



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:12 PM UTC

PDB ID : 1CZI / pdb_00001czi
Title : CHYMOSIN COMPLEX WITH THE INHIBITOR CP-113972
Authors : Groves, M.R.; Dhanaraj, V.; Pitts, J.E.; Badasso, M.; Hoover, D.; Nugent, P.;
Blundell, T.L.
Deposited on : 1997-01-15
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

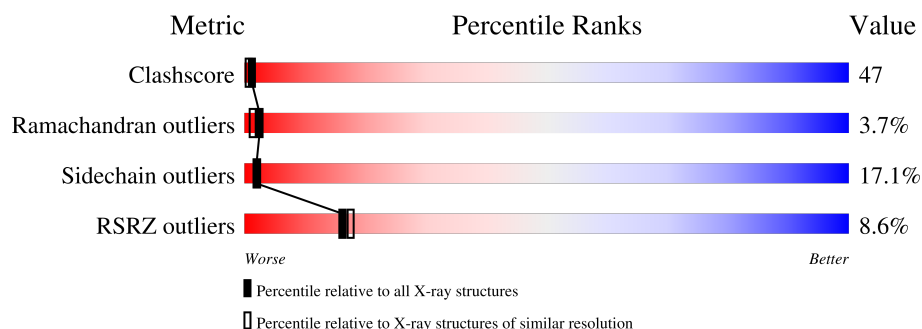
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	323	
2	P	4	

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
2	PHI	P	3	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2745 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 CHYMOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	323	Total	C	N	O	S	0	0	0
			2511	1598	401	498	14			

- Molecule 2 is a protein called CP-113972 (NORSTATINE-S-METHYL CYSTEINE-iodo-PHENYLALANINE-PROLINE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	4	Total	C	I	N	O	S	0	0
			43	31	1	4	6	1		

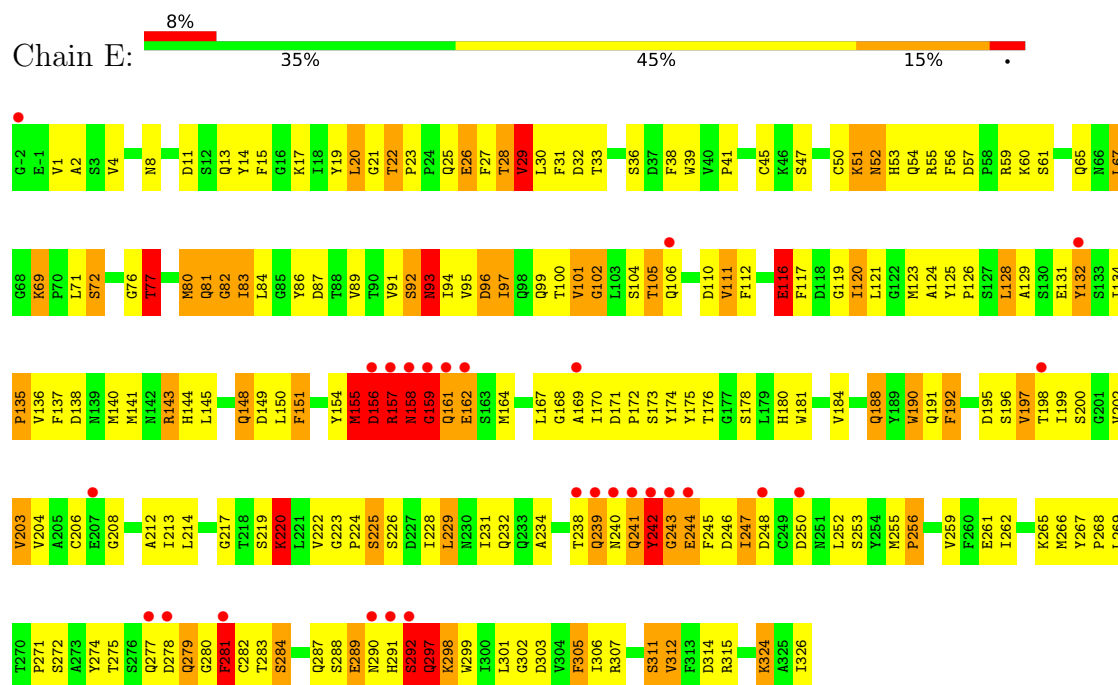
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	191	Total	O	0	0
			191	191		

3 Residue-property plots

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

• Molecule 1: CHYMOSIN



• Molecule 2: CP-113972 (NORSTATINE-S-METHYL CYSTEINE-IODO-PHENYLALANINE-PROLINE)



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	132.78Å 132.78Å 81.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.97 – 2.30 9.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (9.97-2.30) 96.3 (9.97-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 2.30Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.195 , (Not available) 0.265 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.035 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.017 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2745	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SMC, PHI, NOR

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	E	0.59	0/2574	1.92	65/3506 (1.9%)
2	P	0.24	0/7	1.00	0/8
All	All	0.59	0/2581	1.92	65/3514 (1.8%)

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	E	0	4

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	159	GLY	CA-C-N	22.06	161.74	122.92
1	E	159	GLY	C-N-CA	22.06	161.74	122.92
1	E	156	ASP	CA-C-N	14.42	149.09	121.54
1	E	156	ASP	C-N-CA	14.42	149.09	121.54
1	E	157	ARG	CA-C-N	9.82	140.30	121.54
1	E	157	ARG	C-N-CA	9.82	140.30	121.54
1	E	289	GLU	CA-C-O	-9.24	110.47	120.36
1	E	102	GLY	CA-C-O	-9.00	113.36	121.64
1	E	155	MET	N-CA-C	8.96	123.30	107.80
1	E	220	LYS	CA-C-O	7.27	128.96	120.89
1	E	289	GLU	O-C-N	7.24	131.48	123.22
1	E	248	ASP	CA-C-N	7.22	130.92	120.38
1	E	248	ASP	C-N-CA	7.22	130.92	120.38
1	E	188	GLN	O-C-N	7.06	131.98	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	154	TYR	CA-C-O	-6.95	112.66	120.66
1	E	28	THR	CA-C-N	-6.77	112.94	122.75
1	E	28	THR	C-N-CA	-6.77	112.94	122.75
1	E	151	PHE	CA-CB-CG	6.60	120.40	113.80
1	E	20	LEU	CA-C-O	-6.46	113.15	120.32
1	E	155	MET	CA-C-O	-6.27	112.35	120.25
1	E	20	LEU	O-C-N	6.26	130.64	123.31
1	E	242	TYR	CA-C-N	6.20	133.56	121.41
1	E	242	TYR	C-N-CA	6.20	133.56	121.41
1	E	102	GLY	O-C-N	6.19	129.28	122.96
1	E	312	VAL	CA-C-O	-6.06	114.15	120.27
1	E	192	PHE	O-C-N	5.97	129.81	123.42
1	E	190	TRP	O-C-N	5.94	130.22	122.38
1	E	93	ASN	CA-C-O	5.92	126.46	119.48
1	E	82	GLY	CA-C-N	5.91	131.21	123.06
1	E	82	GLY	C-N-CA	5.91	131.21	123.06
1	E	256	PRO	CA-C-O	5.78	129.29	122.12
1	E	77	THR	O-C-N	5.78	129.98	123.28
1	E	76	GLY	N-CA-C	-5.71	107.84	115.32
1	E	158	ASN	CA-CB-CG	-5.70	106.90	112.60
1	E	156	ASP	CA-CB-CG	-5.69	106.91	112.60
1	E	252	LEU	CA-C-N	5.64	128.62	120.38
1	E	252	LEU	C-N-CA	5.64	128.62	120.38
1	E	178	SER	CA-C-N	5.55	128.72	120.95
1	E	178	SER	C-N-CA	5.55	128.72	120.95
1	E	72	SER	CA-C-N	-5.49	115.32	122.94
1	E	72	SER	C-N-CA	-5.49	115.32	122.94
1	E	157	ARG	N-CA-C	5.49	122.49	110.80
1	E	305	PHE	O-C-N	5.48	129.35	122.23
1	E	220	LYS	CA-C-N	-5.40	115.15	123.14
1	E	220	LYS	C-N-CA	-5.40	115.15	123.14
1	E	239	GLN	CA-C-N	5.33	130.56	121.29
1	E	239	GLN	C-N-CA	5.33	130.56	121.29
1	E	96	ASP	CA-C-N	5.31	127.73	120.35
1	E	96	ASP	C-N-CA	5.31	127.73	120.35
1	E	135	PRO	CA-C-N	5.29	127.71	120.46
1	E	135	PRO	C-N-CA	5.29	127.71	120.46
1	E	145	LEU	N-CA-C	-5.27	106.86	113.72
1	E	241	GLN	CA-C-N	5.26	131.58	121.54
1	E	241	GLN	C-N-CA	5.26	131.58	121.54
1	E	132	TYR	CA-C-O	5.25	124.25	119.00
1	E	111	VAL	N-CA-CB	5.23	117.26	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	197	VAL	CA-C-O	5.23	125.83	120.39
1	E	289	GLU	CA-C-N	5.20	131.46	121.54
1	E	289	GLU	C-N-CA	5.20	131.46	121.54
1	E	29	VAL	CA-CB-CG2	5.19	119.23	110.40
1	E	143	ARG	CD-NE-CZ	-5.19	117.13	124.40
1	E	242	TYR	O-C-N	5.19	129.50	122.59
1	E	116	GLU	CA-C-O	5.07	125.61	119.38
1	E	208	GLY	CA-C-O	5.04	124.66	119.27
1	E	281	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	143	ARG	Sidechain
1	E	155	MET	Peptide
1	E	157	ARG	Sidechain
1	E	159	GLY	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	E	2511	0	2383	231	6
2	P	43	0	36	19	0
3	E	191	0	0	25	3
All	All	2745	0	2419	236	9

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 47.

All (236) 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:P:3:PHI:I	2:P:3:PHI:CZ	1.36	1.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:PHI:I	2:P:3:PHI:CE2	2.42	1.36
2:P:3:PHI:I	2:P:3:PHI:CE1	2.44	1.35
1:E:77:THR:HG22	1:E:77:THR:O	1.54	1.03
1:E:243:GLY:O	1:E:244:GLU:HB2	1.58	1.02
1:E:297:GLN:HG3	1:E:298:LYS:N	1.69	1.02
1:E:278:ASP:HB3	1:E:281:PHE:HD1	1.25	1.01
1:E:91:VAL:O	1:E:92:SER:HB3	1.60	1.00
1:E:25:GLN:HE22	1:E:57:ASP:H	1.17	0.91
1:E:278:ASP:HB3	1:E:281:PHE:CD1	2.07	0.90
1:E:214:LEU:HD21	1:E:311:SER:HB3	1.55	0.88
1:E:77:THR:O	1:E:77:THR:CG2	2.27	0.82
1:E:171:ASP:HB3	1:E:174:TYR:CD2	2.15	0.81
1:E:176:THR:CG2	1:E:324:LYS:HB3	2.11	0.81
1:E:224:PRO:HB3	1:E:292:SER:OG	1.83	0.79
1:E:13:GLN:NE2	2:P:3:PHI:I	2.85	0.79
1:E:156:ASP:HB2	1:E:157:ARG:HD3	1.63	0.79
1:E:292:SER:O	1:E:297:GLN:HB3	1.83	0.79
1:E:157:ARG:HA	1:E:161:GLN:HE21	1.49	0.78
1:E:240:ASN:CG	1:E:241:GLN:H	1.92	0.77
1:E:277:GLN:NE2	1:E:280:GLY:H	1.84	0.76
1:E:181:TRP:HH2	1:E:312:VAL:HG11	1.49	0.76
1:E:2:ALA:HB2	1:E:94:ILE:HG13	1.69	0.75
1:E:222:VAL:HG12	1:E:289:GLU:HG3	1.69	0.74
1:E:171:ASP:HB3	1:E:174:TYR:HD2	1.50	0.74
1:E:195:ASP:HB2	1:E:261:GLU:HG2	1.70	0.73
1:E:265:LYS:HB3	3:E:613:HOH:O	1.88	0.72
1:E:71:LEU:HD22	1:E:102:GLY:HA3	1.71	0.71
1:E:67:LEU:HG	3:E:438:HOH:O	1.91	0.71
1:E:220:LYS:CE	2:P:4:PRO:HG3	2.22	0.70
1:E:128:LEU:HD13	1:E:188:GLN:C	2.17	0.70
1:E:150:LEU:HB3	3:E:549:HOH:O	1.89	0.70
1:E:222:VAL:CG1	1:E:289:GLU:HG3	2.22	0.70
1:E:220:LYS:CD	2:P:4:PRO:HG3	2.22	0.70
1:E:156:ASP:CB	1:E:157:ARG:HD3	2.22	0.70
1:E:161:GLN:C	1:E:162:GLU:HG2	2.16	0.70
1:E:30:LEU:HD11	3:E:594:HOH:O	1.91	0.69
1:E:176:THR:HG22	1:E:324:LYS:HB3	1.74	0.69
1:E:297:GLN:CG	1:E:298:LYS:N	2.52	0.69
1:E:71:LEU:CD2	1:E:102:GLY:HA3	2.22	0.69
1:E:181:TRP:CH2	1:E:312:VAL:HG11	2.28	0.68
2:P:3:PHI:I	2:P:3:PHI:HE2	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LEU:HD23	1:E:314:ASP:HA	1.74	0.68
1:E:259:VAL:HG11	1:E:266:MET:HE3	1.76	0.68
1:E:220:LYS:HG2	2:P:4:PRO:HB3	1.75	0.67
1:E:277:GLN:HE21	1:E:280:GLY:H	1.42	0.67
1:E:157:ARG:C	1:E:161:GLN:HB2	2.20	0.67
1:E:128:LEU:CD1	1:E:188:GLN:HB3	2.25	0.67
1:E:4:VAL:HG23	3:E:557:HOH:O	1.96	0.66
1:E:121:LEU:C	1:E:121:LEU:HD23	2.21	0.65
1:E:156:ASP:CG	1:E:157:ARG:HD3	2.21	0.65
1:E:22:THR:HA	1:E:23:PRO:C	2.21	0.65
1:E:19:TYR:CE1	1:E:26:GLU:HB2	2.32	0.65
1:E:111:VAL:HB	3:E:532:HOH:O	1.97	0.65
1:E:176:THR:HG23	1:E:324:LYS:HB3	1.80	0.64
1:E:240:ASN:CG	1:E:241:GLN:N	2.55	0.64
1:E:128:LEU:HG	3:E:581:HOH:O	1.96	0.64
1:E:269:LEU:HD13	3:E:491:HOH:O	1.96	0.64
1:E:91:VAL:O	1:E:92:SER:CB	2.34	0.63
1:E:156:ASP:HB3	1:E:307:ARG:HG2	1.80	0.63
1:E:229:LEU:HD22	3:E:597:HOH:O	1.99	0.62
1:E:259:VAL:HA	1:E:268:PRO:HA	1.80	0.62
1:E:2:ALA:HB2	1:E:94:ILE:CD1	2.29	0.62
1:E:51:LYS:HA	1:E:55:ARG:NH1	2.13	0.62
1:E:228:ILE:O	1:E:232:GLN:HG2	2.00	0.61
1:E:21:GLY:HA2	1:E:87:ASP:OD1	2.00	0.61
1:E:303:ASP:O	1:E:307:ARG:HB2	2.00	0.61
1:E:2:ALA:HB2	1:E:94:ILE:CG1	2.31	0.61
1:E:206:CYS:HA	3:E:590:HOH:O	2.02	0.60
1:E:57:ASP:HB3	1:E:60:LYS:HD2	1.83	0.60
1:E:157:ARG:HB2	1:E:158:ASN:OD1	2.01	0.60
1:E:155:MET:O	1:E:156:ASP:HB3	1.99	0.60
1:E:126:PRO:HG3	1:E:138:ASP:OD2	2.03	0.59
1:E:39:TRP:CE2	1:E:80:MET:HG2	2.37	0.59
1:E:80:MET:C	1:E:80:MET:SD	2.86	0.59
2:P:3:PHI:I	2:P:3:PHI:HE1	2.63	0.59
1:E:289:GLU:HG2	3:E:507:HOH:O	2.02	0.59
1:E:241:GLN:O	1:E:242:TYR:HB2	2.03	0.59
1:E:156:ASP:CG	1:E:157:ARG:HH11	2.11	0.58
1:E:77:THR:HG21	2:P:3:PHI:HA	1.84	0.58
1:E:95:VAL:HG12	1:E:97:ILE:HD12	1.84	0.58
1:E:214:LEU:CD2	1:E:311:SER:HB3	2.33	0.58
1:E:8:ASN:OD1	1:E:11:ASP:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:GLN:HB3	1:E:86:TYR:HB2	1.85	0.58
1:E:15:PHE:CE1	1:E:116:GLU:HB3	2.40	0.57
1:E:161:GLN:O	1:E:162:GLU:HG2	2.04	0.57
1:E:162:GLU:HB2	3:E:377:HOH:O	2.05	0.56
1:E:222:VAL:HA	1:E:287:GLN:O	2.05	0.56
1:E:197:VAL:O	1:E:203:VAL:HA	2.05	0.55
1:E:225:SER:HA	1:E:288:SER:HB2	1.87	0.55
1:E:274:TYR:HD1	1:E:274:TYR:O	1.90	0.55
1:E:155:MET:O	1:E:307:ARG:HG2	2.07	0.54
1:E:13:GLN:OE1	1:E:116:GLU:HB2	2.07	0.54
1:E:29:VAL:HG11	1:E:121:LEU:HB2	1.89	0.54
1:E:150:LEU:HD13	3:E:549:HOH:O	2.06	0.54
1:E:51:LYS:HA	1:E:55:ARG:HH11	1.71	0.54
1:E:156:ASP:HB2	1:E:157:ARG:CD	2.35	0.54
1:E:67:LEU:CD2	1:E:86:TYR:CE2	2.91	0.54
1:E:155:MET:O	1:E:156:ASP:CB	2.55	0.54
1:E:148:GLN:HG3	1:E:168:GLY:O	2.08	0.54
1:E:297:GLN:HG3	1:E:298:LYS:H	1.68	0.54
1:E:213:ILE:HD13	3:E:593:HOH:O	2.08	0.54
1:E:120:ILE:HD11	2:P:1:NOR:HE22	1.89	0.53
1:E:291:HIS:O	1:E:292:SER:HB2	2.07	0.53
1:E:198:THR:HA	1:E:202:VAL:O	2.09	0.53
1:E:190:TRP:O	1:E:213:ILE:HA	2.08	0.53
1:E:324:LYS:HG2	3:E:621:HOH:O	2.08	0.53
1:E:144:HIS:O	1:E:144:HIS:CD2	2.61	0.52
1:E:31:PHE:CE1	1:E:121:LEU:HD13	2.44	0.52
1:E:150:LEU:HD23	1:E:314:ASP:CA	2.40	0.52
1:E:199:ILE:HD12	1:E:234:ALA:HB1	1.91	0.52
1:E:271:PRO:HA	1:E:274:TYR:CE2	2.44	0.52
1:E:141:MET:SD	1:E:149:ASP:HB3	2.49	0.52
1:E:184:VAL:HG13	1:E:191:GLN:O	2.10	0.52
1:E:128:LEU:HD13	1:E:188:GLN:O	2.10	0.52
1:E:213:ILE:O	1:E:213:ILE:HG13	2.08	0.52
1:E:126:PRO:HD3	1:E:315:ARG:HH12	1.75	0.52
1:E:83:ILE:HD13	1:E:83:ILE:N	2.25	0.52
1:E:38:PHE:CE2	1:E:101:VAL:HB	2.45	0.51
1:E:277:GLN:HE21	1:E:279:GLN:HA	1.75	0.51
1:E:39:TRP:CG	1:E:80:MET:HE3	2.45	0.51
1:E:212:ALA:HA	1:E:299:TRP:O	2.11	0.51
1:E:128:LEU:HD13	1:E:188:GLN:HB3	1.93	0.51
1:E:196:SER:HB2	1:E:203:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ILE:HG21	3:E:593:HOH:O	2.10	0.51
1:E:247:ILE:O	1:E:282:CYS:HB2	2.11	0.51
1:E:269:LEU:HD11	1:E:305:PHE:HD1	1.75	0.50
1:E:125:TYR:HB3	1:E:126:PRO:HD2	1.92	0.50
1:E:223:GLY:O	1:E:288:SER:HA	2.12	0.50
1:E:67:LEU:HD22	1:E:86:TYR:CD2	2.46	0.50
1:E:36:SER:HB3	1:E:135:PRO:HG3	1.93	0.50
1:E:45:CYS:HB2	1:E:104:SER:O	2.12	0.50
1:E:100:THR:HG23	3:E:538:HOH:O	2.12	0.49
1:E:19:TYR:HA	1:E:25:GLN:O	2.12	0.49
1:E:277:GLN:HG3	1:E:278:ASP:N	2.27	0.49
1:E:52:ASN:C	1:E:52:ASN:ND2	2.69	0.49
1:E:72:SER:HB2	1:E:81:GLN:HE21	1.78	0.49
1:E:14:TYR:O	1:E:30:LEU:HD12	2.12	0.48
1:E:297:GLN:HG2	3:E:502:HOH:O	2.13	0.48
1:E:150:LEU:HD22	1:E:312:VAL:CG1	2.43	0.48
1:E:69:LYS:O	1:E:84:LEU:HB2	2.13	0.48
1:E:86:TYR:CE1	1:E:100:THR:HG22	2.48	0.48
1:E:22:THR:CA	1:E:23:PRO:C	2.86	0.48
1:E:157:ARG:O	1:E:161:GLN:HB2	2.13	0.48
1:E:245:PHE:O	1:E:283:THR:HG23	2.14	0.48
1:E:170:ILE:HG13	3:E:549:HOH:O	2.13	0.47
1:E:220:LYS:CG	2:P:4:PRO:HG3	2.44	0.47
1:E:271:PRO:HA	1:E:274:TYR:CZ	2.49	0.47
1:E:82:GLY:C	1:E:83:ILE:HD13	2.40	0.47
1:E:41:PRO:HA	1:E:104:SER:OG	2.15	0.47
1:E:131:GLU:O	1:E:132:TYR:HB2	2.15	0.47
1:E:262:ILE:HB	1:E:267:TYR:CE2	2.49	0.47
1:E:51:LYS:HE2	1:E:51:LYS:HB3	1.76	0.47
1:E:176:THR:HG23	1:E:324:LYS:HE2	1.96	0.47
1:E:274:TYR:HB3	3:E:491:HOH:O	2.14	0.47
1:E:33:THR:HA	1:E:123:MET:HB2	1.96	0.47
1:E:291:HIS:O	1:E:292:SER:CB	2.63	0.47
1:E:277:GLN:HE21	1:E:280:GLY:N	2.11	0.47
1:E:99:GLN:NE2	1:E:136:VAL:HA	2.29	0.46
1:E:158:ASN:C	1:E:161:GLN:HB3	2.39	0.46
1:E:279:GLN:CG	1:E:279:GLN:O	2.62	0.46
1:E:39:TRP:CB	1:E:80:MET:HE3	2.45	0.46
1:E:274:TYR:O	1:E:274:TYR:CD1	2.68	0.46
1:E:172:PRO:HA	1:E:175:TYR:CE2	2.51	0.46
1:E:67:LEU:HD21	1:E:86:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ALA:HB1	1:E:128:LEU:HD22	1.97	0.45
1:E:167:LEU:HG	3:E:557:HOH:O	2.16	0.45
1:E:1:VAL:O	1:E:93:ASN:ND2	2.50	0.45
1:E:195:ASP:O	1:E:196:SER:HB3	2.17	0.45
1:E:271:PRO:O	1:E:275:THR:HB	2.16	0.45
1:E:151:PHE:HB2	1:E:167:LEU:HD23	1.99	0.45
1:E:128:LEU:HD13	1:E:188:GLN:CA	2.47	0.45
1:E:128:LEU:HD13	1:E:188:GLN:CB	2.47	0.45
1:E:124:ALA:CB	1:E:128:LEU:HD22	2.47	0.44
1:E:25:GLN:NE2	1:E:56:PHE:HD1	2.15	0.44
1:E:121:LEU:C	1:E:121:LEU:CD2	2.90	0.44
1:E:180:HIS:HB3	3:E:458:HOH:O	2.18	0.44
1:E:199:ILE:O	1:E:200:SER:HB2	2.17	0.44
1:E:277:GLN:HB2	1:E:282:CYS:SG	2.58	0.44
1:E:269:LEU:HD11	1:E:305:PHE:CD1	2.53	0.44
1:E:244:GLU:HG3	1:E:245:PHE:H	1.83	0.44
1:E:199:ILE:HG13	1:E:204:VAL:HG11	2.00	0.44
1:E:232:GLN:OE1	1:E:232:GLN:HA	2.18	0.44
1:E:283:THR:HG22	1:E:284:SER:N	2.33	0.43
1:E:238:THR:O	1:E:245:PHE:HA	2.18	0.43
1:E:36:SER:OG	1:E:124:ALA:HB3	2.18	0.43
1:E:302:GLY:O	1:E:306:ILE:HG13	2.18	0.43
1:E:220:LYS:O	1:E:302:GLY:HA3	2.19	0.43
1:E:71:LEU:HD22	1:E:102:GLY:CA	2.43	0.43
1:E:105:THR:O	1:E:106:GLN:HG2	2.18	0.43
1:E:131:GLU:O	1:E:132:TYR:CB	2.67	0.43
1:E:184:VAL:HA	1:E:191:GLN:O	2.19	0.43
1:E:220:LYS:HE3	2:P:4:PRO:HG3	2.01	0.43
1:E:28:THR:OG1	1:E:117:PHE:HA	2.19	0.42
1:E:291:HIS:HB2	1:E:292:SER:H	1.60	0.42
1:E:255:MET:HB3	1:E:256:PRO:HD2	2.01	0.42
1:E:19:TYR:CD1	1:E:26:GLU:HB2	2.54	0.42
1:E:22:THR:O	1:E:61:SER:HA	2.19	0.42
1:E:67:LEU:HB2	1:E:84:LEU:O	2.18	0.42
1:E:199:ILE:HD12	1:E:234:ALA:CB	2.49	0.42
1:E:124:ALA:HB1	3:E:575:HOH:O	2.19	0.42
1:E:112:PHE:CE1	2:P:1:NOR:HE21	2.55	0.42
1:E:52:ASN:C	1:E:52:ASN:HD22	2.28	0.42
1:E:77:THR:HB	2:P:2:SMC:N	2.35	0.42
1:E:83:ILE:N	1:E:83:ILE:CD1	2.80	0.42
1:E:100:THR:HG21	1:E:134:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:PHE:O	1:E:140:MET:HB2	2.19	0.42
1:E:2:ALA:CB	1:E:94:ILE:CD1	2.98	0.41
1:E:36:SER:OG	1:E:128:LEU:HB3	2.19	0.41
1:E:112:PHE:HE1	1:E:120:ILE:HD11	1.85	0.41
1:E:156:ASP:OD1	1:E:156:ASP:C	2.62	0.41
1:E:26:GLU:HG2	1:E:27:PHE:N	2.35	0.41
1:E:239:GLN:HA	1:E:244:GLU:O	2.20	0.41
1:E:129:ALA:CB	1:E:135:PRO:HD3	2.50	0.41
1:E:32:ASP:OD2	2:P:1:NOR:HC	2.20	0.41
1:E:38:PHE:CD2	1:E:101:VAL:HB	2.56	0.41
1:E:89:VAL:HG13	1:E:96:ASP:HB3	2.02	0.41
1:E:100:THR:CG2	1:E:134:ILE:HD12	2.50	0.41
1:E:151:PHE:CB	1:E:167:LEU:HD23	2.51	0.41
1:E:52:ASN:ND2	1:E:53:HIS:ND1	2.68	0.41
1:E:32:ASP:OD2	2:P:1:NOR:HB1	2.21	0.41
1:E:20:LEU:HD12	1:E:20:LEU:HA	1.83	0.41
1:E:67:LEU:HD13	1:E:67:LEU:HA	1.88	0.41
1:E:217:GLY:HA3	2:P:1:NOR:HB2	2.02	0.40
1:E:269:LEU:O	1:E:274:TYR:HD2	2.04	0.40
1:E:1:VAL:HG11	1:E:169:ALA:HB3	2.03	0.40
1:E:2:ALA:CB	1:E:94:ILE:HD12	2.51	0.40
1:E:13:GLN:HE21	2:P:3:PHI:CE1	2.34	0.40
1:E:29:VAL:HA	1:E:119:GLY:O	2.21	0.40
1:E:123:MET:HB3	1:E:151:PHE:CZ	2.56	0.40
1:E:47:SER:O	1:E:50:CYS:HB2	2.22	0.40
1:E:67:LEU:HD22	1:E:86:TYR:CE2	2.56	0.40
1:E:112:PHE:HB3	3:E:399:HOH:O	2.21	0.40
1:E:124:ALA:HA	3:E:575:HOH:O	2.22	0.40
1:E:192:PHE:HZ	1:E:301:LEU:HD12	1.86	0.40
1:E:266:MET:C	1:E:268:PRO:HD3	2.47	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:568:HOH:O	3:E:568:HOH:O[6_766]	0.58	1.62
1:E:242:TYR:CD2	1:E:244:GLU:CG[18_655]	1.47	0.73
1:E:241:GLN:O	1:E:246:ASP:OD2[18_655]	1.69	0.51
1:E:240:ASN:OD1	1:E:240:ASN:OD1[18_655]	1.87	0.33
3:E:450:HOH:O	3:E:450:HOH:O[10_546]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:TYR:CD2	1:E:244:GLU:CD[18_655]	2.08	0.12
1:E:242:TYR:CE2	1:E:244:GLU:OE2[18_655]	2.09	0.11
3:E:521:HOH:O	3:E:521:HOH:O[17_555]	2.09	0.11
1:E:240:ASN:ND2	1:E:240:ASN:ND2[18_655]	2.11	0.09

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	E	321/323 (99%)	284 (88%)	25 (8%)	12 (4%)	2 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	157	ARG
1	E	158	ASN
1	E	242	TYR
1	E	244	GLU
1	E	297	GLN
1	E	92	SER
1	E	159	GLY
1	E	243	GLY
1	E	290	ASN
1	E	292	SER
1	E	156	ASP
1	E	279	GLN

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	E	280/280 (100%)	232 (83%)	48 (17%)	2	2
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	281/281 (100%)	233 (83%)	48 (17%)	2	2

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	17	LYS
1	E	22	THR
1	E	26	GLU
1	E	29	VAL
1	E	51	LYS
1	E	52	ASN
1	E	54	GLN
1	E	59	ARG
1	E	67	LEU
1	E	69	LYS
1	E	77	THR
1	E	80	MET
1	E	81	GLN
1	E	83	ILE
1	E	93	ASN
1	E	97	ILE
1	E	101	VAL
1	E	105	THR
1	E	110	ASP
1	E	116	GLU
1	E	120	ILE
1	E	128	LEU
1	E	148	GLN
1	E	157	ARG
1	E	161	GLN
1	E	162	GLU
1	E	164	MET
1	E	173	SER
1	E	203	VAL
1	E	219	SER
1	E	220	LYS
1	E	225	SER
1	E	226	SER

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Mol	Chain	Res	Type
1	E	229	LEU
1	E	231	ILE
1	E	242	TYR
1	E	247	ILE
1	E	250	ASP
1	E	253	SER
1	E	272	SER
1	E	281	PHE
1	E	284	SER
1	E	292	SER
1	E	297	GLN
1	E	298	LYS
1	E	311	SER
1	E	324	LYS
1	E	326	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	25	GLN
1	E	52	ASN
1	E	54	GLN
1	E	65	GLN
1	E	81	GLN
1	E	93	ASN
1	E	99	GLN
1	E	139	ASN
1	E	142	ASN
1	E	144	HIS
1	E	148	GLN
1	E	161	GLN
1	E	180	HIS
1	E	187	GLN
1	E	251	ASN
1	E	277	GLN
1	E	297	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NOR	P	1	2	17,17,17	2.84	1 (5%)	18,22,22	2.42	5 (27%)
2	PHI	P	3	2	11,12,13	8.64	1 (9%)	10,15,17	2.88	5 (50%)
2	SMC	P	2	2	5,6,7	0.49	0	3,6,8	4.35	2 (66%)

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	NOR	P	1	2	-	7/16/24/24	0/1/1/1
2	PHI	P	3	2	-	1/5/6/8	0/1/1/1
2	SMC	P	2	2	-	2/3/5/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	3	PHI	CZ-I	-28.54	1.36	2.10
2	P	1	NOR	CH-CA	-11.23	1.41	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	2	SMC	CA-CB-SG	-7.05	102.64	114.04
2	P	1	NOR	CE2-CD2-CG	-6.30	98.82	112.08
2	P	3	PHI	CE2-CZ-CE1	-5.82	112.95	120.64
2	P	1	NOR	OXT-C-CH	4.73	118.64	111.13
2	P	1	NOR	CM-OXT-C	-4.13	111.84	117.71
2	P	3	PHI	CD1-CE1-CZ	3.78	124.40	119.55
2	P	3	PHI	CE1-CZ-I	3.15	124.39	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	PHI	CD2-CE2-CZ	2.96	123.34	119.55
2	P	1	NOR	CD2-CG-CD1	2.63	115.71	109.29
2	P	1	NOR	OXT-CM-CM2	2.61	114.08	107.13
2	P	3	PHI	CD2-CG-CD1	-2.60	114.37	118.23
2	P	2	SMC	CB-CA-C	-2.16	104.94	110.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	3	PHI	O-C-CA-CB
2	P	2	SMC	N-CA-CB-SG
2	P	1	NOR	CA-CB-CG-CD2
2	P	1	NOR	CM2-CM-OXT-C
2	P	1	NOR	CA-CB-CG-CD1
2	P	1	NOR	OXT-C-CH-CA
2	P	1	NOR	O-C-OXT-CM
2	P	1	NOR	O-C-CH-CA
2	P	1	NOR	CM1-CM-OXT-C
2	P	2	SMC	CA-CB-SG-CS

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	NOR	5	0
2	P	3	PHI	8	0
2	P	2	SMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	E	323/323 (100%)	0.82	27 (8%) 17 18	0, 0, 0, 1	0
2	P	1/4 (25%)	4.10	1 (100%) 0 0	1, 1, 1, 1	0
All	All	324/327 (99%)	0.83	28 (8%) 16 17	0, 0, 0, 1	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	242	TYR	10.0
1	E	243	GLY	7.5
1	E	292	SER	7.5
1	E	290	ASN	6.4
1	E	241	GLN	6.2
1	E	156	ASP	6.0
1	E	159	GLY	5.6
1	E	244	GLU	4.9
1	E	291	HIS	4.8
1	E	161	GLN	4.8
1	E	158	ASN	4.4
2	P	4	PRO	4.1
1	E	250	ASP	3.7
1	E	106	GLN	3.4
1	E	281	PHE	3.2
1	E	240	ASN	3.2
1	E	238	THR	3.2
1	E	239	GLN	3.1
1	E	157	ARG	3.0
1	E	-2	GLY	2.7
1	E	198	THR	2.6
1	E	169	ALA	2.6
1	E	162	GLU	2.4
1	E	132	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	248	ASP	2.2
1	E	207	GLU	2.1
1	E	278	ASP	2.0
1	E	277	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NOR	P	1	17/17	0.76	0.12	0,0,0,0	0
2	SMC	P	2	7/8	0.92	0.10	0,0,0,0	0
2	PHI	P	3	12/13	0.97	0.15	0,0,0,1	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.