



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:26 AM GMT

PDB ID : 3ENS
Title : Crystal structure of human FXA in complex with methyl (2Z)-3-[(3-chloro-1H-indol-7-yl)amino]-2-cyano-3-{[(3S)-2-oxo-1-(2-oxo-2-pyrrolidin-1-ylethyl)azepan-3-yl]amino}acrylate
Authors : Klei, H.E.
Deposited on : 2008-09-25
Resolution : 2.30 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

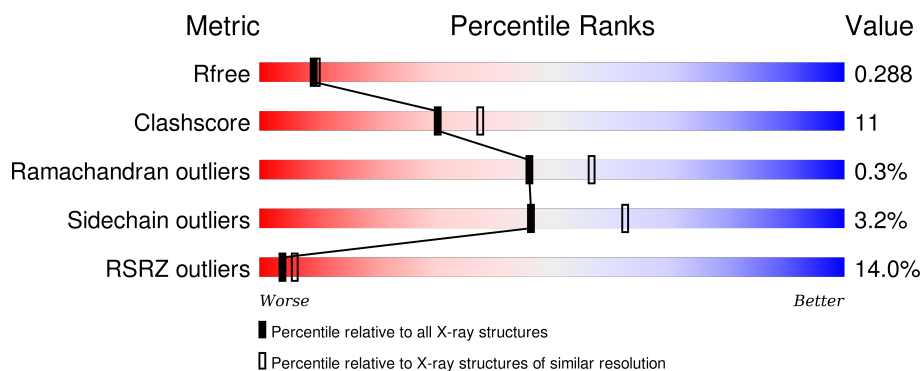
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	94	<div> <div>21%</div> <div>66%</div> <div>22%</div> <div>11%</div> </div>
1	C	94	<div> <div>26%</div> <div>72%</div> <div>15%</div> <div>11%</div> </div>
2	B	238	<div> <div>8%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>
2	D	238	<div> <div>12%</div> <div>84%</div> <div>15%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	203	-	-	-	X
7	GOL	D	306	-	-	-	X
7	GOL	D	307	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5432 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.

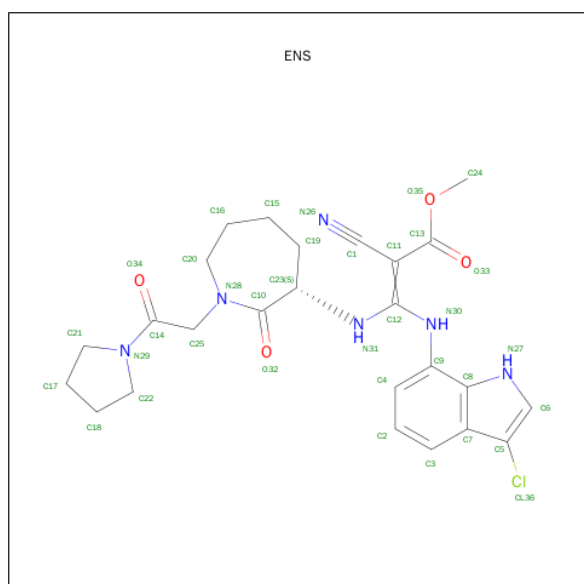
- Molecule 1 is a protein called Factor X light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	84	Total	C	N	O	S	0	0	0
			625	375	106	131	13			
1	C	84	Total	C	N	O	S	0	0	1
			610	366	104	127	13			

- Molecule 2 is a protein called Activated factor Xa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1879	1183	329	353	14			
2	D	238	Total	C	N	O	S	0	0	0
			1864	1175	324	351	14			

- Molecule 3 is METHYL (2Z)-3-[(3-CHLORO-1H-INDOL-7-YL)AMINO]-2-CYANO-3-[[[(3S)-2-OXO-1-(2-OXO-2-PYRROLIDIN-1-YLETHYL)AZEPAN-3-YL]AMINO}ACRYLATE (three-letter code: ENS) (formula: C₂₅H₂₉ClN₆O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			36	25	1	6	4		
3	D	1	Total	C	Cl	N	O	0	0
			36	25	1	6	4		

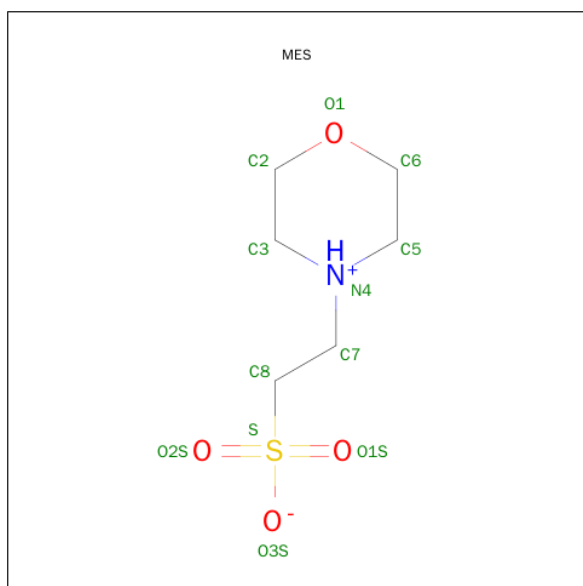
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

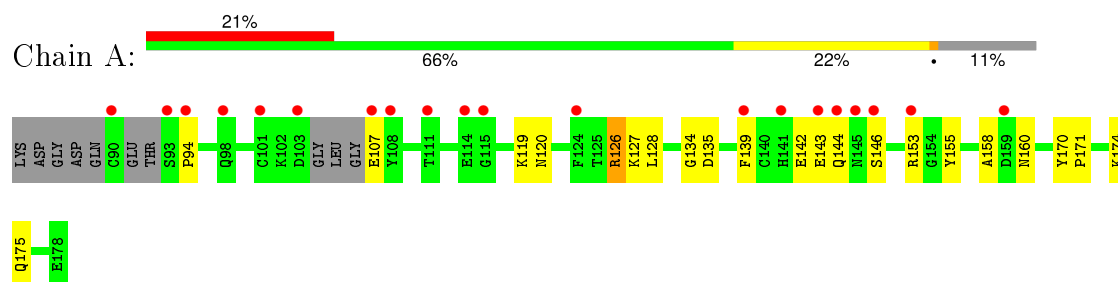
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	28	Total	O	0	0
			28	28		
9	B	126	Total	O	0	0
			126	126		
9	C	26	Total	O	0	0
			26	26		
9	D	124	Total	O	0	0
			124	124		

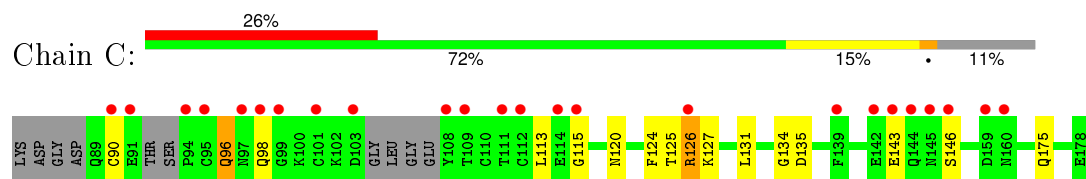
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

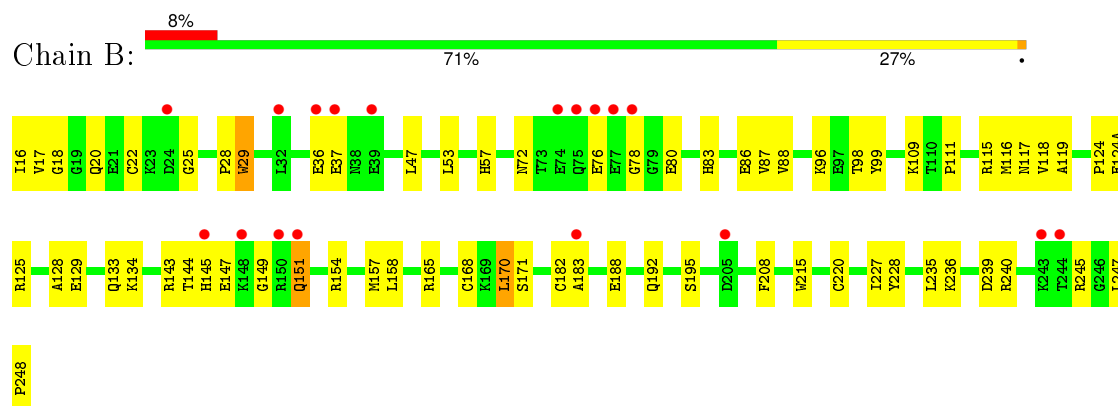
- Molecule 1: Factor X light chain



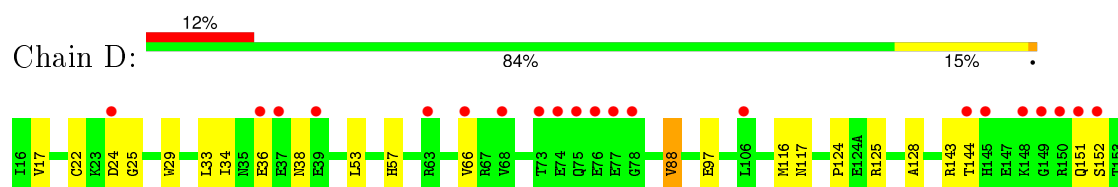
- Molecule 1: Factor X light chain



- Molecule 2: Activated factor Xa heavy chain



- Molecule 2: Activated factor Xa heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.31Å 78.86Å 73.85Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	19.03 – 2.30 19.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.03-2.30) 97.3 (19.03-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.223 , 0.286 0.223 , 0.288	Depositor DCC
R_{free} test set	1000 reflections (3.42%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.7	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 30225 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5432	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, CA, ENS, MES, ACT

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	0.32	0/633	0.47	0/850
1	C	0.30	0/618	0.47	0/830
2	B	0.32	0/1918	0.52	0/2583
2	D	0.33	0/1903	0.51	0/2566
All	All	0.32	0/5072	0.50	0/6829

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	625	0	550	19	0
1	C	610	0	533	16	0
2	B	1879	0	1836	47	0
2	D	1864	0	1805	26	0
3	B	36	0	29	4	0
3	D	36	0	29	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	B	12	0	12	2	0
6	D	12	0	12	2	0
7	A	18	0	24	3	0
7	B	6	0	8	0	0
7	D	18	0	24	1	0
8	B	4	0	3	0	0
8	D	4	0	3	0	0
9	A	28	0	0	3	0
9	B	126	0	0	4	0
9	C	26	0	0	1	0
9	D	124	0	0	6	0
All	All	5432	0	4868	110	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 11.

All (110) 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)
3:B:301:ENS:C4	3:B:301:ENS:HN31	2.03	0.71
2:D:232:THR:HG23	9:D:337:HOH:O	1.92	0.69
2:B:145:HIS:HB3	2:B:149:GLY:HA3	1.74	0.69
2:D:22:CYS:SG	2:D:157:MET:HG2	2.33	0.69
2:B:125:ARG:O	2:B:129:GLU:HG3	1.95	0.67
1:A:174:LYS:HB3	7:A:203:GOL:H31	1.78	0.66
2:B:22:CYS:SG	2:B:157:MET:HG2	2.37	0.64
2:B:72:ASN:ND2	2:B:154:ARG:HD3	2.13	0.64
2:B:170:LEU:HD12	2:B:170:LEU:C	2.18	0.63
2:B:72:ASN:HD22	2:B:154:ARG:HD3	1.61	0.63
2:B:86:GLU:HB2	2:B:109:LYS:HG2	1.82	0.62
2:B:86:GLU:HG2	2:B:87:VAL:HG23	1.83	0.60
2:D:36:GLU:CD	2:D:36:GLU:H	2.04	0.60
1:C:96:GLN:NE2	1:C:96:GLN:H	2.00	0.60
1:C:98:GLN:O	1:C:113:LEU:HD21	2.03	0.59
2:B:134:LYS:HE3	9:D:425:HOH:O	2.04	0.57
2:D:88:VAL:O	7:D:307:GOL:H11	2.05	0.57
2:D:158:LEU:HD11	2:D:188:GLU:HB3	1.86	0.56
2:B:47:LEU:HD11	2:B:53:LEU:HB2	1.87	0.56
2:B:18:GLY:HA3	2:B:188:GLU:HG2	1.88	0.56
1:A:158:ALA:HB1	9:A:221:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:ASP:O	2:D:243:LYS:HG2	2.06	0.55
2:D:34:ILE:HD12	2:D:38:ASN:HD22	1.72	0.55
2:B:195:SER:HB2	9:B:424:HOH:O	2.05	0.55
2:B:57:HIS:CE1	2:B:195:SER:OG	2.60	0.55
2:D:143:ARG:HA	2:D:151:GLN:HA	1.90	0.54
2:B:192:GLN:HB2	3:B:301:ENS:O33	2.07	0.54
2:B:57:HIS:CE1	2:B:195:SER:HG	2.26	0.54
3:B:301:ENS:N31	3:B:301:ENS:C4	2.69	0.53
2:D:33:LEU:HD22	2:D:66:VAL:HG22	1.89	0.53
2:B:236:LYS:HG2	2:B:240:ARG:HH12	1.74	0.53
2:D:178:GLN:HG2	9:D:395:HOH:O	2.09	0.52
2:D:116:MET:O	2:D:117:ASN:HB2	2.09	0.52
2:B:116:MET:O	2:B:117:ASN:HB2	2.09	0.52
1:A:127:LYS:HE3	1:A:135:ASP:OD1	2.09	0.52
2:D:124:PRO:HB2	2:D:128:ALA:HB2	1.91	0.52
1:A:119:LYS:HG2	1:A:120:ASN:ND2	2.26	0.51
2:B:115:ARG:CZ	2:B:118:VAL:HG21	2.40	0.51
1:C:96:GLN:HG2	1:C:120:ASN:O	2.11	0.50
1:C:126:ARG:HB3	9:C:207:HOH:O	2.11	0.50
1:A:119:LYS:C	1:A:120:ASN:HD22	2.14	0.50
2:B:124:PRO:HB2	2:B:128:ALA:HB2	1.93	0.49
2:D:144:THR:CG2	2:D:152:SER:HB2	2.41	0.49
2:B:36:GLU:H	2:B:36:GLU:CD	2.15	0.49
2:B:28:PRO:HB2	2:B:119:ALA:HB3	1.95	0.48
2:D:24:ASP:HB3	2:D:116:MET:CE	2.44	0.48
1:C:96:GLN:H	1:C:96:GLN:HE21	1.60	0.48
1:A:174:LYS:HG3	7:A:203:GOL:H11	1.96	0.48
2:B:28:PRO:HD2	2:B:29:TRP:CE3	2.49	0.47
6:B:304:MES:H51	9:B:412:HOH:O	2.15	0.47
1:A:120:ASN:HD22	1:A:120:ASN:N	2.12	0.47
2:B:170:LEU:HD12	2:B:171:SER:N	2.30	0.47
2:B:236:LYS:HG2	2:B:240:ARG:NH1	2.29	0.47
1:A:155:TYR:CZ	1:A:171:PRO:HB2	2.50	0.47
2:B:124:PRO:HG3	2:B:208:PHE:HB3	1.96	0.47
2:B:183:ALA:HB3	2:B:228:TYR:CE1	2.50	0.46
2:B:16:ILE:O	2:B:144:THR:HA	2.15	0.46
2:D:243:LYS:HA	2:D:243:LYS:HD3	1.67	0.46
2:B:98:THR:O	2:B:99:TYR:HB2	2.15	0.46
1:C:115:GLY:HA2	1:C:125:THR:OG1	2.16	0.46
2:B:124:PRO:HD2	2:B:235:LEU:HD21	1.98	0.46
1:A:139:PHE:CD2	2:B:124(A):GLU:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TYR:CZ	2:B:115:ARG:HA	2.51	0.45
1:A:143:GLU:O	1:A:146:SER:HB3	2.16	0.45
3:B:301:ENS:H23	3:B:301:ENS:C1	2.47	0.45
1:C:113:LEU:H	1:C:113:LEU:CD2	2.29	0.45
2:D:57:HIS:CE1	2:D:195:SER:OG	2.69	0.45
2:B:215:TRP:CE2	2:B:227:ILE:HG21	2.52	0.45
1:A:134:GLY:O	1:A:135:ASP:HB2	2.17	0.44
1:C:126:ARG:NH2	1:C:146:SER:OG	2.50	0.44
1:C:143:GLU:O	1:C:146:SER:HB3	2.17	0.44
6:D:304:MES:H81	9:D:418:HOH:O	2.16	0.44
2:D:185(B):THR:HA	2:D:223:LYS:HD2	2.00	0.44
1:A:119:LYS:HE2	2:D:174:PHE:CE1	2.53	0.43
2:B:78:GLY:C	2:B:80:GLU:H	2.21	0.43
1:C:134:GLY:O	1:C:135:ASP:HB2	2.19	0.43
2:D:97:GLU:H	2:D:97:GLU:CD	2.21	0.43
1:A:126:ARG:HB3	9:A:211:HOH:O	2.18	0.42
1:A:128:LEU:HB3	1:A:142:GLU:OE1	2.19	0.42
2:B:115:ARG:HG2	2:B:118:VAL:HB	2.01	0.42
1:C:175:GLN:HB3	2:D:25:GLY:O	2.19	0.42
2:D:125:ARG:NH2	9:D:432:HOH:O	2.53	0.42
1:C:113:LEU:N	1:C:113:LEU:HD22	2.34	0.42
2:B:147:GLU:HB2	2:B:220:CYS:HB2	2.01	0.42
2:B:72:ASN:HB2	2:B:154:ARG:HH21	1.85	0.42
2:B:96:LYS:HG3	9:B:393:HOH:O	2.20	0.42
2:B:245:ARG:HB3	9:B:386:HOH:O	2.20	0.42
1:A:153:ARG:HG3	1:A:153:ARG:O	2.19	0.42
2:D:57:HIS:CE1	2:D:195:SER:HG	2.36	0.42
1:C:124:PHE:N	1:C:124:PHE:CD2	2.87	0.42
2:B:170:LEU:C	2:B:170:LEU:CD1	2.88	0.41
1:C:124:PHE:N	1:C:124:PHE:HD2	2.18	0.41
2:B:83:HIS:HE1	2:B:111:PRO:O	2.03	0.41
2:B:17:VAL:O	2:B:188:GLU:HA	2.20	0.41
1:A:160:ASN:C	1:A:160:ASN:OD1	2.58	0.41
1:A:143:GLU:O	1:A:144:GLN:HB2	2.19	0.41
1:A:175:GLN:HB3	2:B:25:GLY:O	2.21	0.41
6:D:304:MES:H31	9:D:418:HOH:O	2.19	0.41
7:A:203:GOL:H2	9:A:209:HOH:O	2.20	0.41
2:D:17:VAL:HG22	2:D:144:THR:O	2.20	0.41
2:B:143:ARG:HA	2:B:151:GLN:HA	2.03	0.41
2:B:165:ARG:O	2:B:168:CYS:HB3	2.21	0.41
1:C:90:CYS:SG	1:C:90:CYS:O	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:ASN:HD22	2:D:166:ASN:HA	1.64	0.41
2:B:168:CYS:HB2	2:B:182:CYS:HB2	1.97	0.40
2:D:247:LEU:HA	2:D:248:PRO:HD3	1.86	0.40
2:B:236:LYS:HD3	6:B:304:MES:O3S	2.22	0.40
1:C:127:LYS:HD3	1:C:131:LEU:O	2.22	0.40
2:D:53:LEU:HD21	2:D:212:ILE:HD11	2.02	0.40
2:B:247:LEU:HA	2:B:248:PRO:HD3	1.85	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	79/94 (84%)	72 (91%)	6 (8%)	1 (1%)	15	15
1	C	78/94 (83%)	75 (96%)	3 (4%)	0	100	100
2	B	236/238 (99%)	224 (95%)	11 (5%)	1 (0%)	39	48
2	D	236/238 (99%)	226 (96%)	10 (4%)	0	100	100
All	All	629/664 (95%)	597 (95%)	30 (5%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	PRO
2	B	76	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	71/80 (89%)	69 (97%)	2 (3%)	51	68
1	C	68/80 (85%)	66 (97%)	2 (3%)	50	66
2	B	201/202 (100%)	192 (96%)	9 (4%)	34	46
2	D	197/202 (98%)	193 (98%)	4 (2%)	63	79
All	All	537/564 (95%)	520 (97%)	17 (3%)	46	62

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	126	ARG
2	B	20	GLN
2	B	29	TRP
2	B	37	GLU
2	B	88	VAL
2	B	133	GLN
2	B	151	GLN
2	B	158	LEU
2	B	170	LEU
2	B	239	ASP
1	C	96	GLN
1	C	126	ARG
2	D	29	TRP
2	D	88	VAL
2	D	158	LEU
2	D	239	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	144	GLN
2	B	151	GLN
1	C	96	GLN
1	C	141	HIS
1	C	145	ASN
2	D	38	ASN
2	D	133	GLN

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Mol	Chain	Res	Type
2	D	151	GLN
2	D	166	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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$
7	GOL	A	201	-	5,5,5	0.33	0	5,5,5	0.35	0
7	GOL	A	202	-	5,5,5	0.30	0	5,5,5	0.20	0
7	GOL	A	203	-	5,5,5	0.34	0	5,5,5	0.44	0
3	ENS	B	301	-	34,39,39	4.00	11 (32%)	34,54,54	1.49	7 (20%)
6	MES	B	304	-	11,12,12	0.60	0	14,16,16	2.56	5 (35%)
7	GOL	B	305	-	5,5,5	0.31	0	5,5,5	0.24	0
8	ACT	B	306	-	1,3,3	1.20	0	0,3,3	0.00	-
3	ENS	D	301	-	34,39,39	3.96	8 (23%)	34,54,54	1.44	6 (17%)
6	MES	D	304	-	11,12,12	0.57	0	14,16,16	2.42	6 (42%)
7	GOL	D	305	-	5,5,5	0.27	0	5,5,5	0.16	0
7	GOL	D	306	-	5,5,5	0.29	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	D	307	-	5,5,5	0.34	0	5,5,5	0.12	0
8	ACT	D	308	-	1,3,3	0.99	0	0,3,3	0.00	-

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
7	GOL	A	201	-	-	0/4/4/4	0/0/0/0
7	GOL	A	202	-	-	0/4/4/4	0/0/0/0
7	GOL	A	203	-	-	0/4/4/4	0/0/0/0
3	ENS	B	301	-	-	0/26/50/50	0/4/4/4
6	MES	B	304	-	-	0/6/14/14	0/1/1/1
7	GOL	B	305	-	-	0/4/4/4	0/0/0/0
8	ACT	B	306	-	-	0/0/0/0	0/0/0/0
3	ENS	D	301	-	-	0/26/50/50	0/4/4/4
6	MES	D	304	-	-	0/6/14/14	0/1/1/1
7	GOL	D	305	-	-	0/4/4/4	0/0/0/0
7	GOL	D	306	-	-	0/4/4/4	0/0/0/0
7	GOL	D	307	-	-	0/4/4/4	0/0/0/0
8	ACT	D	308	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	ENS	C1-C11	-10.25	1.24	1.43
3	B	301	ENS	C1-C11	-10.20	1.24	1.43
3	D	301	ENS	C23-C10	-9.19	1.39	1.53
3	B	301	ENS	C23-C10	-9.18	1.39	1.53
3	D	301	ENS	C11-C13	-4.35	1.36	1.47
3	B	301	ENS	C11-C13	-4.23	1.36	1.47
3	B	301	ENS	O35-C13	-2.59	1.27	1.33
3	D	301	ENS	O35-C13	-2.52	1.27	1.33
3	B	301	ENS	C12-N30	-2.11	1.30	1.35
3	B	301	ENS	C14-N29	-2.09	1.30	1.35
3	B	301	ENS	C4-C9	2.18	1.43	1.38
3	B	301	ENS	O34-C14	5.58	1.35	1.23
3	D	301	ENS	O34-C14	5.80	1.36	1.23
3	D	301	ENS	O33-C13	7.11	1.36	1.21
3	B	301	ENS	O33-C13	7.45	1.37	1.21
3	D	301	ENS	O32-C10	7.70	1.36	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	ENS	O32-C10	7.91	1.36	1.22
3	D	301	ENS	C1-N26	12.05	1.35	1.14
3	B	301	ENS	C1-N26	12.24	1.35	1.14

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	304	MES	C2-C3-N4	-2.79	105.89	110.12
6	D	304	MES	C6-C5-N4	-2.76	105.94	110.12
3	D	301	ENS	O33-C13-C11	-2.70	118.93	125.04
3	B	301	ENS	O33-C13-C11	-2.61	119.12	125.04
3	B	301	ENS	C9-N30-C12	-2.36	120.92	126.11
3	B	301	ENS	C2-C3-C7	-2.33	117.59	120.88
3	D	301	ENS	C2-C3-C7	-2.07	117.96	120.88
6	D	304	MES	O2S-S-C8	2.09	108.69	106.91
3	B	301	ENS	C23-N31-C12	2.26	128.61	121.89
3	D	301	ENS	C8-C9-N30	2.40	120.89	115.50
6	B	304	MES	C7-N4-C5	2.53	117.76	111.27
3	D	301	ENS	C3-C7-C8	2.55	122.30	117.03
3	B	301	ENS	C3-C7-C8	2.69	122.59	117.03
6	D	304	MES	C7-N4-C5	2.83	118.53	111.27
3	D	301	ENS	C25-C14-N29	2.98	121.39	117.04
6	D	304	MES	O1S-S-C8	3.35	109.76	106.91
3	B	301	ENS	C25-C14-N29	3.52	122.19	117.04
3	B	301	ENS	O35-C13-C11	3.53	118.71	111.44
3	D	301	ENS	O35-C13-C11	3.81	119.29	111.44
6	D	304	MES	C7-N4-C3	3.90	121.28	111.27
6	B	304	MES	C7-N4-C3	4.05	121.65	111.27
6	B	304	MES	O2S-S-C8	4.14	110.44	106.91
6	D	304	MES	C5-N4-C3	5.22	120.20	108.90
6	B	304	MES	C5-N4-C3	5.40	120.58	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	203	GOL	3	0
3	B	301	ENS	4	0
6	B	304	MES	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	304	MES	2	0
7	D	307	GOL	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	84/94 (89%)	1.09	20 (23%) 1 1	21, 30, 52, 57	0
1	C	84/94 (89%)	1.42	24 (28%) 1 1	20, 32, 58, 63	0
2	B	238/238 (100%)	0.67	18 (7%) 17 24	20, 24, 35, 46	0
2	D	238/238 (100%)	0.86	28 (11%) 6 10	19, 24, 37, 43	0
All	All	644/664 (96%)	0.89	90 (13%) 4 6	19, 25, 44, 63	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	CYS	8.1
2	D	145	HIS	6.0
2	D	148	LYS	5.9
1	A	101	CYS	5.6
2	D	150	ARG	4.8
1	C	144	GLN	4.7
1	C	98	GLN	4.7
1	C	108	TYR	4.6
2	D	149	GLY	4.5
1	A	107	GLU	4.4
1	A	144	GLN	4.3
2	D	76	GLU	4.3
1	C	94	PRO	4.2
1	C	114	GLU	4.1
1	C	103	ASP	4.0
2	D	77	GLU	3.8
1	C	146	SER	3.7
1	C	95	CYS	3.7
1	C	115	GLY	3.5
1	C	101	CYS	3.5
2	B	78	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	108	TYR	3.4
1	A	90	CYS	3.4
1	C	159	ASP	3.2
1	A	146	SER	3.2
2	D	144	THR	3.1
2	D	75	GLN	3.1
1	C	145	ASN	3.0
1	A	103	ASP	3.0
2	D	74	GLU	3.0
2	B	150	ARG	3.0
1	C	142	GLU	3.0
2	D	152	SER	3.0
2	D	151	GLN	2.9
1	A	94	PRO	2.9
2	D	39	GLU	2.8
2	B	151	GLN	2.8
2	B	145	HIS	2.8
2	B	75	GLN	2.8
1	A	141	HIS	2.8
2	D	37	GLU	2.8
2	B	77	GLU	2.8
2	B	74	GLU	2.7
2	B	24	ASP	2.7
1	A	114	GLU	2.7
1	C	111	THR	2.7
2	D	243	LYS	2.7
1	C	139	PHE	2.7
2	D	166	ASN	2.6
2	B	37	GLU	2.6
2	B	243	LYS	2.6
1	C	109	THR	2.6
2	D	154	ARG	2.5
1	A	93	SER	2.5
1	C	126	ARG	2.5
1	C	91	GLU	2.5
2	D	68	VAL	2.5
2	B	148	LYS	2.5
1	A	153	ARG	2.4
2	B	76	GLU	2.4
2	D	183	ALA	2.4
1	A	98	GLN	2.4
2	D	66	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	139	PHE	2.3
1	A	145	ASN	2.3
2	D	73	THR	2.3
1	C	99	GLY	2.3
1	C	143	GLU	2.3
1	C	97	ASN	2.3
2	B	205	ASP	2.3
1	A	159	ASP	2.2
2	D	231	VAL	2.2
2	B	39	GLU	2.2
2	D	24	ASP	2.2
1	A	111	THR	2.2
2	D	185(B)	THR	2.2
1	A	124	PHE	2.2
2	B	183	ALA	2.2
2	D	78	GLY	2.2
2	B	244	THR	2.1
1	C	112	CYS	2.1
2	D	36	GLU	2.1
1	A	143	GLU	2.1
1	C	160	ASN	2.0
2	D	223(A)	GLY	2.0
2	B	36	GLU	2.0
1	A	115	GLY	2.0
2	D	63	ARG	2.0
2	B	32	LEU	2.0
2	D	106	LEU	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
7	GOL	D	307	6/6	0.91	0.33	7.06	23,23,24,24	0
7	GOL	A	203	6/6	0.93	0.31	4.81	23,23,24,25	0
7	GOL	D	306	6/6	0.92	0.22	3.13	20,20,20,20	0
6	MES	D	304	12/12	0.92	0.18	0.35	20,21,23,24	0
4	CA	B	302	1/1	0.62	0.29	0.19	44,44,44,44	0
3	ENS	D	301	36/36	0.86	0.18	0.09	24,28,31,33	0
5	NA	B	303	1/1	0.63	0.19	0.02	29,29,29,29	0
5	NA	D	303	1/1	0.69	0.18	-0.11	31,31,31,31	0
4	CA	D	302	1/1	0.64	0.27	-0.36	45,45,45,45	0
7	GOL	A	201	6/6	0.96	0.13	-0.43	20,21,21,22	0
6	MES	B	304	12/12	0.94	0.16	-0.58	21,22,23,24	0
3	ENS	B	301	36/36	0.91	0.14	-0.66	23,27,30,31	0
7	GOL	B	305	6/6	0.88	0.14	-0.88	22,23,24,24	0
7	GOL	D	305	6/6	0.87	0.15	-1.65	22,23,23,24	0
8	ACT	D	308	4/4	0.93	0.15	-	31,31,31,31	0
8	ACT	B	306	4/4	0.91	0.12	-	27,27,27,28	0
7	GOL	A	202	6/6	0.84	0.36	-	28,29,29,30	0

6.5 Other polymers

There are no such residues in this entry.