W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:49 am GMT

PDB ID	:	4ZG9
Title	:	Structural basis for inhibition of human autotaxin by four novel compounds
Authors	:	Stein, A.J.; Bain, G.; Hutchinson, J.H.; Evans, J.F.
Deposited on	:	2015-04-22
Resolution	:	2.95 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 2.95 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		5
Ramachandran outliers		0.9%
Sidechain outliers		7.5%
RSRZ outliers		2.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
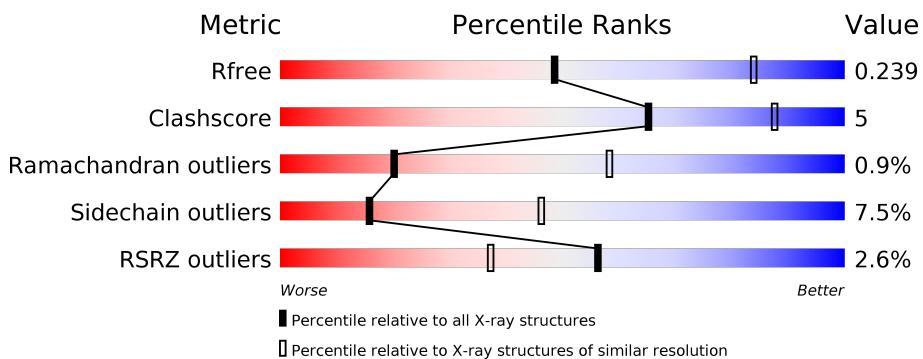
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	863	2% 72% 13% • 13%
1	B	863	2% 76% 11% • 11%
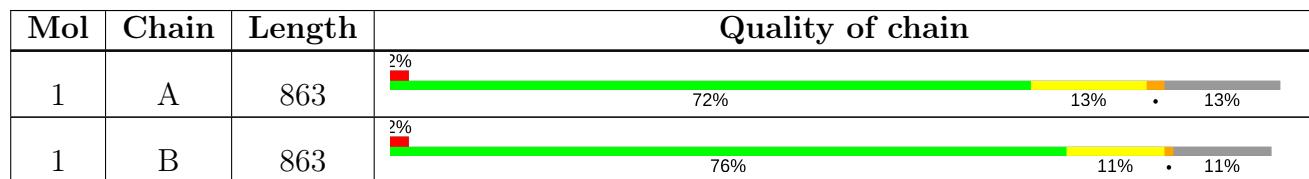
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	4O2	A	909	-	-	-	X

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 12241 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	2	0
			5932	3783	1010	1093	46			
1	B	764	Total	C	N	O	S	0	0	0
			6045	3851	1029	1118	47			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
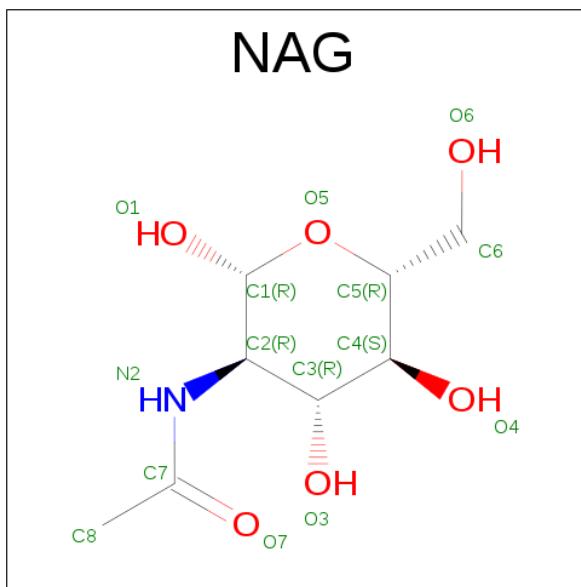
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Na 2	0	0
5	A	2	Total 2	Na 2	0	0

- Molecule 6 is 3-[(11aS)-6-(4-fluorobenzyl)-1,3-dioxo-5,6,11,11a-tetrahydro-1H-imidaz o[1',5':1,6]pyrido[3,4-b]indol-2(3H)-yl]propanoic acid (three-letter code: 4O2) (formula: $C_{23}H_{20}FN_3O_4$).
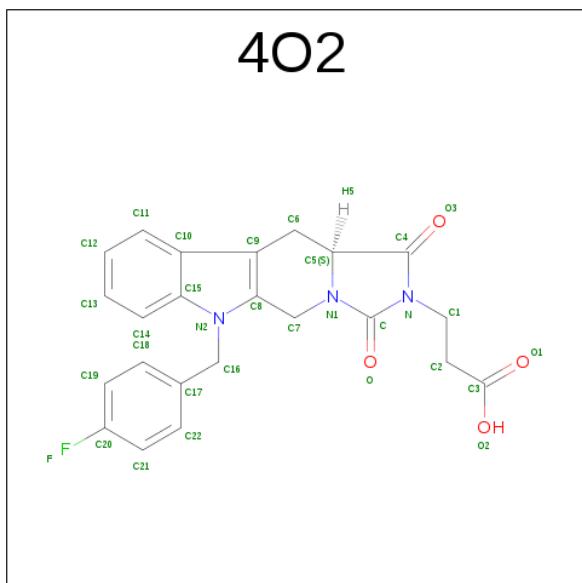
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			31	23	1	3	4		
6	A	1	Total	C	F	N	O	0	0
			31	23	1	3	4		
6	B	1	Total	C	F	N	O	0	0
			31	23	1	3	4		
6	B	1	Total	C	F	N	O	0	0
			31	23	1	3	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
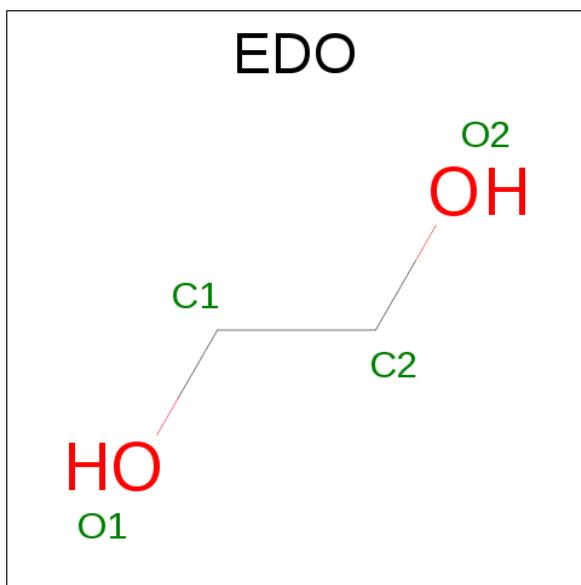
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).
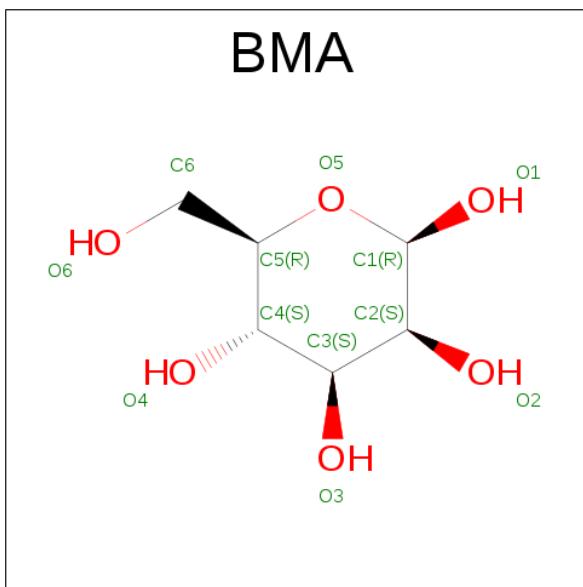
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 11	C 6	O 5	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	19	Total 19	O 19	0	0
9	B	32	Total 32	O 32	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2
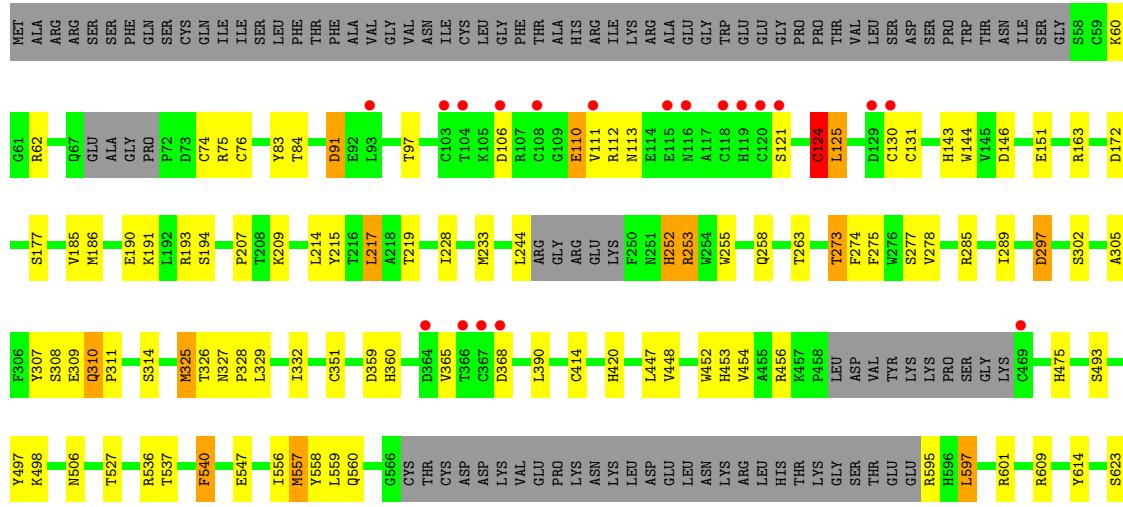
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2
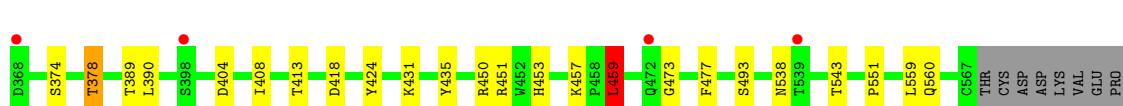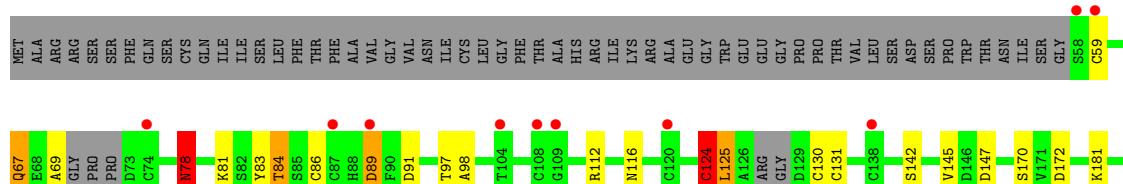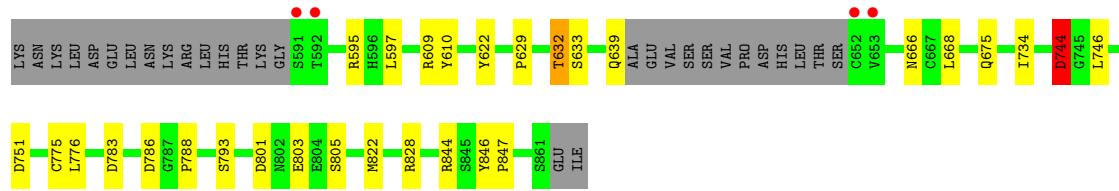
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	127.46Å　　209.99Å　　188.19Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	43.86　–　2.95 43.86　–　2.92	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.86-2.95) 97.9 (43.86-2.92)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179　,　0.244 0.181　,　0.239	Depositor DCC
R_{free} test set	2699 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.016 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12241	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, 4O2, NA, CA, EDO

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	0.57	0/6113	0.75	2/8323 (0.0%)
1	B	0.58	0/6218	0.75	3/8456 (0.0%)
All	All	0.57	0/12331	0.75	5/16779 (0.0%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	459	LEU	CA-CB-CG	5.81	128.66	115.30
1	B	744	ASP	CB-CA-C	-5.10	100.19	110.40
1	A	325	MET	CG-SD-CE	-5.09	92.06	100.20
1	A	826	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	744	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	424	TYR	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	5932	0	5534	58	0
1	B	6045	0	5674	49	0
2	A	28	0	25	0	0
2	B	28	0	24	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	62	0	38	4	0
6	B	62	0	38	4	0
7	A	8	0	12	0	0
7	B	4	0	5	0	0
8	B	11	0	10	0	0
9	A	19	0	0	1	0
9	B	32	0	0	1	0
All	All	12241	0	11360	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (111) 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:124:CYS:SG	1:B:125:LEU:N	2.53	0.82
6:A:909:4O2:H9	6:A:909:4O2:H15	1.67	0.77
1:A:121:SER:O	1:A:124:CYS:HB3	1.85	0.77
1:B:639:GLN:N	1:B:639:GLN:OE1	2.19	0.75
1:B:83:TYR:OH	1:B:249:LYS:HG2	1.90	0.72
6:B:909:4O2:H4	6:B:909:4O2:O3	1.89	0.71
1:A:844:ARG:HD3	1:A:848:GLU:OE2	1.93	0.69
1:B:378:THR:HA	9:B:1015:HOH:O	1.93	0.68
1:A:310:GLN:HE22	1:A:314:SER:H	1.43	0.66
1:A:110:GLU:HB3	1:A:121:SER:HA	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASP:N	1:B:297:ASP:OD1	2.29	0.65
1:B:457:LYS:HD3	1:B:459:LEU:HD21	1.79	0.64
1:A:190:GLU:OE2	1:A:193:ARG:NH1	2.31	0.64
1:A:62:ARG:NH2	1:A:76:CYS:SG	2.71	0.63
1:B:185:VAL:HG13	1:B:330:ARG:HG2	1.80	0.62
1:A:365:VAL:HG11	1:A:453:HIS:CD2	2.37	0.60
1:B:413:THR:HG21	1:B:803:GLU:HG3	1.84	0.60
1:B:81:LYS:HG2	1:B:86:CYS:SG	2.42	0.59
1:B:83:TYR:O	1:B:84:THR:OG1	2.18	0.59
1:B:325:MET:O	1:B:328:PRO:HD2	2.03	0.59
1:B:744:ASP:HB3	1:B:746:LEU:H	1.66	0.58
1:B:632:THR:O	1:B:734:ILE:HA	2.03	0.58
1:B:83:TYR:C	1:B:84:THR:OG1	2.40	0.58
1:A:314:SER:HB3	1:A:325:MET:HE1	1.86	0.58
1:A:110:GLU:HB3	1:A:121:SER:CA	2.35	0.56
1:A:609:ARG:HD2	1:A:624:GLU:OE1	2.05	0.56
1:B:98:ALA:HB3	1:B:116:ASN:HA	1.88	0.56
1:A:310:GLN:HE21	1:A:310:GLN:HA	1.72	0.55
1:B:314:SER:CB	1:B:325:MET:HE1	2.36	0.55
1:B:78:ASN:HD22	1:B:78:ASN:C	2.11	0.53
1:A:297:ASP:OD1	1:A:297:ASP:N	2.41	0.53
1:A:255:TRP:CH2	6:A:909:4O2:H16	2.43	0.53
1:B:363:GLU:O	1:B:473:GLY:HA2	2.08	0.52
1:A:497:TYR:CE2	1:A:498:LYS:HD2	2.45	0.52
1:A:91:ASP:N	1:A:91:ASP:OD1	2.43	0.51
1:B:622:TYR:HA	1:B:629:PRO:HA	1.92	0.51
1:A:124:CYS:SG	1:A:125:LEU:N	2.84	0.51
1:A:310:GLN:NE2	1:A:314:SER:H	2.07	0.51
1:B:210:THR:HG22	1:B:214:LEU:HD22	1.93	0.51
1:A:274:PHE:HA	1:A:305:ALA:HB3	1.91	0.50
1:A:172:ASP:OD2	1:A:307:TYR:OH	2.30	0.49
1:A:151:GLU:HA	1:A:497:TYR:CD1	2.47	0.49
1:B:67:GLN:HE22	1:B:69:ALA:HB2	1.76	0.49
1:A:143:HIS:HB2	1:A:146:ASP:OD2	2.11	0.49
1:B:78:ASN:C	1:B:78:ASN:ND2	2.64	0.49
1:A:163:ARG:NH1	1:A:302:SER:OG	2.45	0.49
1:A:274:PHE:O	6:A:908:4O2:H17	2.13	0.48
1:B:308:SER:OG	1:B:310:GLN:O	2.28	0.48
1:B:78:ASN:OD1	1:B:273:THR:HG21	2.13	0.48
1:B:801:ASP:OD1	1:B:803:GLU:HB2	2.14	0.48
1:A:497:TYR:CZ	1:A:498:LYS:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:HIS:CE1	1:B:299:GLU:OE1	2.66	0.48
1:A:207:PRO:HB2	1:A:209:LYS:HG2	1.97	0.47
1:B:207:PRO:HD3	1:B:435:TYR:CE1	2.49	0.47
1:B:89:ASP:N	1:B:89:ASP:OD1	2.47	0.47
1:B:551:PRO:HB3	1:B:610:TYR:CE2	2.50	0.47
1:B:450:ARG:O	1:B:451:ARG:HB2	2.14	0.47
1:B:81:LYS:NZ	1:B:91:ASP:OD1	2.41	0.47
1:B:363:GLU:OE2	1:B:450:ARG:NH2	2.47	0.47
1:A:172:ASP:O	1:A:311:PRO:HD2	2.14	0.47
1:A:217:LEU:HD13	1:A:506:ASN:HB2	1.97	0.47
1:A:558:TYR:O	1:A:657:VAL:HG22	2.14	0.47
1:B:325:MET:C	1:B:328:PRO:HD2	2.34	0.46
1:B:275:PHE:HA	6:B:909:4O2:O	2.15	0.46
1:A:536:ARG:HG2	1:A:537:THR:HG23	1.98	0.46
1:B:310:GLN:OE1	1:B:311:PRO:HA	2.15	0.46
1:A:556:ILE:HG23	1:A:657:VAL:CG1	2.45	0.46
6:B:910:4O2:O3	6:B:910:4O2:H4	2.15	0.46
1:A:258:GLN:OE1	1:A:263:THR:HA	2.16	0.45
1:A:360:HIS:CE1	1:A:475:HIS:CE1	3.05	0.45
1:A:83:TYR:O	1:A:84:THR:OG1	2.34	0.45
1:A:308:SER:OG	1:A:332:ILE:HD11	2.17	0.44
1:A:614:TYR:C	1:A:614:TYR:CD1	2.91	0.44
1:A:106:ASP:OD1	1:A:106:ASP:N	2.49	0.44
1:A:770:SER:HB2	1:A:794:PHE:CZ	2.53	0.44
1:B:314:SER:HB3	1:B:325:MET:HE1	1.99	0.44
1:A:215:TYR:O	1:A:219:THR:HG23	2.18	0.44
1:B:431:LYS:HD2	1:B:431:LYS:HA	1.76	0.44
1:A:151:GLU:HA	1:A:497:TYR:CE1	2.53	0.43
6:A:909:4O2:C7	6:A:909:4O2:H15	2.41	0.43
1:A:111:VAL:O	1:A:113:ASN:N	2.42	0.43
1:B:776:LEU:CD2	1:B:788:PRO:HB2	2.49	0.43
1:B:666:ASN:OD1	1:B:668:LEU:HB3	2.19	0.43
1:B:97:THR:O	1:B:97:THR:HG22	2.17	0.43
1:B:83:TYR:HE2	1:B:249:LYS:HD3	1.84	0.43
1:A:327:ASN:HB2	1:A:328:PRO:HD3	2.00	0.43
1:B:170:SER:HA	1:B:357:VAL:O	2.18	0.43
1:A:359:ASP:OD1	1:A:360:HIS:N	2.53	0.42
1:A:144:TRP:CH2	1:A:191:LYS:HG2	2.55	0.42
1:B:190:GLU:OE2	1:B:193:ARG:NH1	2.53	0.42
1:A:557:MET:HB3	1:A:558:TYR:CD1	2.55	0.42
1:A:527:THR:OG1	1:A:828:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:SER:OG	1:B:147:ASP:OD1	2.35	0.42
1:A:228:ILE:HG23	1:A:244:LEU:HD11	2.02	0.41
1:A:448:VAL:HG22	1:A:454:VAL:HG21	2.02	0.41
1:A:595:ARG:NH1	1:A:783:ASP:OD2	2.53	0.41
1:A:597:LEU:HD11	1:A:601:ARG:HB3	2.01	0.41
1:A:186:MET:SD	1:A:329:LEU:HB3	2.60	0.41
1:A:252[B]:HIS:CE1	1:A:253:ARG:HD3	2.55	0.41
1:A:273:THR:HB	1:A:275:PHE:H	1.86	0.41
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.92	0.41
1:A:285:ARG:O	1:A:289:ILE:HG13	2.21	0.41
1:A:540:PHE:HA	9:A:1007:HOH:O	2.21	0.41
1:A:623:SER:HB2	1:A:630:LEU:HD21	2.03	0.41
1:B:389:THR:HG22	1:B:477:PHE:CZ	2.56	0.41
1:B:285:ARG:NH2	6:B:909:4O2:O1	2.54	0.40
1:B:404:ASP:O	1:B:408:ILE:HG12	2.21	0.40
1:A:420:HIS:CD2	1:A:452:TRP:CZ2	3.09	0.40
1:B:83:TYR:CE2	1:B:249:LYS:HD3	2.57	0.40
1:B:846:TYR:N	1:B:847:PRO:CD	2.85	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	740/863 (86%)	682 (92%)	52 (7%)	6 (1%)	22	61
1	B	754/863 (87%)	695 (92%)	52 (7%)	7 (1%)	20	58
All	All	1494/1726 (87%)	1377 (92%)	104 (7%)	13 (1%)	20	58

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	124	CYS
1	B	78	ASN
1	A	414	CYS
1	B	124	CYS
1	B	181	LYS
1	B	248	GLU
1	B	374	SER
1	A	112	ARG
1	B	112	ARG
1	B	751	ASP
1	A	815	TRP
1	A	729	ASN

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	642/780 (82%)	593 (92%)	49 (8%)	15	46
1	B	656/780 (84%)	607 (92%)	49 (8%)	16	46
All	All	1298/1560 (83%)	1200 (92%)	98 (8%)	16	46

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	CYS
1	A	75	ARG
1	A	91	ASP
1	A	97	THR
1	A	110	GLU
1	A	124	CYS
1	A	125	LEU
1	A	130	CYS
1	A	131	CYS
1	A	177	SER
1	A	185	VAL

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Mol	Chain	Res	Type
1	A	194	SER
1	A	217	LEU
1	A	233	MET
1	A	252[A]	HIS
1	A	252[B]	HIS
1	A	253	ARG
1	A	273	THR
1	A	277	SER
1	A	278	VAL
1	A	297	ASP
1	A	309	GLU
1	A	310	GLN
1	A	326	THR
1	A	351	CYS
1	A	368	ASP
1	A	390	LEU
1	A	447	LEU
1	A	456	ARG
1	A	493	SER
1	A	540	PHE
1	A	547	GLU
1	A	557	MET
1	A	559	LEU
1	A	560	GLN
1	A	597	LEU
1	A	639	GLN
1	A	652	CYS
1	A	657	VAL
1	A	749	THR
1	A	773	THR
1	A	774	SER
1	A	775	CYS
1	A	793	SER
1	A	799	ARG
1	A	805	SER
1	A	828	ARG
1	A	844	ARG
1	A	858	THR
1	B	59	CYS
1	B	67	GLN
1	B	78	ASN
1	B	84	THR

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Mol	Chain	Res	Type
1	B	89	ASP
1	B	124	CYS
1	B	125	LEU
1	B	130	CYS
1	B	131	CYS
1	B	145	VAL
1	B	172	ASP
1	B	193	ARG
1	B	214	LEU
1	B	217	LEU
1	B	244	LEU
1	B	247	ARG
1	B	253	ARG
1	B	270	LYS
1	B	291	GLN
1	B	297	ASP
1	B	308	SER
1	B	317	LYS
1	B	330	ARG
1	B	366	THR
1	B	378	THR
1	B	390	LEU
1	B	418	ASP
1	B	453	HIS
1	B	459	LEU
1	B	493	SER
1	B	538	ASN
1	B	543	THR
1	B	559	LEU
1	B	560	GLN
1	B	595	ARG
1	B	597	LEU
1	B	609	ARG
1	B	632	THR
1	B	633	SER
1	B	675	GLN
1	B	744	ASP
1	B	775	CYS
1	B	783	ASP
1	B	786	ASP
1	B	793	SER
1	B	805	SER

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Mol	Chain	Res	Type
1	B	822	MET
1	B	828	ARG
1	B	844	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	GLN
1	A	338	GLN
1	A	434	HIS
1	A	453	HIS
1	A	732	ASN
1	B	67	GLN
1	B	298	HIS
1	B	538	ASN

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 ⓘ

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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
2	NAG	A	901	1,2	14,14,15	0.67	0	15,19,21	1.72	3 (20%)
2	NAG	A	902	2	14,14,15	0.44	0	15,19,21	1.51	3 (20%)
6	4O2	A	908	-	29,35,35	1.89	5 (17%)	29,52,52	4.21	9 (31%)
6	4O2	A	909	-	29,35,35	2.02	5 (17%)	29,52,52	4.34	13 (44%)
7	EDO	A	910	3	3,3,3	0.58	0	2,2,2	0.45	0
7	EDO	A	911	-	3,3,3	0.63	0	2,2,2	0.35	0
2	NAG	B	901	1,2	14,14,15	0.74	1 (7%)	15,19,21	1.70	3 (20%)
2	NAG	B	902	8,2	14,14,15	0.93	1 (7%)	15,19,21	1.89	4 (26%)
8	BMA	B	903	2	11,11,12	1.15	1 (9%)	13,15,17	1.89	2 (15%)
6	4O2	B	909	-	29,35,35	2.34	10 (34%)	29,52,52	4.93	10 (34%)
6	4O2	B	910	-	29,35,35	2.21	10 (34%)	29,52,52	4.97	7 (24%)
7	EDO	B	911	3	3,3,3	0.74	0	2,2,2	0.29	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
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	2	-	0/6/23/26	0/1/1/1
6	4O2	A	908	-	-	0/7/37/37	0/5/5/5
6	4O2	A	909	-	-	0/7/37/37	0/5/5/5
7	EDO	A	910	3	-	0/1/1/1	0/0/0/0
7	EDO	A	911	-	-	0/1/1/1	0/0/0/0
2	NAG	B	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	902	8,2	-	0/6/23/26	0/1/1/1
8	BMA	B	903	2	-	0/2/19/22	0/1/1/1
6	4O2	B	909	-	-	0/7/37/37	0/5/5/5
6	4O2	B	910	-	-	0/7/37/37	0/5/5/5
7	EDO	B	911	3	-	0/1/1/1	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	910	4O2	C4-N	-5.42	1.31	1.38
6	B	909	4O2	C4-N	-5.24	1.31	1.38
6	A	909	4O2	C5-C4	-5.11	1.45	1.52
6	B	909	4O2	C-N	-5.06	1.30	1.40
6	B	909	4O2	C5-C4	-4.80	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	908	4O2	C5-C4	-4.72	1.45	1.52
6	B	910	4O2	C5-C4	-4.46	1.46	1.52
6	B	910	4O2	C-N	-4.38	1.31	1.40
6	B	909	4O2	C-N1	-3.76	1.29	1.37
6	B	909	4O2	C11-C10	-3.11	1.35	1.42
6	B	910	4O2	C-N1	-2.61	1.32	1.37
6	B	910	4O2	C11-C10	-2.48	1.37	1.42
6	A	908	4O2	C11-C10	-2.40	1.37	1.42
6	B	909	4O2	C14-C15	-2.40	1.36	1.41
6	B	910	4O2	C16-N2	-2.33	1.44	1.48
2	B	902	NAG	O5-C1	-2.27	1.40	1.43
2	B	901	NAG	O5-C1	-2.08	1.40	1.43
6	B	910	4O2	C14-C15	-2.04	1.36	1.41
6	B	909	4O2	F-C20	-2.04	1.31	1.36
6	B	909	4O2	C16-N2	-2.03	1.44	1.48
6	B	909	4O2	C9-C10	2.22	1.45	1.41
6	B	910	4O2	O3-C4	2.30	1.26	1.22
6	B	910	4O2	C9-C10	2.61	1.46	1.41
8	B	903	BMA	C2-C3	2.83	1.56	1.52
6	A	909	4O2	O-C	3.13	1.28	1.22
6	A	908	4O2	O-C	3.29	1.28	1.22
6	A	909	4O2	C9-C10	3.52	1.48	1.41
6	A	909	4O2	O3-C4	3.89	1.29	1.22
6	A	908	4O2	O3-C4	4.01	1.29	1.22
6	B	909	4O2	C8-C9	4.38	1.45	1.38
6	B	910	4O2	C8-C9	4.38	1.45	1.38
6	A	909	4O2	C8-C9	5.32	1.47	1.38
6	A	908	4O2	C8-C9	5.33	1.47	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	909	4O2	C4-N-C	-20.22	99.06	111.73
6	A	908	4O2	C4-N-C	-18.68	100.02	111.73
6	B	910	4O2	C4-N-C	-18.59	100.08	111.73
6	A	909	4O2	C4-N-C	-18.09	100.39	111.73
6	B	910	4O2	C4-C5-N1	-12.95	88.85	101.70
6	B	909	4O2	C4-C5-N1	-12.87	88.93	101.70
6	A	909	4O2	C4-C5-N1	-7.86	93.91	101.70
6	A	908	4O2	C4-C5-N1	-7.49	94.27	101.70
6	B	910	4O2	C2-C1-N	-7.27	104.75	112.22
6	B	910	4O2	O3-C4-N	-7.03	115.29	124.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	909	4O2	O3-C4-N	-4.87	118.03	124.19
2	B	901	NAG	O5-C1-C2	-4.56	105.13	111.47
2	B	902	NAG	O4-C4-C3	-3.44	102.86	110.36
6	A	909	4O2	C17-C16-N2	-3.44	107.15	112.62
6	A	908	4O2	O3-C4-N	-3.26	120.06	124.19
6	A	909	4O2	C14-C15-C10	-3.05	116.78	120.94
6	B	909	4O2	O3-C4-C5	-3.05	118.45	125.32
6	A	908	4O2	C14-C15-C10	-3.04	116.81	120.94
2	A	902	NAG	O5-C1-C2	-2.85	107.51	111.47
6	A	909	4O2	O3-C4-N	-2.76	120.69	124.19
6	A	909	4O2	O3-C4-C5	-2.72	119.19	125.32
6	A	908	4O2	O3-C4-C5	-2.63	119.41	125.32
2	B	901	NAG	O7-C7-C8	-2.49	117.53	122.06
6	B	909	4O2	O-C-N1	-2.37	122.23	125.80
6	A	909	4O2	C21-C20-C19	-2.34	119.61	122.86
2	A	902	NAG	O7-C7-C8	-2.33	117.83	122.06
6	B	909	4O2	C2-C1-N	-2.21	109.95	112.22
2	A	902	NAG	C3-C4-C5	-2.14	106.44	110.22
2	A	901	NAG	O7-C7-C8	-2.13	118.19	122.06
6	A	909	4O2	O-C-N1	-2.11	122.62	125.80
6	B	909	4O2	C14-C15-C10	-2.04	118.16	120.94
6	A	908	4O2	C17-C16-N2	2.01	115.81	112.62
2	A	901	NAG	O7-C7-N2	2.26	126.27	121.92
2	B	902	NAG	C4-C3-C2	2.35	114.46	111.02
6	A	909	4O2	C1-N-C4	2.42	127.47	123.27
6	A	909	4O2	C9-C8-N2	2.58	110.18	107.01
6	A	909	4O2	C16-C17-C18	2.64	125.34	120.42
6	A	908	4O2	C9-C8-N2	2.90	110.57	107.01
8	B	903	BMA	C2-C3-C4	3.14	116.35	110.88
2	B	901	NAG	C1-O5-C5	3.14	116.50	112.17
6	A	909	4O2	C2-C1-N	3.24	115.55	112.22
6	B	910	4O2	C1-N-C4	3.37	129.11	123.27
2	B	902	NAG	O4-C4-C5	3.43	117.92	109.28
2	B	902	NAG	C1-O5-C5	3.48	116.96	112.17
6	B	909	4O2	C1-N-C	3.51	127.34	123.63
6	B	909	4O2	C9-C8-N2	3.65	111.49	107.01
6	A	908	4O2	C1-N-C4	4.11	130.38	123.27
6	B	910	4O2	C9-C8-N2	4.23	112.20	107.01
2	A	901	NAG	C1-O5-C5	4.24	118.02	112.17
8	B	903	BMA	C1-C2-C3	4.81	115.75	109.65
6	A	908	4O2	C1-N-C	5.64	129.59	123.63
6	B	909	4O2	C1-N-C4	5.96	133.59	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	910	4O2	C1-N-C	6.76	130.78	123.63
6	A	909	4O2	C1-N-C	8.04	132.14	123.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	908	4O2	1	0
6	A	909	4O2	3	0
6	B	909	4O2	3	0
6	B	910	4O2	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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	750/863 (86%)	-0.15	19 (2%)	58	39	35, 56, 104, 135	0
1	B	764/863 (88%)	-0.18	21 (2%)	55	36	35, 57, 102, 124	0
All	All	1514/1726 (87%)	-0.16	40 (2%)	56	37	35, 57, 102, 135	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	CYS	4.4
1	B	539	THR	4.1
1	A	93	LEU	4.0
1	B	59	CYS	3.7
1	A	469	CYS	3.7
1	A	116	ASN	3.4
1	A	118	CYS	3.3
1	B	366	THR	3.2
1	B	652	CYS	3.0
1	B	653	VAL	2.9
1	A	367	CYS	2.8
1	A	119	HIS	2.8
1	A	108	CYS	2.8
1	B	104	THR	2.8
1	B	58	SER	2.7
1	A	111	VAL	2.7
1	A	368	ASP	2.6
1	B	74	CYS	2.5
1	B	87	CYS	2.5
1	B	592	THR	2.5
1	B	89	ASP	2.5
1	B	108	CYS	2.5
1	B	318	TYR	2.5
1	B	368	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	364	ASP	2.4
1	B	120	CYS	2.4
1	A	106	ASP	2.4
1	B	591	SER	2.3
1	A	129	ASP	2.3
1	B	398	SER	2.3
1	A	104	THR	2.2
1	A	103	CYS	2.2
1	B	472	GLN	2.2
1	B	321	PHE	2.2
1	A	366	THR	2.2
1	A	130	CYS	2.1
1	A	121	SER	2.1
1	B	138	CYS	2.0
1	A	115	GLU	2.0
1	B	109	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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
6	4O2	A	909	31/31	0.92	0.29	2.50	53,70,99,108	0
7	EDO	A	910	4/4	0.97	0.19	1.70	48,53,55,59	0
6	4O2	B	910	31/31	0.94	0.20	0.62	50,58,87,88	0
7	EDO	B	911	4/4	0.97	0.21	0.24	46,55,61,62	0
2	NAG	A	901	14/15	0.96	0.17	-0.09	44,47,53,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
6	4O2	A	908	31/31	0.97	0.17	-0.19	37,41,54,64	0
6	4O2	B	909	31/31	0.97	0.16	-0.27	42,46,69,74	0
7	EDO	A	911	4/4	0.98	0.15	-0.29	44,46,48,49	0
2	NAG	B	901	14/15	0.97	0.13	-0.61	42,47,52,59	0
5	NA	A	907	1/1	0.96	0.13	-0.89	50,50,50,50	0
4	CA	A	905	1/1	0.98	0.11	-1.02	58,58,58,58	0
4	CA	B	906	1/1	0.99	0.12	-1.07	45,45,45,45	0
5	NA	B	907	1/1	0.96	0.11	-1.47	56,56,56,56	0
3	ZN	B	905	1/1	0.98	0.13	-1.83	93,93,93,93	0
5	NA	A	906	1/1	0.92	0.10	-2.00	72,72,72,72	0
3	ZN	A	903	1/1	1.00	0.10	-2.03	46,46,46,46	0
5	NA	B	908	1/1	0.96	0.07	-2.49	56,56,56,56	0
3	ZN	B	904	1/1	0.98	0.10	-2.63	57,57,57,57	0
3	ZN	A	904	1/1	0.97	0.06	-3.86	99,99,99,99	0
2	NAG	B	902	14/15	0.95	0.14	-	51,58,72,80	0
2	NAG	A	902	14/15	0.96	0.26	-	51,58,72,74	0
8	BMA	B	903	11/12	0.83	0.20	-	83,91,97,101	0

6.5 Other polymers ⓘ

There are no such residues in this entry.