



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID : 1P4A
Title : Crystal Structure of the PurR complexed with cPRPP
Authors : Bera, A.K.; Zhu, J.; Zalkin, H.; Smith, J.L.
Deposited on : 2003-04-22
Resolution : 2.22 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

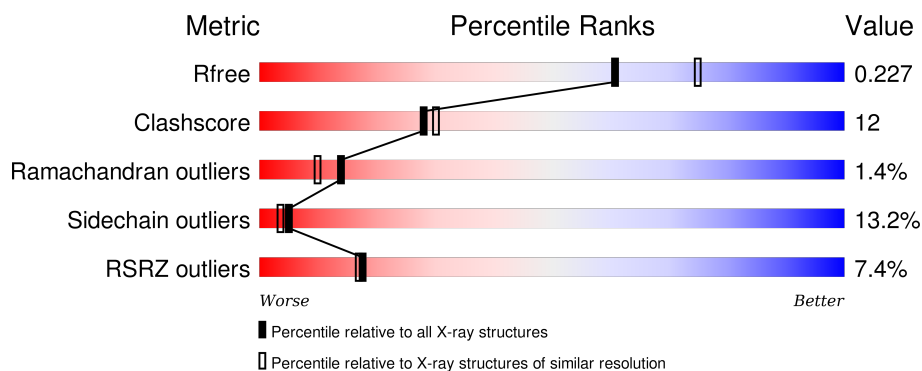
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	285	<div> <div>7%</div> <div>65% 20% 8% • 6%</div> </div>
1	B	285	<div> <div>5%</div> <div>74% 17% • 6%</div> </div>
1	C	285	<div> <div>6%</div> <div>67% 21% 5% • 6%</div> </div>
1	D	285	<div> <div>9%</div> <div>68% 19% 6% • 6%</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
2	PCP	A	604	X	-	-	X
2	PCP	B	605	X	-	-	X
2	PCP	C	606	X	-	-	X
2	PCP	D	607	X	-	-	X

2 Entry composition [i](#)

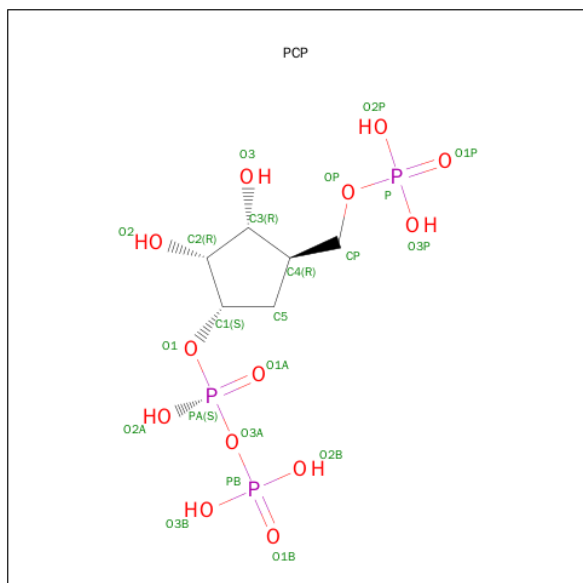
There are 3 unique types of molecules in this entry. The entry contains 8926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pur operon repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2073	1323	345	397	8			
1	B	268	Total	C	N	O	S	0	0	0
			2061	1316	342	395	8			
1	C	269	Total	C	N	O	S	0	0	0
			2069	1320	344	397	8			
1	D	268	Total	C	N	O	S	0	0	0
			2061	1316	342	395	8			

- Molecule 2 is 1-ALPHA-PYROPHOSPHORYL-2-ALPHA,3-ALPHA-DIHYDROXY-4-BETA-CYCLOPENTANE-METHANOL-5-PHOSPHATE (three-letter code: PCP) (formula: $C_6H_{15}O_{13}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			22	6	13	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			22	6	13	3		
2	C	1	Total	C	O	P	0	0
			22	6	13	3		
2	D	1	Total	C	O	P	0	0
			22	6	13	3		

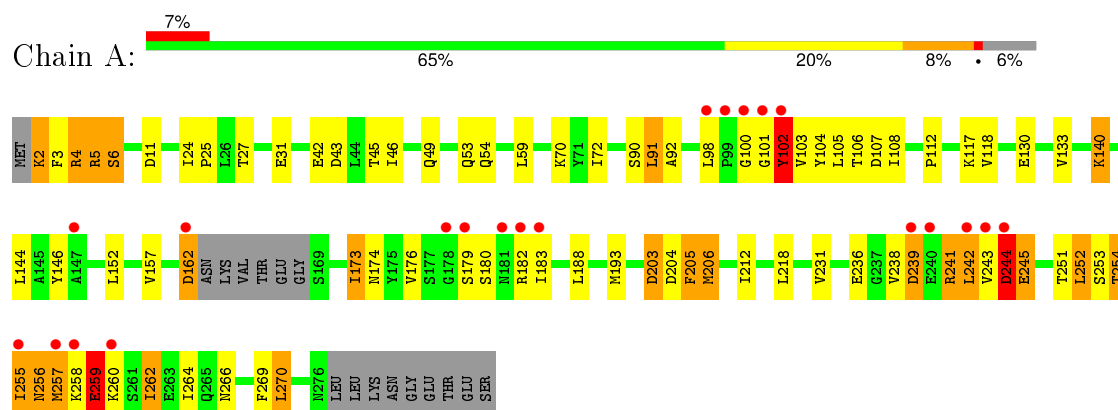
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total	O	0	0
			162	162		
3	B	155	Total	O	0	0
			155	155		
3	C	139	Total	O	0	0
			139	139		
3	D	118	Total	O	0	0
			118	118		

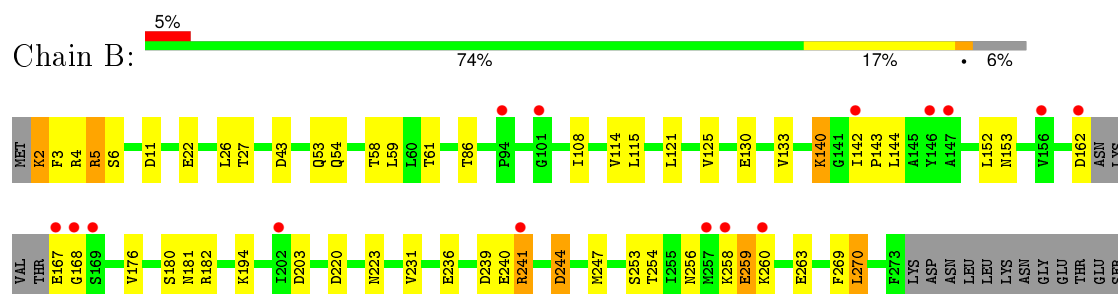
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

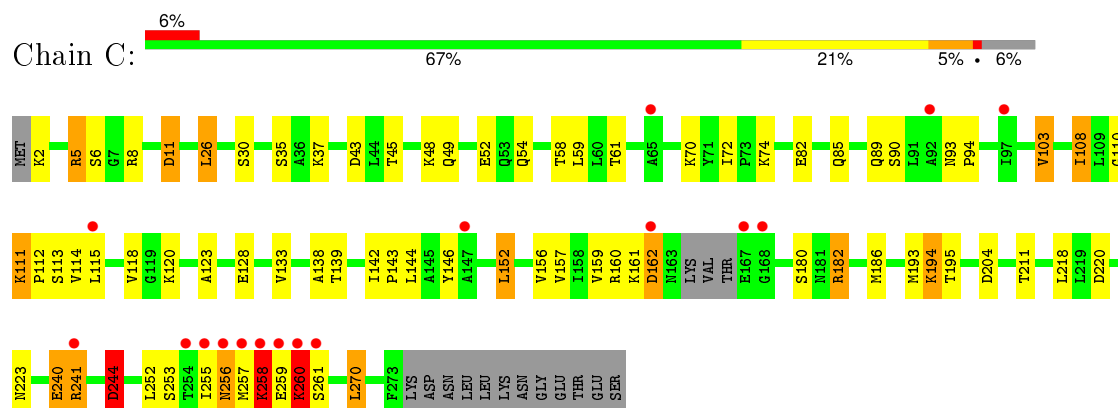
• Molecule 1: Pur operon repressor



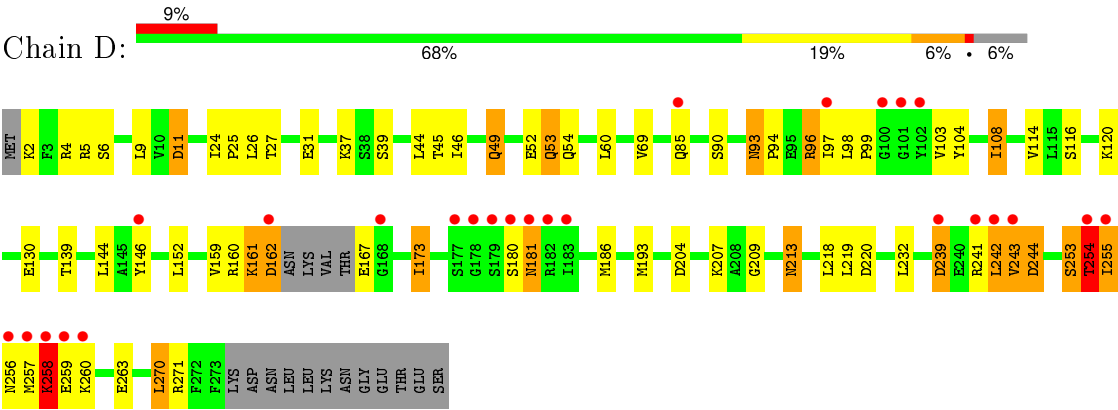
• Molecule 1: Pur operon repressor



• Molecule 1: Pur operon repressor



● Molecule 1: Pur operon repressor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.37Å 135.72Å 82.07Å 90.00° 95.10° 90.00°	Depositor
Resolution (Å)	37.80 – 2.22 37.80 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.80-2.22) 98.5 (37.80-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.177 , 0.234 0.176 , 0.227	Depositor DCC
R_{free} test set	3137 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 61770 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8926	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCP

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	0.44	0/2103	0.69	7/2840 (0.2%)
1	B	0.46	0/2091	0.70	3/2824 (0.1%)
1	C	0.40	0/2099	0.66	3/2835 (0.1%)
1	D	0.39	0/2091	0.67	5/2824 (0.2%)
All	All	0.42	0/8384	0.68	18/11323 (0.2%)

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	D	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ASP	CB-CG-OD2	7.13	124.72	118.30
1	C	204	ASP	CB-CG-OD2	6.03	123.72	118.30
1	D	220	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	244	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	244	ASP	CB-CG-OD2	5.85	123.57	118.30
1	C	244	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	107	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	11	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	11	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	162	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	11	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	239	ASP	CB-CG-OD2	5.31	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	162	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	239	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	239	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	11	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	43	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	253	SER	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	2073	0	2128	72	0
1	B	2061	0	2114	35	0
1	C	2069	0	2120	53	0
1	D	2061	0	2114	46	0
2	A	22	0	10	0	0
2	B	22	0	10	3	0
2	C	22	0	10	2	0
2	D	22	0	10	1	0
3	A	162	0	0	13	0
3	B	155	0	0	13	0
3	C	139	0	0	13	0
3	D	118	0	0	11	0
All	All	8926	0	8516	198	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 12.

All (198) 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:58:THR:HB	3:B:753:HOH:O	1.30	1.26
1:A:112:PRO:HD2	3:A:735:HOH:O	1.30	1.24
2:B:605:PCP:O1A	3:B:760:HOH:O	1.64	1.15
1:A:112:PRO:HG3	3:A:710:HOH:O	1.50	1.09
1:A:42:GLU:HB3	3:A:743:HOH:O	1.56	1.05
1:D:27:THR:HG22	1:D:37:LYS:HE2	1.47	0.95
1:A:251:THR:HG22	3:A:678:HOH:O	1.72	0.90
1:A:101:GLY:O	1:A:102:TYR:HB2	1.78	0.84
1:D:45:THR:O	1:D:49:GLN:HG2	1.83	0.79
1:A:206:MET:HG3	1:A:212:ILE:HD12	1.67	0.77
1:C:110:GLY:HA2	1:D:146:TYR:OH	1.84	0.77
1:A:258:LYS:O	1:A:259:GLU:HB2	1.84	0.75
1:C:241:ARG:HB2	3:C:731:HOH:O	1.87	0.73
1:D:4:ARG:HB2	3:D:656:HOH:O	1.87	0.73
1:B:236:GLU:HG3	1:B:253:SER:HA	1.70	0.73
1:A:4:ARG:HG3	1:A:5:ARG:N	2.02	0.73
1:A:53:GLN:HG2	1:A:54:GLN:HE21	1.54	0.72
1:C:5:ARG:HD2	3:D:614:HOH:O	1.89	0.71
1:B:53:GLN:HG2	1:B:54:GLN:HE21	1.56	0.71
1:C:118:VAL:HG11	1:C:144:LEU:HD21	1.72	0.71
1:A:243:VAL:O	1:A:244:ASP:HB2	1.91	0.70
1:B:256:ASN:HD22	1:B:259:GLU:HB2	1.57	0.69
1:C:146:TYR:HA	1:C:156:VAL:HG21	1.75	0.69
1:B:256:ASN:HD22	1:B:259:GLU:CB	2.04	0.69
1:D:5:ARG:O	3:D:708:HOH:O	2.10	0.69
1:C:244:ASP:OD1	3:C:721:HOH:O	2.12	0.68
1:C:240:GLU:O	3:C:719:HOH:O	2.11	0.68
2:C:606:PCP:H1	3:C:659:HOH:O	1.92	0.68
2:B:605:PCP:H2	2:B:605:PCP:O2A	1.95	0.67
1:C:143:PRO:HG3	1:D:146:TYR:CE1	2.29	0.67
1:A:70:LYS:HD3	1:A:72:ILE:HD11	1.78	0.66
1:B:22:GLU:OE2	3:B:738:HOH:O	2.14	0.66
1:D:5:ARG:HG2	3:D:708:HOH:O	1.96	0.66
1:A:183:ILE:HG13	1:A:183:ILE:O	1.94	0.66
1:B:61:THR:HG23	3:B:666:HOH:O	1.94	0.65
3:A:755:HOH:O	1:B:140:LYS:HG3	1.95	0.65
1:D:49:GLN:HB2	3:D:646:HOH:O	1.96	0.65
1:B:5:ARG:NH1	1:B:43:ASP:OD1	2.30	0.65
1:A:27:THR:O	1:A:31:GLU:HG3	1.96	0.65
1:C:58:THR:HA	3:C:730:HOH:O	1.97	0.65
1:B:2:LYS:O	1:B:3:PHE:HB2	1.95	0.65
1:A:173:ILE:CG2	1:A:218:LEU:HD13	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD11	1:A:105:LEU:CD2	2.27	0.64
1:D:99:PRO:HG3	1:D:258:LYS:HZ1	1.63	0.63
1:C:6:SER:HB3	1:D:46:ILE:HG21	1.79	0.62
1:D:53:GLN:HG3	1:D:54:GLN:HE21	1.64	0.62
1:B:153:ASN:CG	3:B:633:HOH:O	2.38	0.62
1:C:120:LYS:HE3	3:C:661:HOH:O	1.99	0.61
1:A:241:ARG:HD2	3:A:675:HOH:O	2.00	0.61
1:D:218:LEU:HD13	3:D:705:HOH:O	2.01	0.61
1:C:143:PRO:CG	1:D:146:TYR:CE1	2.85	0.60
1:B:203:ASP:OD2	2:B:605:PCP:O2	2.19	0.60
1:C:156:VAL:HB	3:D:659:HOH:O	2.00	0.60
1:A:238:VAL:O	1:A:241:ARG:HG2	2.02	0.59
1:A:45:THR:O	1:A:49:GLN:HG3	2.01	0.59
1:A:256:ASN:HD21	1:A:260:LYS:H	1.49	0.59
1:B:182:ARG:NE	3:B:752:HOH:O	2.36	0.59
1:D:161:LYS:O	1:D:162:ASP:HB2	2.03	0.58
1:A:42:GLU:CB	3:A:743:HOH:O	2.33	0.58
1:D:96:ARG:HB2	1:D:104:TYR:HB3	1.85	0.58
1:C:5:ARG:NE	1:C:43:ASP:OD1	2.31	0.57
1:D:97:ILE:HG21	1:D:258:LYS:HA	1.85	0.57
1:A:256:ASN:HD21	1:A:260:LYS:N	2.03	0.56
1:D:160:ARG:NH2	3:D:625:HOH:O	2.36	0.56
1:A:256:ASN:O	1:A:257:MET:HE1	2.05	0.56
1:A:173:ILE:HG22	1:A:218:LEU:HD13	1.87	0.56
1:A:112:PRO:CD	3:A:735:HOH:O	2.11	0.55
1:A:103:VAL:HG21	1:A:252:LEU:HD11	1.87	0.55
1:A:176:VAL:HG22	3:A:650:HOH:O	2.06	0.55
1:C:85:GLN:O	1:C:89:GLN:HG3	2.07	0.55
1:B:142:ILE:HB	1:B:143:PRO:HD3	1.89	0.55
1:A:173:ILE:HG12	1:A:174:ASN:N	2.22	0.54
1:C:85:GLN:NE2	3:C:740:HOH:O	2.41	0.54
1:D:139:THR:N	2:D:607:PCP:O1B	2.40	0.54
1:A:257:MET:HE3	1:A:257:MET:HA	1.88	0.54
1:A:4:ARG:HG3	1:A:6:SER:H	1.73	0.54
1:B:176:VAL:HG22	3:B:660:HOH:O	2.07	0.53
1:A:236:GLU:HB2	3:A:678:HOH:O	2.08	0.53
1:A:91:LEU:HD11	1:A:105:LEU:HD21	1.90	0.53
1:C:182:ARG:HG3	1:C:182:ARG:NH1	2.25	0.52
1:A:262:ILE:HG13	1:A:264:ILE:HD12	1.90	0.52
1:A:146:TYR:CE2	1:B:115:LEU:HD11	2.45	0.52
1:A:146:TYR:CE2	1:B:115:LEU:CD1	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:OE1	3:A:756:HOH:O	2.19	0.52
1:C:45:THR:O	1:C:49:GLN:HG3	2.09	0.51
1:B:86:THR:HB	3:B:655:HOH:O	2.10	0.51
1:A:255:ILE:O	1:A:256:ASN:HB2	2.09	0.51
1:B:2:LYS:N	3:B:749:HOH:O	2.42	0.51
1:D:242:LEU:O	1:D:243:VAL:HB	2.10	0.51
1:A:243:VAL:O	1:A:244:ASP:CB	2.59	0.51
1:A:53:GLN:HG2	1:A:54:GLN:NE2	2.23	0.51
1:A:133:VAL:HG21	1:A:157:VAL:HG23	1.93	0.50
1:C:70:LYS:HD3	1:C:72:ILE:HD11	1.92	0.50
1:D:53:GLN:HE21	1:D:54:GLN:NE2	2.10	0.50
1:A:5:ARG:NH2	1:A:46:ILE:CD1	2.75	0.50
1:C:115:LEU:CD1	1:D:146:TYR:CE2	2.95	0.50
1:B:256:ASN:ND2	1:B:259:GLU:HB2	2.25	0.50
1:C:103:VAL:CG2	1:C:252:LEU:HD22	2.42	0.50
1:C:182:ARG:HG3	1:C:182:ARG:HH11	1.77	0.49
1:C:30:SER:HB2	1:C:35:SER:O	2.11	0.49
1:C:211:THR:OG1	2:C:606:PCP:H3	2.12	0.49
1:A:257:MET:CE	1:A:257:MET:HA	2.43	0.49
1:C:256:ASN:HB3	1:C:261:SER:H	1.77	0.49
1:B:27:THR:HG23	3:B:750:HOH:O	2.13	0.48
1:D:270:LEU:HA	1:D:270:LEU:HD12	1.68	0.48
1:D:254:THR:HG22	1:D:255:ILE:H	1.78	0.48
1:A:91:LEU:HB3	1:A:264:ILE:HD13	1.96	0.48
1:C:160:ARG:O	1:C:186:MET:HA	2.14	0.48
1:D:96:ARG:CB	1:D:104:TYR:HB3	2.44	0.47
1:B:180:SER:O	3:B:657:HOH:O	2.20	0.47
1:A:253:SER:O	1:A:254:THR:C	2.53	0.47
1:C:270:LEU:HD22	3:C:655:HOH:O	2.14	0.47
1:C:111:LYS:HB2	1:C:111:LYS:HE2	1.46	0.47
1:D:27:THR:O	1:D:31:GLU:HG3	2.15	0.47
1:C:48:LYS:NZ	3:C:693:HOH:O	2.47	0.47
1:A:46:ILE:HG21	1:B:6:SER:HB3	1.97	0.46
1:A:5:ARG:HB3	3:A:723:HOH:O	2.16	0.46
1:A:91:LEU:HD11	1:A:105:LEU:HD22	1.95	0.46
1:A:203:ASP:O	1:A:231:VAL:HA	2.15	0.46
1:C:142:ILE:HB	1:C:143:PRO:HD3	1.98	0.46
1:A:257:MET:O	1:A:258:LYS:HB3	2.16	0.46
1:B:269:PHE:CE1	1:B:270:LEU:HD13	2.51	0.46
1:A:238:VAL:HG23	1:A:238:VAL:O	2.15	0.46
1:B:153:ASN:ND2	3:B:633:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NH2	1:A:242:LEU:O	2.48	0.46
1:B:162:ASP:C	3:B:653:HOH:O	2.54	0.46
1:B:240:GLU:HG3	1:B:241:ARG:NH1	2.31	0.45
1:A:5:ARG:HH21	1:A:46:ILE:CD1	2.29	0.45
1:B:108:ILE:HG23	1:B:114:VAL:HG11	1.98	0.45
1:D:120:LYS:HE3	3:D:674:HOH:O	2.17	0.45
1:C:194:LYS:NZ	3:C:667:HOH:O	2.36	0.44
1:A:262:ILE:CG1	1:A:264:ILE:HD12	2.47	0.44
1:C:11:ASP:OD1	1:D:54:GLN:HG3	2.16	0.44
1:D:44:LEU:HD13	1:D:69:VAL:HG11	1.98	0.44
1:A:100:GLY:O	1:A:101:GLY:C	2.56	0.44
1:D:159:VAL:CG1	1:D:186:MET:HB2	2.47	0.44
1:A:205:PHE:HZ	1:A:252:LEU:HD22	1.82	0.44
1:D:108:ILE:HG23	1:D:114:VAL:HG11	2.00	0.44
1:A:157:VAL:HG11	1:A:188:LEU:HD21	2.00	0.44
1:A:2:LYS:CG	1:A:3:PHE:H	2.30	0.44
1:D:5:ARG:NH2	1:D:46:ILE:CD1	2.81	0.43
1:D:53:GLN:CG	1:D:54:GLN:HE21	2.29	0.43
1:B:241:ARG:HA	1:B:241:ARG:HD3	1.51	0.43
1:A:24:ILE:HA	1:A:25:PRO:HD3	1.85	0.43
1:B:240:GLU:OE2	1:B:241:ARG:NH2	2.51	0.43
1:A:236:GLU:OE1	1:A:236:GLU:HA	2.19	0.43
1:A:252:LEU:HD21	1:A:255:ILE:HD13	2.01	0.43
1:D:181:ASN:HD22	1:D:181:ASN:HA	1.52	0.43
1:D:193:MET:HE3	1:D:219:LEU:HD22	2.01	0.43
1:B:203:ASP:O	1:B:231:VAL:HA	2.19	0.43
1:A:256:ASN:ND2	1:A:260:LYS:N	2.67	0.43
1:A:262:ILE:CG1	1:A:264:ILE:CD1	2.97	0.42
1:C:157:VAL:HG21	1:C:193:MET:HG3	1.99	0.42
1:C:74:LYS:HE3	1:C:74:LYS:HB3	1.83	0.42
1:A:269:PHE:CE1	1:A:270:LEU:HD13	2.55	0.42
1:D:5:ARG:O	1:D:5:ARG:HG2	2.20	0.42
1:A:104:TYR:CZ	1:A:106:THR:HB	2.55	0.42
1:C:255:ILE:CG2	1:C:256:ASN:N	2.83	0.42
1:B:167:GLU:HB3	1:B:168:GLY:H	1.58	0.42
1:D:173:ILE:HA	1:D:173:ILE:HD13	1.80	0.42
1:D:209:GLY:O	1:D:213:ASN:HB2	2.20	0.42
1:C:54:GLN:HG3	1:D:11:ASP:OD1	2.19	0.42
1:A:49:GLN:HB3	3:A:682:HOH:O	2.18	0.42
1:C:256:ASN:OD1	1:C:259:GLU:N	2.53	0.42
1:C:138:ALA:HA	1:C:139:THR:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLY:O	1:A:102:TYR:CB	2.56	0.42
1:C:143:PRO:HB3	1:D:146:TYR:CZ	2.54	0.42
1:D:186:MET:HG3	3:D:705:HOH:O	2.20	0.42
1:A:256:ASN:O	1:A:257:MET:CE	2.67	0.41
1:B:125:VAL:HG21	1:B:247:MET:SD	2.60	0.41
1:A:92:ALA:O	1:A:262:ILE:HG23	2.19	0.41
1:A:140:LYS:HE2	1:A:140:LYS:HB2	1.42	0.41
1:C:26:LEU:HB3	1:C:37:LYS:HG2	2.02	0.41
1:C:259:GLU:O	1:C:260:LYS:C	2.59	0.41
1:A:256:ASN:ND2	1:A:260:LYS:H	2.17	0.41
1:C:258:LYS:HB3	1:C:258:LYS:HE2	1.36	0.41
1:C:52:GLU:HG3	3:C:730:HOH:O	2.20	0.41
1:D:218:LEU:HD22	3:D:705:HOH:O	2.21	0.41
1:C:159:VAL:CG1	1:C:186:MET:HB2	2.51	0.41
1:C:8:ARG:HD3	3:C:735:HOH:O	2.20	0.41
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.76	0.41
1:B:256:ASN:HD22	1:B:259:GLU:HB3	1.85	0.41
1:D:26:LEU:HA	1:D:26:LEU:HD12	1.96	0.41
1:D:24:ILE:HA	1:D:25:PRO:HD3	1.93	0.41
1:C:108:ILE:HG23	1:C:114:VAL:HG11	2.03	0.41
1:D:204:ASP:O	1:D:232:LEU:HB3	2.20	0.41
1:C:26:LEU:HA	1:C:26:LEU:HD12	1.87	0.41
1:C:123:ALA:HB1	1:C:152:LEU:HD13	2.02	0.41
1:C:111:LYS:HG3	1:C:112:PRO:HD2	2.01	0.40
1:C:61:THR:HG23	3:C:632:HOH:O	2.21	0.40
1:A:118:VAL:CG1	1:A:144:LEU:HD11	2.51	0.40
1:C:255:ILE:HG22	1:C:256:ASN:N	2.37	0.40
1:D:93:ASN:HD22	1:D:94:PRO:HD2	1.87	0.40
1:D:243:VAL:HG22	1:D:243:VAL:O	2.21	0.40
1:C:2:LYS:HD2	1:C:2:LYS:HA	1.86	0.40
1:B:254:THR:HB	1:B:263:GLU:HB2	2.04	0.40
1:A:59:LEU:HD12	1:A:59:LEU:HA	1.93	0.40
1:C:93:ASN:HA	1:C:94:PRO:HD2	1.88	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	265/285 (93%)	247 (93%)	12 (4%)	6 (2%)	8	4
1	B	264/285 (93%)	257 (97%)	6 (2%)	1 (0%)	39	41
1	C	265/285 (93%)	254 (96%)	8 (3%)	3 (1%)	17	14
1	D	264/285 (93%)	249 (94%)	10 (4%)	5 (2%)	10	6
All	All	1058/1140 (93%)	1007 (95%)	36 (3%)	15 (1%)	14	10

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	TYR
1	A	239	ASP
1	A	244	ASP
1	A	256	ASN
1	A	259	GLU
1	B	244	ASP
1	C	162	ASP
1	C	260	LYS
1	D	243	VAL
1	C	258	LYS
1	A	254	THR
1	D	244	ASP
1	D	254	THR
1	D	258	LYS
1	D	259	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	230/244 (94%)	198 (86%)	32 (14%)	4	3
1	B	228/244 (93%)	208 (91%)	20 (9%)	12	11
1	C	229/244 (94%)	199 (87%)	30 (13%)	5	4
1	D	228/244 (93%)	189 (83%)	39 (17%)	2	1
All	All	915/976 (94%)	794 (87%)	121 (13%)	5	3

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	4	ARG
1	A	5	ARG
1	A	6	SER
1	A	90	SER
1	A	91	LEU
1	A	98	LEU
1	A	102	TYR
1	A	108	ILE
1	A	117	LYS
1	A	130	GLU
1	A	140	LYS
1	A	152	LEU
1	A	162	ASP
1	A	173	ILE
1	A	179	SER
1	A	180	SER
1	A	182	ARG
1	A	193	MET
1	A	205	PHE
1	A	206	MET
1	A	241	ARG
1	A	242	LEU
1	A	244	ASP
1	A	245	GLU
1	A	252	LEU
1	A	255	ILE
1	A	257	MET
1	A	259	GLU
1	A	262	ILE
1	A	266	ASN

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Mol	Chain	Res	Type
1	A	270	LEU
1	B	2	LYS
1	B	4	ARG
1	B	5	ARG
1	B	26	LEU
1	B	59	LEU
1	B	121	LEU
1	B	130	GLU
1	B	133	VAL
1	B	140	LYS
1	B	144	LEU
1	B	152	LEU
1	B	181	ASN
1	B	194	LYS
1	B	220	ASP
1	B	223	ASN
1	B	241	ARG
1	B	258	LYS
1	B	259	GLU
1	B	260	LYS
1	B	270	LEU
1	C	5	ARG
1	C	26	LEU
1	C	59	LEU
1	C	82	GLU
1	C	90	SER
1	C	103	VAL
1	C	108	ILE
1	C	111	LYS
1	C	113	SER
1	C	128	GLU
1	C	133	VAL
1	C	152	LEU
1	C	161	LYS
1	C	162	ASP
1	C	180	SER
1	C	182	ARG
1	C	194	LYS
1	C	195	THR
1	C	218	LEU
1	C	220	ASP
1	C	223	ASN

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Mol	Chain	Res	Type
1	C	240	GLU
1	C	241	ARG
1	C	244	ASP
1	C	253	SER
1	C	256	ASN
1	C	257	MET
1	C	258	LYS
1	C	260	LYS
1	C	270	LEU
1	D	2	LYS
1	D	6	SER
1	D	9	LEU
1	D	39	SER
1	D	49	GLN
1	D	52	GLU
1	D	53	GLN
1	D	60	LEU
1	D	85	GLN
1	D	90	SER
1	D	93	ASN
1	D	96	ARG
1	D	98	LEU
1	D	103	VAL
1	D	108	ILE
1	D	116	SER
1	D	130	GLU
1	D	144	LEU
1	D	152	LEU
1	D	161	LYS
1	D	167	GLU
1	D	173	ILE
1	D	180	SER
1	D	181	ASN
1	D	207	LYS
1	D	213	ASN
1	D	239	ASP
1	D	241	ARG
1	D	242	LEU
1	D	253	SER
1	D	254	THR
1	D	255	ILE
1	D	256	ASN

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Mol	Chain	Res	Type
1	D	257	MET
1	D	258	LYS
1	D	260	LYS
1	D	263	GLU
1	D	270	LEU
1	D	271	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	77	GLN
1	A	153	ASN
1	A	217	ASN
1	A	256	ASN
1	A	266	ASN
1	A	276	ASN
1	B	54	GLN
1	B	77	GLN
1	B	89	GLN
1	B	184	GLN
1	B	213	ASN
1	B	217	ASN
1	B	256	ASN
1	B	266	ASN
1	C	53	GLN
1	C	54	GLN
1	C	77	GLN
1	C	89	GLN
1	C	163	ASN
1	C	184	GLN
1	C	217	ASN
1	C	266	ASN
1	D	54	GLN
1	D	77	GLN
1	D	89	GLN
1	D	181	ASN
1	D	217	ASN
1	D	223	ASN
1	D	266	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 ⓘ

4 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	$\# Z > 2$
2	PCP	A	604	-	20,22,22	0.64	0	31,35,35	1.65	6 (19%)
2	PCP	B	605	-	20,22,22	0.64	0	31,35,35	1.35	4 (12%)
2	PCP	C	606	-	20,22,22	0.66	0	31,35,35	1.49	4 (12%)
2	PCP	D	607	-	20,22,22	0.61	0	31,35,35	1.59	6 (19%)

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	PCP	A	604	-	2/2/7/7	0/17/33/33	0/1/1/1
2	PCP	B	605	-	2/2/7/7	0/17/33/33	0/1/1/1
2	PCP	C	606	-	2/2/7/7	0/17/33/33	0/1/1/1
2	PCP	D	607	-	2/2/7/7	0/17/33/33	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	606	PCP	PA-O3A-PB	-3.32	121.55	132.67
2	A	604	PCP	PA-O3A-PB	-3.30	121.61	132.67
2	B	605	PCP	PA-O3A-PB	-3.21	121.90	132.67
2	D	607	PCP	PA-O3A-PB	-3.21	121.90	132.67
2	C	606	PCP	C5-C1-C2	2.08	107.23	103.44
2	C	606	PCP	C5-C4-C3	2.14	107.40	102.24
2	B	605	PCP	C3-C2-C1	2.16	107.06	102.61
2	B	605	PCP	C4-C5-C1	2.19	107.16	103.73
2	A	604	PCP	C4-C5-C1	2.37	107.44	103.73
2	D	607	PCP	C5-C1-C2	2.43	107.87	103.44
2	D	607	PCP	C5-C4-C3	2.44	108.13	102.24
2	A	604	PCP	C3-C2-C1	2.47	107.68	102.61
2	A	604	PCP	C5-C4-C3	2.50	108.28	102.24
2	D	607	PCP	C4-C5-C1	2.59	107.78	103.73
2	D	607	PCP	C3-C2-C1	2.78	108.33	102.61
2	A	604	PCP	C5-C1-C2	2.82	108.58	103.44
2	B	605	PCP	C4-C3-C2	3.05	106.32	103.50
2	D	607	PCP	C4-C3-C2	4.64	107.78	103.50
2	A	604	PCP	C4-C3-C2	4.86	107.99	103.50
2	C	606	PCP	C4-C3-C2	5.02	108.13	103.50

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	605	PCP	C2
2	B	605	PCP	C3
2	C	606	PCP	C2
2	C	606	PCP	C3
2	D	607	PCP	C2
2	D	607	PCP	C3
2	A	604	PCP	C2
2	A	604	PCP	C3

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	605	PCP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	606	PCP	2	0
2	D	607	PCP	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	269/285 (94%)	0.29	21 (7%) 16 15	12, 25, 62, 74	0
1	B	268/285 (94%)	0.04	15 (5%) 28 27	12, 23, 47, 62	0
1	C	269/285 (94%)	0.13	17 (6%) 23 22	13, 25, 49, 75	0
1	D	268/285 (94%)	0.28	26 (9%) 10 9	13, 26, 59, 78	0
All	All	1074/1140 (94%)	0.19	79 (7%) 17 17	12, 25, 54, 78	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	VAL	12.4
1	C	257	MET	12.0
1	A	257	MET	8.2
1	A	239	ASP	7.5
1	D	241	ARG	6.9
1	D	255	ILE	6.6
1	C	258	LYS	6.4
1	D	257	MET	6.0
1	A	240	GLU	5.4
1	A	179	SER	5.3
1	A	255	ILE	5.2
1	D	179	SER	5.2
1	D	258	LYS	5.1
1	A	101	GLY	5.0
1	D	242	LEU	5.0
1	D	259	GLU	4.5
1	D	180	SER	4.5
1	B	258	LYS	4.5
1	C	259	GLU	4.5
1	A	258	LYS	4.3
1	C	254	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	GLY	4.2
1	A	99	PRO	4.2
1	D	182	ARG	4.1
1	A	181	ASN	4.0
1	A	102	TYR	3.9
1	C	260	LYS	3.8
1	D	181	ASN	3.8
1	B	257	MET	3.7
1	D	254	THR	3.7
1	B	162	ASP	3.6
1	D	260	LYS	3.6
1	C	256	ASN	3.6
1	A	182	ARG	3.6
1	C	162	ASP	3.4
1	C	261	SER	3.4
1	C	255	ILE	3.3
1	D	162	ASP	3.3
1	A	178	GLY	3.2
1	A	183	ILE	3.2
1	D	177	SER	3.2
1	A	98	LEU	3.2
1	D	183	ILE	3.1
1	B	167	GLU	3.1
1	B	169	SER	3.1
1	C	168	GLY	3.1
1	D	256	ASN	3.1
1	B	168	GLY	3.0
1	D	100	GLY	3.0
1	D	243	VAL	3.0
1	D	102	TYR	3.0
1	C	167	GLU	2.8
1	D	178	GLY	2.7
1	D	97	ILE	2.7
1	D	101	GLY	2.7
1	A	244	ASP	2.6
1	B	260	LYS	2.6
1	A	260	LYS	2.6
1	C	92	ALA	2.3
1	D	146	TYR	2.3
1	B	142	ILE	2.3
1	A	147	ALA	2.3
1	C	241	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	65	ALA	2.3
1	D	168	GLY	2.2
1	B	156	VAL	2.2
1	B	202	ILE	2.2
1	B	241	ARG	2.2
1	D	239	ASP	2.2
1	C	97	ILE	2.2
1	B	94	PRO	2.1
1	A	162	ASP	2.1
1	B	101	GLY	2.1
1	B	146	TYR	2.1
1	D	85	GLN	2.1
1	A	242	LEU	2.1
1	C	115	LEU	2.1
1	B	147	ALA	2.0
1	C	147	ALA	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(\AA^2)	Q<0.9
2	PCP	C	606	22/22	0.85	0.41	6.16	43,93,100,102	22
2	PCP	A	604	22/22	0.71	0.53	4.33	109,120,125,126	22
2	PCP	B	605	22/22	0.94	0.21	2.82	41,77,82,82	13
2	PCP	D	607	22/22	0.86	0.35	2.13	74,108,112,112	22

6.5 Other polymers

There are no such residues in this entry.