



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:24 PM GMT

PDB ID : 3TSR
Title : X-ray structure of mouse ribonuclease inhibitor complexed with mouse ribonuclease 1
Authors : Chang, A.; Lomax, J.E.; Bingman, C.A.; Raines, R.T.; Phillips Jr., G.N.
Deposited on : 2011-09-13
Resolution : 2.20 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

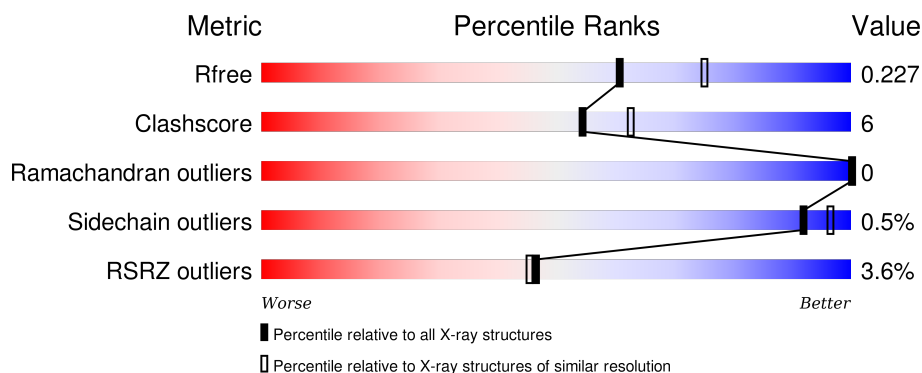
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	125	<div> <div></div> <div>85% 14% .</div> </div>
1	B	125	<div> <div></div> <div>90% 9% .</div> </div>
1	C	125	<div> <div>22%</div> <div>79% 14% 6%</div> </div>
1	D	125	<div> <div>39%</div> <div>76% 14% 10%</div> </div>
2	E	457	<div> <div></div> <div>84% 16%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	457	 85%15%
2	G	457	 86%14%
2	H	457	 %82%17%

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
3	EDO	E	458	-	-	-	X
3	EDO	G	457	-	-	-	X
4	PEG	E	457	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18531 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 Ribonuclease pancreatic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			976	595	179	190	12			
1	B	123	Total	C	N	O	S	0	0	0
			965	589	175	189	12			
1	C	117	Total	C	N	O	S	0	0	0
			925	567	168	178	12			
1	D	113	Total	C	N	O	S	0	0	0
			896	550	164	170	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P00683
B	1	MET	-	EXPRESSION TAG	UNP P00683
C	1	MET	-	EXPRESSION TAG	UNP P00683
D	1	MET	-	EXPRESSION TAG	UNP P00683

- Molecule 2 is a protein called Ribonuclease inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	457	Total	C	N	O	S	0	0	0
			3472	2152	594	690	36			
2	F	457	Total	C	N	O	S	0	0	0
			3472	2152	594	690	36			
2	G	457	Total	C	N	O	S	0	0	0
			3472	2152	594	690	36			
2	H	457	Total	C	N	O	S	0	0	0
			3472	2152	594	690	36			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	EXPRESSION TAG	UNP Q91VI7
F	0	MET	-	EXPRESSION TAG	UNP Q91VI7
G	0	MET	-	EXPRESSION TAG	UNP Q91VI7
H	0	MET	-	EXPRESSION TAG	UNP Q91VI7

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



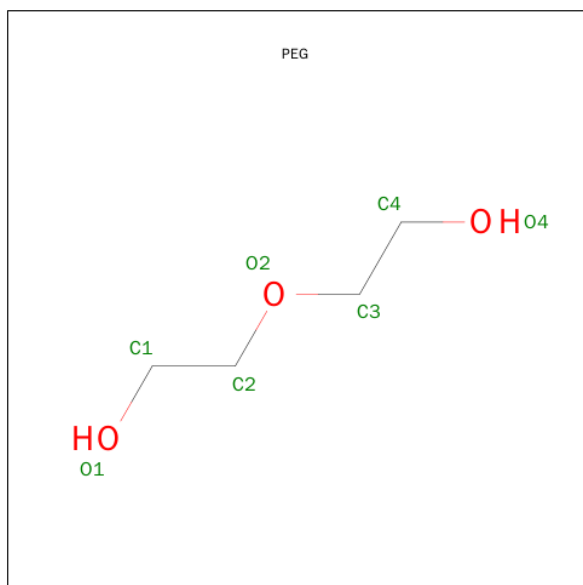
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		
5	B	53	Total	O	0	0
			53	53		
5	C	19	Total	O	0	0
			19	19		
5	D	15	Total	O	0	0
			15	15		
5	E	185	Total	O	0	0
			185	185		

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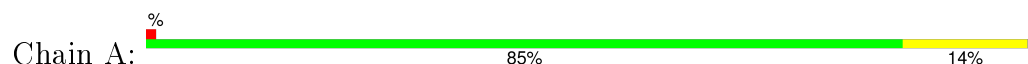
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	178	Total 178	O 178	0	0
5	G	167	Total 167	O 167	0	0
5	H	148	Total 148	O 148	0	0

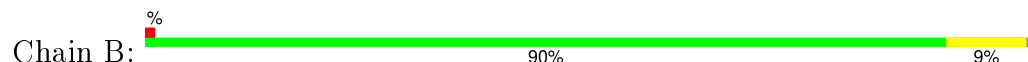
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

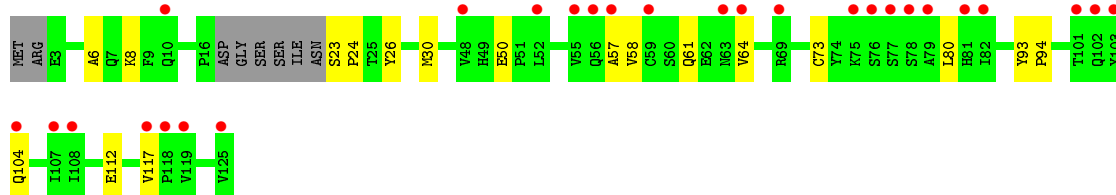
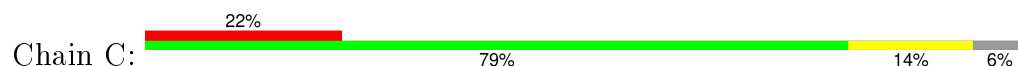
- Molecule 1: Ribonuclease pancreatic



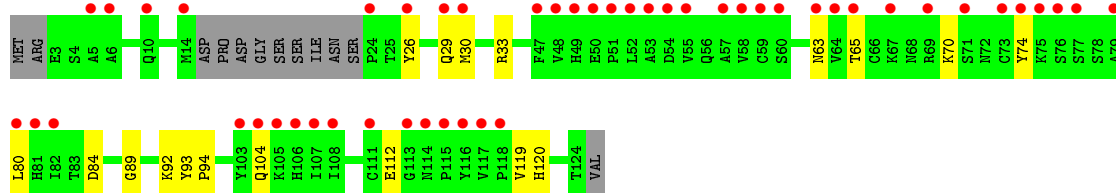
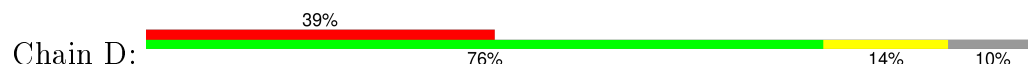
- Molecule 1: Ribonuclease pancreatic



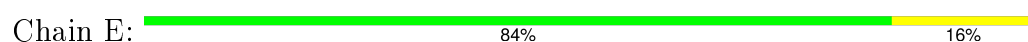
- Molecule 1: Ribonuclease pancreatic

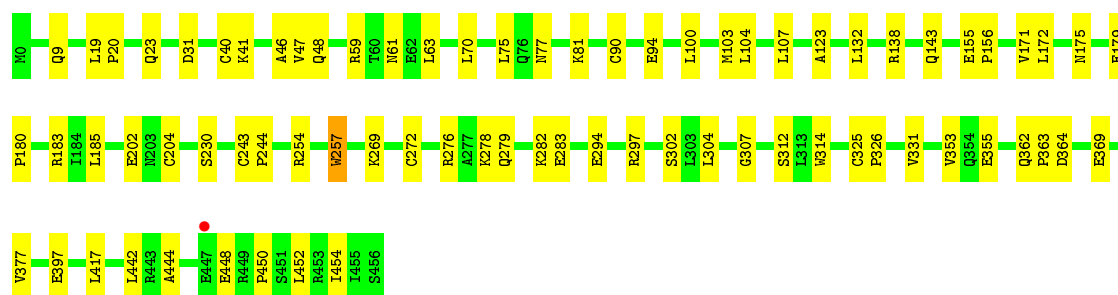


- Molecule 1: Ribonuclease pancreatic



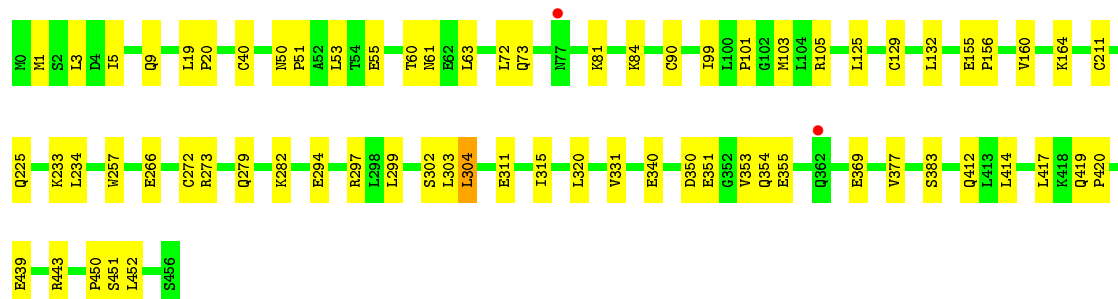
- Molecule 2: Ribonuclease inhibitor





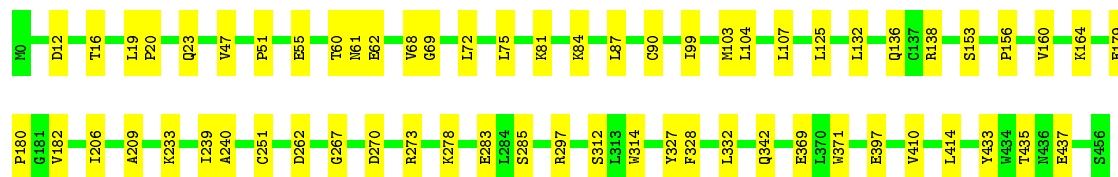
- Molecule 2: Ribonuclease inhibitor

Chain F: 85% 15%



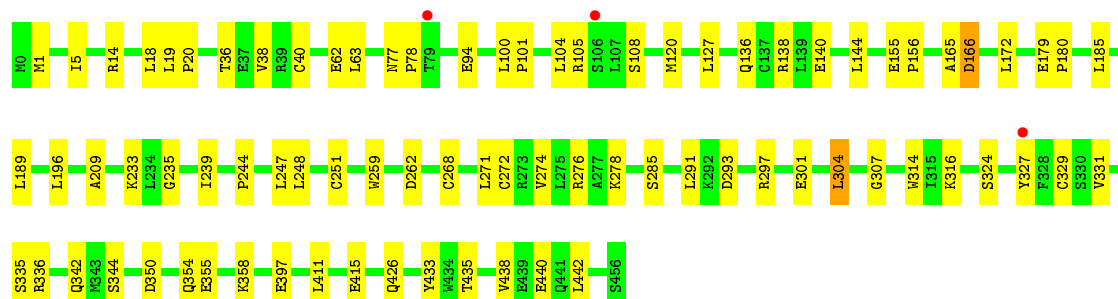
- Molecule 2: Ribonuclease inhibitor

Chain G: 86% 14%



- Molecule 2: Ribonuclease inhibitor

Chain H: 82% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.40 Å 125.34 Å 123.06 Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	34.38 – 2.20 38.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (34.38-2.20) 92.0 (38.87-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.182 , 0.233 0.178 , 0.227	Depositor DCC
R_{free} test set	2002 reflections (2.00%)	DCC
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 108474 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18531	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.42 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.8459e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, 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	0.23	0/997	0.41	0/1346
1	B	0.22	0/986	0.42	0/1332
1	C	0.28	0/945	0.40	0/1275
1	D	0.21	0/915	0.38	0/1233
2	E	0.23	0/3509	0.40	0/4750
2	F	0.22	0/3509	0.39	0/4750
2	G	0.25	0/3509	0.39	0/4750
2	H	0.22	0/3509	0.39	0/4750
All	All	0.23	0/17879	0.39	0/24186

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	976	0	926	10	0
1	B	965	0	913	6	0
1	C	925	0	878	12	0
1	D	896	0	854	12	0
2	E	3472	0	3538	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3472	0	3538	48	0
2	G	3472	0	3538	45	0
2	H	3472	0	3538	57	0
3	A	4	0	6	0	0
3	E	8	0	12	2	0
3	F	12	0	18	2	0
3	G	16	0	24	1	0
3	H	12	0	18	0	0
4	E	7	0	10	3	0
5	A	57	0	0	0	0
5	B	53	0	0	0	0
5	C	19	0	0	0	0
5	D	15	0	0	0	0
5	E	185	0	0	0	0
5	F	178	0	0	2	0
5	G	167	0	0	3	0
5	H	148	0	0	2	0
All	All	18531	0	17811	228	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 6.

All (228) 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:E:450:PRO:HG2	2:G:138:ARG:HD3	1.63	0.79
2:H:108:SER:HB2	2:H:138:ARG:HH12	1.50	0.74
2:F:101:PRO:O	2:F:105:ARG:HG3	1.89	0.72
2:E:94:GLU:HG3	2:E:123:ALA:HB3	1.75	0.68
2:E:23:GLN:HG2	2:E:46:ALA:HA	1.76	0.67
2:E:103:MET:SD	2:E:107:LEU:HD12	2.35	0.66
2:F:294:GLU:HG3	2:F:297:ARG:HH21	1.60	0.66
2:G:62:GLU:HG2	5:G:478:HOH:O	1.94	0.65
1:B:90:ASN:HA	2:F:257:TRP:HE1	1.60	0.65
2:H:101:PRO:O	2:H:105:ARG:HG3	1.94	0.65
1:D:26:TYR:CZ	1:D:30:MET:HG3	2.31	0.65
1:C:93:TYR:CG	1:C:94:PRO:HA	2.33	0.63
2:H:285:SER:HA	2:H:314:TRP:HB2	1.80	0.63
2:F:51:PRO:O	2:F:81:LYS:HD3	1.99	0.62
2:H:355:GLU:O	2:H:358:LYS:HG2	1.99	0.62
2:F:311:GLU:HG2	5:F:855:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:179:GLU:HB3	2:G:180:PRO:HD3	1.81	0.61
2:F:294:GLU:HG3	2:F:297:ARG:NH2	2.15	0.61
2:F:279:GLN:NE2	2:H:336:ARG:HG3	2.14	0.61
2:F:155:GLU:HB3	2:F:156:PRO:HD3	1.82	0.61
2:E:417:LEU:HD13	2:E:452:LEU:HD21	1.82	0.61
2:E:172:LEU:HD12	2:E:185:LEU:HD21	1.83	0.60
2:F:450:PRO:HG2	2:H:166:ASP:OD2	2.02	0.60
2:H:304:LEU:HD11	2:H:331:VAL:HA	1.84	0.59
2:F:5:ILE:HG23	2:H:1:MET:HG2	1.83	0.59
2:F:450:PRO:HG3	2:H:138:ARG:HE	1.66	0.59
2:E:326:PRO:HG3	2:E:355:GLU:OE1	2.02	0.59
2:F:304:LEU:HD11	2:F:331:VAL:HA	1.84	0.59
2:H:297:ARG:HB2	2:H:327:TYR:CE2	2.37	0.59
2:E:183:ARG:NH2	2:H:38:VAL:HG13	2.18	0.59
1:C:93:TYR:CD1	1:C:94:PRO:HA	2.38	0.58
2:H:62:GLU:HG2	5:H:602:HOH:O	2.04	0.58
2:E:362:GLN:HG2	2:E:364:ASP:H	1.69	0.58
2:E:41:LYS:HG3	2:E:70:LEU:HD13	1.86	0.57
2:G:270:ASP:HA	2:G:273:ARG:NH1	2.20	0.57
2:F:72:LEU:HB3	2:F:103:MET:HG3	1.87	0.57
2:E:254:ARG:HD2	2:E:282:LYS:HB2	1.87	0.57
2:G:314:TRP:CE3	2:G:342:GLN:HG2	2.39	0.57
2:E:444:ALA:O	2:E:448:GLU:HG3	2.03	0.56
2:F:417:LEU:HD13	2:F:452:LEU:HD21	1.86	0.56
2:H:411:LEU:O	2:H:415:GLU:HG2	2.06	0.56
2:H:247:LEU:HG	2:H:274:VAL:HG22	1.87	0.55
2:E:294:GLU:HG3	2:E:297:ARG:HH21	1.70	0.55
1:D:93:TYR:CG	1:D:94:PRO:HA	2.42	0.55
2:E:47:VAL:HG11	2:E:75:LEU:HD23	1.89	0.55
2:F:282:LYS:HD2	2:F:311:GLU:HG3	1.89	0.55
1:A:90:ASN:HA	2:E:257:TRP:HE1	1.72	0.55
2:G:239:ILE:HD12	2:G:240:ALA:N	2.21	0.55
2:E:294:GLU:HG3	2:E:297:ARG:NH2	2.22	0.55
1:D:89:GLY:HA3	2:H:259:TRP:CD1	2.43	0.54
2:E:369:GLU:HG2	2:E:397:GLU:HB3	1.89	0.54
2:G:239:ILE:HD11	2:G:267:GLY:HA2	1.90	0.54
2:H:40:CYS:SG	2:H:63:LEU:HD22	2.48	0.54
2:H:314:TRP:CE3	2:H:342:GLN:HG2	2.44	0.53
2:E:442:LEU:HD11	2:E:454:ILE:HG21	1.90	0.53
2:E:19:LEU:O	2:E:23:GLN:HG3	2.09	0.53
2:F:3:LEU:HD11	2:F:5:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:351:GLU:O	2:F:355:GLU:HG3	2.08	0.53
2:H:36:THR:HG22	2:H:62:GLU:HG3	1.89	0.52
1:B:26:TYR:CZ	1:B:30:MET:HG3	2.45	0.52
2:E:100:LEU:O	2:E:104:LEU:HD13	2.10	0.52
2:E:19:LEU:N	2:E:20:PRO:HD2	2.25	0.52
1:D:65:THR:HG23	1:D:70:LYS:O	2.09	0.52
1:A:100:THR:HG22	1:A:102:GLN:NE2	2.25	0.52
2:G:179:GLU:OE2	2:G:209:ALA:HB3	2.10	0.51
2:H:297:ARG:O	2:H:301:GLU:HG3	2.10	0.51
1:B:110:ALA:HB3	1:B:120:HIS:HB3	1.93	0.51
1:C:26:TYR:CZ	1:C:30:MET:HG3	2.46	0.51
2:F:55:GLU:HG3	2:F:84:LYS:HB2	1.93	0.51
2:G:104:LEU:HD23	2:G:132:LEU:HD23	1.93	0.50
2:F:40:CYS:SG	2:F:63:LEU:HD22	2.52	0.50
2:E:442:LEU:HD11	2:E:454:ILE:HD13	1.92	0.50
1:C:6:ALA:HB2	1:C:117:VAL:HG21	1.93	0.50
2:E:269:LYS:HG2	4:E:457:PEG:H41	1.92	0.50
1:D:80:LEU:O	1:D:104:GLN:HA	2.11	0.50
1:D:26:TYR:CE2	1:D:30:MET:HG3	2.45	0.50
2:H:172:LEU:HD12	2:H:185:LEU:HD21	1.93	0.50
2:H:272:CYS:O	2:H:276:ARG:HG2	2.11	0.50
1:B:21:ILE:HG22	1:B:102:GLN:HG3	1.94	0.50
2:F:299:LEU:O	2:F:303:LEU:HG	2.11	0.50
2:G:251:CYS:O	2:G:278:LYS:HE3	2.12	0.49
1:A:26:TYR:CZ	1:A:30:MET:HG3	2.47	0.49
2:E:81:LYS:O	2:E:81:LYS:HG2	2.12	0.49
1:C:64:VAL:HG23	1:C:73:CYS:HB3	1.94	0.49
1:A:14:MET:SD	1:A:55:VAL:HG21	2.53	0.49
2:H:19:LEU:HB2	2:H:20:PRO:HD3	1.95	0.49
2:G:103:MET:O	2:G:107:LEU:HG	2.12	0.49
2:G:369:GLU:HG2	2:G:397:GLU:HB3	1.95	0.48
2:F:211:CYS:SG	2:F:234:LEU:HD22	2.53	0.48
1:A:112:GLU:HB2	1:A:119:VAL:HG21	1.95	0.48
1:C:50:GLU:HG3	1:C:80:LEU:HB3	1.95	0.48
2:H:179:GLU:HB3	2:H:180:PRO:HD3	1.96	0.48
2:G:72:LEU:HD12	2:G:99:ILE:HD11	1.95	0.48
2:F:99:ILE:HD11	2:F:103:MET:CE	2.44	0.48
2:F:353:VAL:HG11	2:F:377:VAL:HG22	1.96	0.48
2:G:55:GLU:HG3	2:G:84:LYS:HB2	1.96	0.47
1:A:93:TYR:CG	1:A:94:PRO:HA	2.49	0.47
1:C:58:VAL:HA	1:C:61:GLN:CD	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:GLN:O	1:D:33:ARG:HG3	2.14	0.47
2:F:450:PRO:HG3	2:H:138:ARG:NE	2.28	0.47
2:G:12:ASP:O	2:G:16:THR:HG23	2.14	0.47
2:E:450:PRO:CG	2:G:138:ARG:HD3	2.38	0.47
2:H:251:CYS:O	2:H:278:LYS:HE3	2.14	0.47
1:C:57:ALA:O	1:C:61:GLN:HG3	2.14	0.47
2:E:31:ASP:OD1	2:E:59:ARG:HG2	2.15	0.47
1:A:29:GLN:O	1:A:33:ARG:HG3	2.15	0.47
2:E:61:ASN:O	2:E:90:CYS:HA	2.15	0.47
2:H:94:GLU:HB3	2:H:120:MET:O	2.15	0.47
2:G:328:PHE:O	2:G:332:LEU:HG	2.15	0.46
2:F:439:GLU:O	2:F:443:ARG:HG2	2.14	0.46
1:D:92:LYS:HB3	2:H:314:TRP:CZ2	2.51	0.46
2:H:314:TRP:HE3	2:H:342:GLN:HG2	1.80	0.46
2:F:272:CYS:HB3	2:F:302:SER:OG	2.16	0.46
2:H:435:THR:OG1	2:H:438:VAL:HG23	2.16	0.46
4:E:457:PEG:H12	2:H:127:LEU:HD11	1.97	0.46
2:H:350:ASP:O	2:H:354:GLN:HG3	2.16	0.46
2:E:94:GLU:HG3	2:E:123:ALA:CB	2.44	0.46
2:E:48:GLN:HG2	2:E:77:ASN:OD1	2.16	0.46
1:B:93:TYR:CG	1:B:94:PRO:HA	2.51	0.46
2:E:179:GLU:N	2:E:180:PRO:HD2	2.31	0.46
2:F:19:LEU:N	2:F:20:PRO:HD2	2.30	0.46
2:F:451:SER:HA	2:H:140:GLU:OE2	2.15	0.46
2:G:283:GLU:HG2	2:G:312:SER:HB3	1.97	0.45
2:H:235:GLY:O	2:H:239:ILE:HD13	2.16	0.45
2:G:160:VAL:O	2:G:164:LYS:HG2	2.16	0.45
1:D:112:GLU:HB2	1:D:119:VAL:HG21	1.99	0.45
2:F:99:ILE:HD11	2:F:103:MET:HE2	1.98	0.45
2:F:61:ASN:O	2:F:90:CYS:HA	2.15	0.45
2:G:233:LYS:HG3	3:G:457:EDO:H11	1.98	0.45
2:G:60:THR:HG22	2:G:60:THR:O	2.16	0.45
2:G:182:VAL:HG21	2:G:206:ILE:HG12	1.97	0.45
2:F:9:GLN:HG2	3:F:459:EDO:O2	2.16	0.45
2:E:353:VAL:HG21	2:E:377:VAL:HG22	1.99	0.45
2:F:350:ASP:O	2:F:354:GLN:HG3	2.16	0.45
2:E:23:GLN:HG2	2:E:46:ALA:CA	2.45	0.45
2:F:1:MET:HG2	2:H:5:ILE:HG23	1.97	0.45
2:E:175:ASN:O	2:E:204:CYS:HA	2.16	0.45
2:H:268:CYS:HB2	2:H:291:LEU:HD22	1.98	0.45
2:G:61:ASN:O	2:G:90:CYS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:51:PRO:O	2:G:81:LYS:HE2	2.17	0.44
2:E:269:LYS:HE2	4:E:457:PEG:H11	2.00	0.44
2:E:48:GLN:HA	2:E:77:ASN:OD1	2.17	0.44
2:G:68:VAL:HG13	2:G:87:LEU:HD13	1.99	0.44
1:A:110:ALA:HB3	1:A:120:HIS:HB3	1.99	0.44
2:H:276:ARG:O	2:H:307:GLY:HA3	2.18	0.44
1:C:80:LEU:O	1:C:104:GLN:HA	2.18	0.44
2:H:233:LYS:HG2	2:H:262:ASP:OD1	2.17	0.44
2:E:104:LEU:HD23	2:E:132:LEU:HD23	1.99	0.44
2:F:50:ASN:ND2	2:F:53:LEU:HB2	2.33	0.44
2:E:450:PRO:HG2	2:G:138:ARG:CD	2.40	0.43
2:E:31:ASP:CG	2:E:59:ARG:HG2	2.38	0.43
2:G:47:VAL:HG11	2:G:75:LEU:HD23	1.99	0.43
2:H:316:LYS:HG3	2:H:344:SER:HB2	2.00	0.43
2:E:304:LEU:HD21	2:E:331:VAL:HA	2.01	0.43
2:H:442:LEU:HD23	2:H:442:LEU:C	2.38	0.43
2:G:435:THR:HB	2:G:437:GLU:OE2	2.18	0.43
2:F:420:PRO:HB3	2:H:165:ALA:CB	2.48	0.43
2:H:397:GLU:HG2	2:H:426:GLN:HB3	1.99	0.43
2:H:293:ASP:OD1	2:H:324:SER:HB3	2.19	0.43
2:H:136:GLN:HA	2:H:138:ARG:HH22	1.84	0.43
2:G:285:SER:HA	2:G:314:TRP:HB2	2.01	0.43
2:G:278:LYS:HA	2:G:278:LYS:HD2	1.90	0.43
2:G:72:LEU:HB3	2:G:103:MET:HG3	2.00	0.43
1:A:68:ASN:O	1:A:69:ARG:HB2	2.18	0.43
2:H:155:GLU:N	2:H:156:PRO:HD2	2.33	0.43
2:H:108:SER:HB2	2:H:138:ARG:NH1	2.26	0.43
2:E:283:GLU:HG2	2:E:312:SER:HB2	2.01	0.43
2:H:331:VAL:O	2:H:335:SER:HB3	2.19	0.42
2:G:342:GLN:HA	2:G:371:TRP:HB2	2.01	0.42
2:G:297:ARG:HD3	2:G:327:TYR:CZ	2.54	0.42
2:E:272:CYS:HB3	2:E:302:SER:OG	2.18	0.42
2:F:340:GLU:HG2	2:F:369:GLU:HB2	2.02	0.42
2:H:189:LEU:HD22	2:H:196:LEU:HD22	2.00	0.42
2:H:440:GLU:HA	2:H:440:GLU:OE1	2.19	0.42
2:G:297:ARG:CD	2:G:327:TYR:CZ	3.02	0.42
1:C:8:LYS:HE2	5:G:532:HOH:O	2.19	0.42
1:C:112:GLU:HG3	2:G:433:TYR:OH	2.20	0.42
1:A:93:TYR:CD1	1:A:94:PRO:HA	2.54	0.42
1:C:23:SER:HA	1:C:24:PRO:HD3	1.78	0.42
2:E:47:VAL:HG11	2:E:75:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:419:GLN:HA	2:F:420:PRO:HD3	1.89	0.42
2:E:279:GLN:HG2	2:E:307:GLY:O	2.19	0.42
2:H:244:PRO:O	2:H:248:LEU:HD13	2.19	0.42
2:G:23:GLN:HG2	5:G:815:HOH:O	2.20	0.42
1:D:120:HIS:CD2	2:H:433:TYR:HB2	2.54	0.42
2:E:183:ARG:HB2	2:E:183:ARG:CZ	2.49	0.42
2:F:73:GLN:HA	2:F:103:MET:HE1	2.02	0.42
2:G:239:ILE:C	2:G:239:ILE:HD12	2.40	0.42
2:E:40:CYS:SG	2:E:63:LEU:HD22	2.60	0.42
2:H:271:LEU:HD12	2:H:271:LEU:HA	1.90	0.42
2:F:233:LYS:NZ	3:F:457:EDO:H22	2.35	0.42
2:G:125:LEU:C	2:G:125:LEU:HD13	2.40	0.41
2:F:125:LEU:C	2:F:125:LEU:HD13	2.41	0.41
2:E:143:GLN:HG2	2:E:171:VAL:HG13	2.01	0.41
1:D:63:ASN:HA	1:D:74:TYR:CD2	2.55	0.41
2:E:362:GLN:HG2	2:E:363:PRO:N	2.35	0.41
2:G:314:TRP:HA	2:G:342:GLN:HB3	2.02	0.41
2:G:47:VAL:CG1	2:G:75:LEU:HD23	2.50	0.41
2:E:278:LYS:HD3	2:E:278:LYS:HA	1.92	0.41
2:E:107:LEU:HA	2:E:107:LEU:HD23	1.81	0.41
2:G:69:GLY:HA2	2:G:99:ILE:CD1	2.50	0.41
2:G:410:VAL:O	2:G:414:LEU:HG	2.20	0.41
2:E:9:GLN:OE1	3:E:459:EDO:H22	2.20	0.41
2:F:99:ILE:HG12	2:F:103:MET:HG2	2.02	0.41
2:H:144:LEU:HB2	2:H:172:LEU:HD23	2.01	0.41
2:H:179:GLU:OE2	2:H:209:ALA:HB3	2.20	0.41
1:B:68:ASN:O	1:B:69:ARG:HB2	2.20	0.41
2:E:155:GLU:HB3	2:E:156:PRO:HD3	2.01	0.41
2:G:233:LYS:HG2	2:G:262:ASP:OD1	2.20	0.41
2:F:225:GLN:HG3	5:H:468:HOH:O	2.19	0.41
2:F:60:THR:HG22	2:F:60:THR:O	2.20	0.41
2:E:325:CYS:N	2:E:326:PRO:CD	2.84	0.41
2:F:129:CYS:HA	2:F:132:LEU:HB2	2.03	0.41
2:F:160:VAL:O	2:F:164:LYS:HG2	2.21	0.41
2:F:273:ARG:HD2	5:F:496:HOH:O	2.20	0.41
1:D:93:TYR:CD1	1:D:94:PRO:HA	2.55	0.41
2:H:100:LEU:O	2:H:104:LEU:HD13	2.21	0.41
2:G:153:SER:C	2:G:156:PRO:HD2	2.41	0.41
2:H:14:ARG:O	2:H:18:LEU:HG	2.20	0.41
2:G:19:LEU:HB2	2:G:20:PRO:HD3	2.02	0.41
2:E:9:GLN:CD	3:E:459:EDO:H22	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77:ASN:HA	2:H:78:PRO:HD3	1.91	0.41
2:F:315:ILE:HD12	2:F:320:LEU:HD21	2.03	0.40
2:E:272:CYS:O	2:E:276:ARG:HG3	2.21	0.40
2:E:202:GLU:HG2	2:E:230:SER:HB2	2.02	0.40
2:E:243:CYS:N	2:E:244:PRO:CD	2.84	0.40
2:H:329:CYS:SG	2:H:355:GLU:O	2.79	0.40
2:F:383:SER:HB3	2:F:412:GLN:OE1	2.21	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	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
1	B	121/125 (97%)	116 (96%)	5 (4%)	0	100	100
1	C	113/125 (90%)	108 (96%)	5 (4%)	0	100	100
1	D	109/125 (87%)	102 (94%)	7 (6%)	0	100	100
2	E	455/457 (100%)	444 (98%)	11 (2%)	0	100	100
2	F	455/457 (100%)	443 (97%)	12 (3%)	0	100	100
2	G	455/457 (100%)	442 (97%)	13 (3%)	0	100	100
2	H	455/457 (100%)	442 (97%)	13 (3%)	0	100	100
All	All	2285/2328 (98%)	2215 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	113/114 (99%)	112 (99%)	1 (1%)	84	92
1	B	112/114 (98%)	112 (100%)	0	100	100
1	C	107/114 (94%)	107 (100%)	0	100	100
1	D	103/114 (90%)	102 (99%)	1 (1%)	82	91
2	E	401/401 (100%)	398 (99%)	3 (1%)	88	94
2	F	401/401 (100%)	398 (99%)	3 (1%)	88	94
2	G	401/401 (100%)	400 (100%)	1 (0%)	95	98
2	H	401/401 (100%)	399 (100%)	2 (0%)	92	96
All	All	2039/2060 (99%)	2028 (100%)	11 (0%)	92	96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	TYR
1	D	84	ASP
2	E	138	ARG
2	E	257	TRP
2	E	314	TRP
2	F	266	GLU
2	F	304	LEU
2	F	414	LEU
2	G	136	GLN
2	H	166	ASP
2	H	304	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	126	-	3,3,3	0.49	0	2,2,2	0.37	0
4	PEG	E	457	-	6,6,6	0.45	0	5,5,5	0.24	0
3	EDO	E	458	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	E	459	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	F	457	-	3,3,3	0.48	0	2,2,2	0.40	0
3	EDO	F	458	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	F	459	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	G	457	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	G	458	-	3,3,3	0.48	0	2,2,2	0.39	0
3	EDO	G	459	-	3,3,3	0.47	0	2,2,2	0.38	0
3	EDO	G	460	-	3,3,3	0.47	0	2,2,2	0.41	0
3	EDO	H	457	-	3,3,3	0.50	0	2,2,2	0.35	0
3	EDO	H	458	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	H	459	-	3,3,3	0.48	0	2,2,2	0.43	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	EDO	A	126	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	E	457	-	-	0/4/4/4	0/0/0/0
3	EDO	E	458	-	-	0/1/1/1	0/0/0/0
3	EDO	E	459	-	-	0/1/1/1	0/0/0/0
3	EDO	F	457	-	-	0/1/1/1	0/0/0/0
3	EDO	F	458	-	-	0/1/1/1	0/0/0/0
3	EDO	F	459	-	-	0/1/1/1	0/0/0/0
3	EDO	G	457	-	-	0/1/1/1	0/0/0/0
3	EDO	G	458	-	-	0/1/1/1	0/0/0/0
3	EDO	G	459	-	-	0/1/1/1	0/0/0/0
3	EDO	G	460	-	-	0/1/1/1	0/0/0/0
3	EDO	H	457	-	-	0/1/1/1	0/0/0/0
3	EDO	H	458	-	-	0/1/1/1	0/0/0/0
3	EDO	H	459	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	457	PEG	3	0
3	E	459	EDO	2	0
3	F	457	EDO	1	0
3	F	459	EDO	1	0
3	G	457	EDO	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	124/125 (99%)	-0.04	1 (0%) 87 87	12, 23, 37, 70	0
1	B	123/125 (98%)	-0.12	1 (0%) 87 87	13, 22, 35, 45	0
1	C	117/125 (93%)	1.24	27 (23%) 1 1	21, 46, 71, 72	0
1	D	113/125 (90%)	1.91	49 (43%) 0 0	21, 53, 78, 91	0
2	E	457/457 (100%)	-0.19	1 (0%) 95 95	7, 18, 38, 59	0
2	F	457/457 (100%)	-0.16	2 (0%) 93 93	9, 20, 37, 50	0
2	G	457/457 (100%)	-0.17	0 100 100	9, 20, 35, 56	0
2	H	457/457 (100%)	-0.08	3 (0%) 89 88	10, 23, 41, 53	0
All	All	2305/2328 (99%)	0.03	84 (3%) 46 45	7, 22, 52, 91	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	125	VAL	9.2
1	D	55	VAL	6.4
1	D	104	GLN	5.7
1	D	64	VAL	5.6
1	D	48	VAL	5.6
1	D	79	ALA	5.5
1	D	103	TYR	5.3
1	C	52	LEU	5.0
1	C	117	VAL	4.9
1	D	58	VAL	4.9
1	D	76	SER	4.7
1	D	54	ASP	4.7
1	D	117	VAL	4.5
1	D	51	PRO	4.4
1	B	125	VAL	4.3
1	D	114	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	79	ALA	4.1
1	D	80	LEU	3.9
1	D	77	SER	3.8
1	D	82	ILE	3.8
1	C	75	LYS	3.7
1	C	64	VAL	3.7
1	D	63	ASN	3.7
1	D	74	TYR	3.7
1	D	49	HIS	3.6
1	D	53	ALA	3.5
1	C	55	VAL	3.4
1	C	57	ALA	3.4
1	C	77	SER	3.4
1	D	113	GLY	3.4
1	C	76	SER	3.3
1	C	78	SER	3.3
1	D	75	LYS	3.3
1	D	14	MET	3.3
1	D	81	HIS	3.2
1	D	60	SER	3.1
1	C	69	ARG	3.1
1	C	81	HIS	3.1
1	D	65	THR	3.1
1	C	63	ASN	3.1
1	D	69	ARG	3.0
1	D	59	CYS	3.0
1	D	108	ILE	3.0
2	F	362	GLN	2.9
1	C	119	VAL	2.9
1	D	118	PRO	2.8
1	D	107	ILE	2.8
2	H	79	THR	2.8
1	D	52	LEU	2.7
1	D	6	ALA	2.7
1	C	10	GLN	2.6
1	D	116	TYR	2.6
2	E	447	GLU	2.5
1	D	10	GLN	2.5
1	C	101	THR	2.5
1	C	102	GLN	2.4
1	D	57	ALA	2.4
1	D	50	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	115	PRO	2.3
2	H	327	TYR	2.3
1	C	103	TYR	2.3
1	D	30	MET	2.3
1	C	59	CYS	2.3
1	C	56	GLN	2.3
1	D	111	CYS	2.2
1	D	5	ALA	2.2
1	D	26	TYR	2.2
1	D	67	LYS	2.2
1	C	104	GLN	2.2
1	C	82	ILE	2.2
1	D	24	PRO	2.2
1	C	108	ILE	2.2
2	F	77	ASN	2.1
1	A	125	VAL	2.1
1	D	47	PHE	2.1
1	D	106	HIS	2.1
1	D	71	SER	2.1
1	C	48	VAL	2.1
1	D	105	LYS	2.1
1	D	73	CYS	2.1
1	C	107	ILE	2.0
2	H	106	SER	2.0
1	C	118	PRO	2.0
1	D	29	GLN	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
3	EDO	E	458	4/4	0.88	0.18	3.69	18,23,27,34	0
4	PEG	E	457	7/7	0.92	0.14	2.30	20,26,31,39	0
3	EDO	G	457	4/4	0.87	0.17	2.17	22,23,24,29	0
3	EDO	G	458	4/4	0.88	0.18	1.73	23,29,34,35	0
3	EDO	G	459	4/4	0.86	0.18	1.15	37,41,45,46	0
3	EDO	F	458	4/4	0.91	0.15	0.82	26,27,35,41	0
3	EDO	E	459	4/4	0.90	0.15	0.52	28,29,35,37	0
3	EDO	G	460	4/4	0.93	0.14	0.15	27,37,39,40	0
3	EDO	H	457	4/4	0.91	0.13	0.05	18,25,27,30	0
3	EDO	H	458	4/4	0.93	0.13	-0.13	29,30,31,40	0
3	EDO	A	126	4/4	0.95	0.09	-0.54	16,24,27,32	0
3	EDO	F	459	4/4	0.89	0.09	-1.36	24,30,34,34	0
3	EDO	F	457	4/4	0.96	0.08	-1.45	20,24,29,31	0
3	EDO	H	459	4/4	0.89	0.12	-	32,36,42,46	0

6.5 Other polymers

There are no such residues in this entry.