0/2641
3	F	0.61	0/1914	0.78	0/2603
All	All	0.60	0/10683	0.76	0/14539

There are no bond length outliers.

There are no bond angle outliers.

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	1606	0	1540	9	0
1	C	1589	0	1524	10	0
1	E	1582	0	1516	8	0
2	B	1883	0	1836	24	0
2	D	1893	0	1851	18	0
3	F	1876	0	1829	12	0
4	A	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	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	10184	71	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 (71) 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
2:B:473:LYS:NZ	10:B:814:HOH:O	2.37	0.58
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:368:ASN:HD22	2:D:368:ASN:C	2.12	0.56
2:D:369:ASN:H	2:D:422:ASN:HD22	1.53	0.56
2:B:368:ASN:C	2:B:368:ASN:HD22	2.13	0.56
1:C:19[A]:ILE:HD12	2:D:426:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG21	1:C:106:LEU:HD21	1.88	0.55
2:B:478:LEU:HD23	2:B:478:LEU:C	2.32	0.54
3:F:416:LEU:HB2	5:F:606:BME:H22	1.89	0.54
2:D:478:LEU:C	2:D:478:LEU:HD23	2.32	0.54
2:B:318:LYS:NZ	10:B:883:HOH:O	2.42	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:415:TYR:HB2	10:B:890:HOH:O	2.10	0.51
2:D:361:HIS:CD2	2:D:361:HIS:H	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:356:PHE:CZ	2:D:430[B]:LEU:HG	2.47	0.49
2:B:361:HIS:H	2:B:361:HIS:CD2	2.30	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:E:51:LEU:HD12	1:E:106:LEU:HD23	1.98	0.45
1:C:19[A]:ILE:CD1	2:D:400:TRP:HB2	2.46	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:B:497:ASN:C	2:B:497:ASN:HD22	2.25	0.44
2:D:368:ASN:ND2	2:D:370:GLY:H	2.15	0.44
3:F:478:LEU:C	3:F:478:LEU:HD23	2.43	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
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
2:D:368:ASN:C	2:D:368:ASN:ND2	2.77	0.43
1:A:92:PHE:CZ	5:A:302:BME:H11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:497:ASN:C	3:F:497:ASN:HD22	2.26	0.43
1:A:20:GLY:HA2	2:B:426:VAL:HG13	2.01	0.42
2:D:497:ASN:HD22	2:D:497:ASN:C	2.27	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
1:A:50:LEU:O	1:A:182:ALA:HA	2.22	0.40
5:A:302:BME:H21	2:B:466:SER:CB	2.51	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 ⓘ

5.3.1 Protein backbone ⓘ

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
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%)	160 (96%)	7 (4%)	26	4
1	C	165/163 (101%)	162 (98%)	3 (2%)	51	23
1	E	164/163 (101%)	160 (98%)	4 (2%)	43	13
2	B	201/201 (100%)	194 (96%)	7 (4%)	32	6
2	D	202/201 (100%)	195 (96%)	7 (4%)	32	6
3	F	199/200 (100%)	195 (98%)	4 (2%)	48	20
All	All	1098/1091 (101%)	1066 (97%)	32 (3%)	40	8

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
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	114	VAL
1	E	158	LEU
1	E	178	ASP
1	C	19[A]	ILE
1	C	19[B]	ILE
1	C	100	ASP
2	D	372	LEU
2	D	390	LYS
2	D	395	THR
2	D	411	LYS
2	D	473	LYS

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Mol	Chain	Res	Type
2	D	497	ASN
2	D	522	ARG
2	B	368	ASN
2	B	372	LEU
2	B	395	THR
2	B	411	LYS
2	B	442	ILE
2	B	511	ASN
2	B	512	ASN
3	F	372	LEU
3	F	395	THR
3	F	411	LYS
3	F	416	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	537	ASN
2	B	361	HIS
2	B	368	ASN
2	B	412	ASN
2	B	422	ASN
2	B	497	ASN
2	B	512	ASN
2	B	530	GLN
3	F	314	ASN
3	F	361	HIS
3	F	368	ASN
3	F	412	ASN
3	F	422	ASN
3	F	497	ASN
3	F	503	GLN
3	F	530	GLN

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	1.14	0	1,6,8	0.45	0
2	CSO	B	429	2	3,6,7	1.47	0	1,6,8	0.33	0
3	MHO	F	488	3	6,8,9	0.98	0	3,9,11	2.34	1 (33%)
2	CSO	D	429	2	3,6,7	1.56	0	1,6,8	0.40	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
3	CSO	F	429	3	-	0/1/5/7	-
2	CSO	B	429	2	-	0/1/5/7	-
3	MHO	F	488	3	-	2/6/7/9	-
2	CSO	D	429	2	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	488	MHO	CE-SD-CG	3.69	106.68	97.45

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 oligosaccharides 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	F	601	-	9,9,9	0.68	0	12,12,12	1.12	1 (8%)
4	3N8	B	605	-	9,9,9	0.71	0	12,12,12	1.17	1 (8%)
8	3NJ	B	607	-	9,10,10	2.35	4 (44%)	7,13,13	2.79	4 (57%)
4	3N8	A	301	-	9,9,9	0.84	0	12,12,12	0.85	0
5	BME	A	302	-	3,3,3	0.22	0	2,2,2	0.33	0
4	3N8	B	603	-	9,9,9	0.77	0	12,12,12	0.95	0
5	BME	F	605	-	3,3,3	0.34	0	2,2,2	0.54	0
4	3N8	D	602	-	9,9,9	0.80	0	12,12,12	1.42	3 (25%)
5	BME	B	606	-	3,3,3	0.36	0	2,2,2	0.07	0
4	3N8	C	301	-	9,9,9	0.86	0	12,12,12	0.97	0
4	3N8	D	603	-	9,9,9	0.72	0	12,12,12	1.04	1 (8%)
4	3N8	F	603	-	9,9,9	0.84	0	12,12,12	0.91	0
4	3N8	F	602	-	9,9,9	0.98	0	12,12,12	1.21	1 (8%)
5	BME	F	606	-	3,3,3	0.28	0	2,2,2	0.69	0
4	3N8	E	301	-	9,9,9	0.79	0	12,12,12	0.95	1 (8%)
4	3N8	D	606	-	9,9,9	0.85	0	12,12,12	1.25	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	3N8	D	605	-	9,9,9	0.88	0	12,12,12	1.13	1 (8%)
4	3N8	D	604	-	9,9,9	0.82	0	12,12,12	0.92	0
4	3N8	B	602	-	9,9,9	0.90	0	12,12,12	1.02	1 (8%)
7	TRS	B	604	-	7,7,7	0.90	0	9,9,9	4.04	8 (88%)

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	F	601	-	-	-	0/1/1/1
4	3N8	B	605	-	-	-	0/1/1/1
8	3NJ	B	607	-	-	-	0/1/1/1
5	BME	A	302	-	-	0/1/1/1	-
4	3N8	A	301	-	-	-	0/1/1/1
4	3N8	B	603	-	-	-	0/1/1/1
5	BME	F	605	-	-	1/1/1/1	-
4	3N8	D	602	-	-	-	0/1/1/1
5	BME	B	606	-	-	1/1/1/1	-
4	3N8	D	603	-	-	-	0/1/1/1
4	3N8	C	301	-	-	-	0/1/1/1
4	3N8	F	603	-	-	-	0/1/1/1
4	3N8	F	602	-	-	-	0/1/1/1
5	BME	F	606	-	-	0/1/1/1	-
4	3N8	E	301	-	-	-	0/1/1/1
4	3N8	D	606	-	-	-	0/1/1/1
4	3N8	D	605	-	-	-	0/1/1/1
4	3N8	D	604	-	-	-	0/1/1/1
4	3N8	B	602	-	-	-	0/1/1/1
7	TRS	B	604	-	-	6/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	607	3NJ	O2-C2	-4.35	1.12	1.21
8	B	607	3NJ	O3-C1	3.18	1.44	1.38
8	B	607	3NJ	O3-C2	2.80	1.43	1.38
8	B	607	3NJ	C5-C4	2.70	1.46	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	604	TRS	C2-C-N	-6.24	92.26	108.17
7	B	604	TRS	C1-C-N	-5.47	94.23	108.17
7	B	604	TRS	C3-C-N	-5.38	94.44	108.17
8	B	607	3NJ	C6-C5-C4	-4.63	123.57	130.61
8	B	607	3NJ	O3-C2-O2	-4.08	106.78	116.25
7	B	604	TRS	C2-C-C1	3.82	120.84	110.66
7	B	604	TRS	C3-C-C2	3.79	120.75	110.66
8	B	607	3NJ	O3-C1-C6	3.25	129.01	122.17
4	D	602	3N8	C5-C4-C3	-2.93	119.36	123.23
4	D	606	3N8	C5-C4-C3	-2.78	119.56	123.23
7	B	604	TRS	O1-C1-C	-2.76	103.19	110.88
4	F	602	3N8	C5-C4-C3	-2.73	119.62	123.23
4	D	605	3N8	C5-C4-C3	-2.57	119.83	123.23
7	B	604	TRS	C3-C-C1	2.47	117.22	110.66
4	D	602	3N8	F9-C4-C3	2.43	121.74	118.28
4	D	602	3N8	C6-C5-C4	2.36	120.81	118.38
4	D	603	3N8	C5-C4-C3	-2.36	120.12	123.23
4	B	605	3N8	C5-C4-C3	-2.32	120.17	123.23
7	B	604	TRS	O2-C2-C	-2.28	104.52	110.88
4	F	601	3N8	C5-C4-C3	-2.27	120.23	123.23
8	B	607	3NJ	O3-C1-O1	-2.26	111.00	116.25
4	B	602	3N8	C5-C4-C3	-2.22	120.30	123.23
4	D	606	3N8	F9-C4-C3	2.19	121.39	118.28
4	E	301	3N8	C5-C4-C3	-2.05	120.52	123.23

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
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	F	602	3N8	1	0
5	F	606	BME	1	0
4	D	605	3N8	1	0
7	B	604	TRS	2	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%)	0.77	17 (8%)	16 25	10, 22, 43, 64	4 (2%)
1	C	200/200 (100%)	0.73	16 (8%)	18 27	10, 22, 38, 55	2 (1%)
1	E	200/200 (100%)	1.04	25 (12%)	8 13	16, 29, 50, 69	1 (0%)
2	B	237/238 (99%)	0.54	8 (3%)	48 60	16, 19, 36, 56	0
2	D	236/238 (99%)	0.50	7 (2%)	52 65	9, 19, 32, 51	2 (0%)
3	F	234/238 (98%)	0.54	9 (3%)	44 55	11, 21, 36, 61	2 (0%)
All	All	1307/1314 (99%)	0.67	82 (6%)	26 35	9, 21, 40, 69	11 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	GLY	5.8
1	C	19[A]	ILE	5.4
1	A	25	ALA	4.3
1	E	98[A]	THR	4.2
1	A	99	PHE	4.1
1	E	25	ALA	4.1
2	B	301	PRO	4.0
1	E	19	ILE	3.9
1	E	15	PRO	3.8
1	A	27	GLY	3.8
1	E	67	PHE	3.6
1	E	27	GLY	3.6
1	A	98[A]	THR	3.5
2	B	416	LEU	3.5
2	B	371	GLY	3.4
1	E	36	TRP	3.4
1	A	19	ILE	3.4
1	E	23	LEU	3.4
1	A	29	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	21	LEU	3.3
1	E	102	GLY	3.2
1	A	67	PHE	3.2
1	E	99	PHE	3.2
1	E	16	TYR	3.0
3	F	400	TRP	2.9
1	E	118	ALA	2.9
2	D	416	LEU	2.9
1	E	42	PRO	2.8
1	E	114	VAL	2.8
1	C	25	ALA	2.8
1	A	36	TRP	2.8
1	E	106	LEU	2.8
3	F	416	LEU	2.8
1	A	40	ALA	2.7
1	E	26	ALA	2.7
1	C	21	LEU	2.7
1	C	23	LEU	2.7
1	A	23	LEU	2.6
2	B	372	LEU	2.6
1	E	101	ALA	2.6
1	A	22	ALA	2.6
2	B	411	LYS	2.6
1	A	177	VAL	2.6
1	C	99	PHE	2.5
1	C	101	ALA	2.5
2	D	302	ALA	2.5
2	D	374	ILE	2.5
3	F	372	LEU	2.5
1	E	20	GLY	2.4
2	D	447	TYR	2.4
1	E	179	GLY	2.4
2	D	535	PHE	2.4
1	E	14	GLY	2.3
1	C	26	ALA	2.3
1	A	20	GLY	2.3
3	F	430	LEU	2.3
3	F	505	ILE	2.3
1	C	42	PRO	2.3
3	F	355	GLY	2.3
1	E	52	LEU	2.3
2	B	435	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	499	GLU	2.2
1	E	21	LEU	2.2
1	E	85	LEU	2.2
2	B	442	ILE	2.2
2	D	411	LYS	2.2
3	F	370	GLY	2.2
1	C	120	VAL	2.2
3	F	354	LEU	2.2
2	D	400	TRP	2.2
1	C	28	ASN	2.2
1	A	114[A]	VAL	2.2
1	E	30	THR	2.1
1	C	36	TRP	2.1
1	A	18	HIS	2.1
1	C	98	THR	2.1
1	E	175	CYS	2.1
1	C	14	GLY	2.1
1	C	177	VAL	2.1
1	A	52	LEU	2.0
2	B	538	CYS	2.0
1	C	106	LEU	2.0

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

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
3	MHO	F	488	9/10	0.89	0.15	18,21,46,51	0
2	CSO	D	429	7/8	0.90	0.13	19,21,25,30	0
3	CSO	F	429	7/8	0.93	0.13	21,26,29,30	0
2	CSO	B	429	7/8	0.96	0.09	18,21,25,29	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
8	3NJ	B	607	10/10	0.80	0.20	15,27,36,40	10
7	TRS	B	604	8/8	0.83	0.18	40,44,49,54	0
4	3N8	D	605	9/9	0.86	0.12	29,32,36,52	0
4	3N8	D	603	9/9	0.88	0.11	30,34,46,48	0
4	3N8	B	602	9/9	0.88	0.10	29,31,36,48	0
4	3N8	B	603	9/9	0.89	0.12	29,33,42,53	0
4	3N8	F	601	9/9	0.89	0.12	34,37,44,46	0
4	3N8	D	606	9/9	0.89	0.12	34,40,44,55	0
4	3N8	C	301	9/9	0.89	0.11	30,31,34,39	0
5	BME	F	606	4/4	0.90	0.11	38,45,47,63	0
4	3N8	F	603	9/9	0.90	0.11	31,35,39,45	0
5	BME	F	605	4/4	0.90	0.12	41,44,52,53	0
4	3N8	D	604	9/9	0.91	0.11	28,31,41,45	0
4	3N8	F	602	9/9	0.91	0.12	28,33,36,50	0
4	3N8	B	605	9/9	0.91	0.10	31,33,42,44	0
5	BME	B	606	4/4	0.91	0.10	36,42,46,57	0
4	3N8	E	301	9/9	0.92	0.11	32,33,40,41	0
5	BME	A	302	4/4	0.93	0.08	34,37,38,45	0
4	3N8	A	301	9/9	0.93	0.10	24,26,30,34	0
4	3N8	D	602	9/9	0.94	0.09	28,32,40,45	0
9	CL	F	604	1/1	0.94	0.09	54,54,54,54	0
6	FE	D	601	1/1	1.00	0.03	18,18,18,18	1
6	FE	B	601	1/1	1.00	0.03	19,19,19,19	1
6	FE	F	607	1/1	1.00	0.03	18,18,18,18	1

6.5 Other polymers ⓘ

There are no such residues in this entry.