



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:52 pm GMT

PDB ID : 2OX8
Title : Human Scavenger Receptor C-type Lectin carbohydrate-recognition domain.
Authors : Weis, W.I.; Feinberg, H.; Drickamer, K.; Taylor, M.E.
Deposited on : 2007-02-20
Resolution : 2.50 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

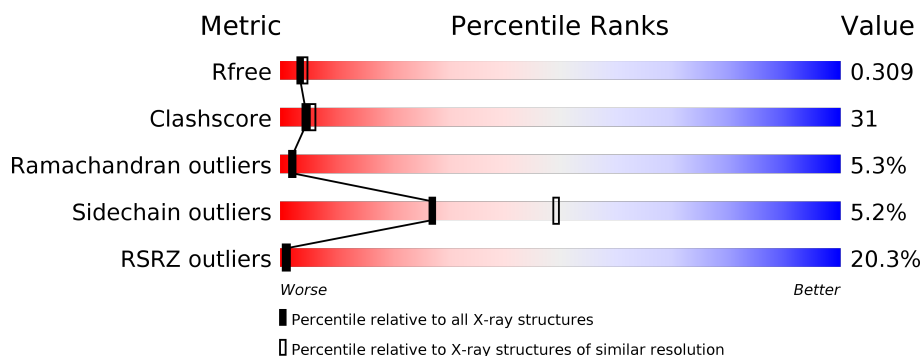
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	140	<div> <div>46%</div> <div>41%</div> <div>5%</div> <div>8%</div> </div>
1	B	140	<div> <div>48%</div> <div>41%</div> <div>•</div> <div>8%</div> </div>
1	C	140	<div> <div>33%</div> <div>34%</div> <div>49%</div> <div>9%</div> <div>8%</div> </div>
1	D	140	<div> <div>41%</div> <div>43%</div> <div>39%</div> <div>9%</div> <div>•</div> <div>8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4379 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 Scavenger receptor with C-type lectin type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1078	681	184	206	7			
1	B	129	Total	C	N	O	S	0	0	0
			1078	681	184	206	7			
1	C	129	Total	C	N	O	S	0	0	0
			1078	681	184	206	7			
1	D	129	Total	C	N	O	S	0	0	0
			1078	681	184	206	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	5	Total	Zn	0	0
			5	5		
2	D	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Cl	0	0
			3	3		
3	A	3	Total	Cl	0	0
			3	3		
3	D	3	Total	Cl	0	0
			3	3		
3	C	3	Total	Cl	0	0
			3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	Ca 3	0	0
4	C	3	Total 3	Ca 3	0	0

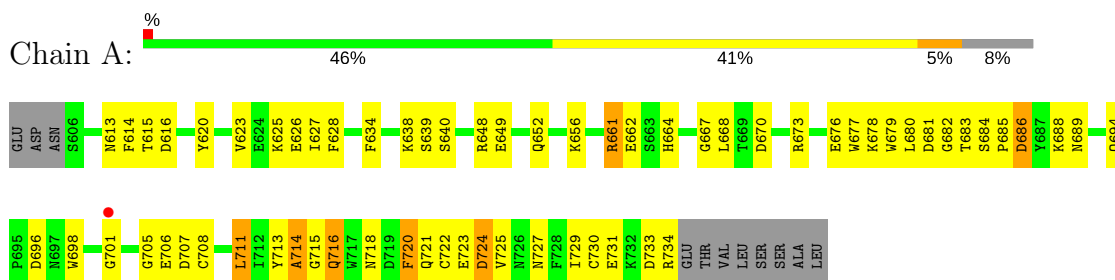
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total 21	O 21	0	0
5	B	10	Total 10	O 10	0	0
5	C	1	Total 1	O 1	0	0
5	D	1	Total 1	O 1	0	0

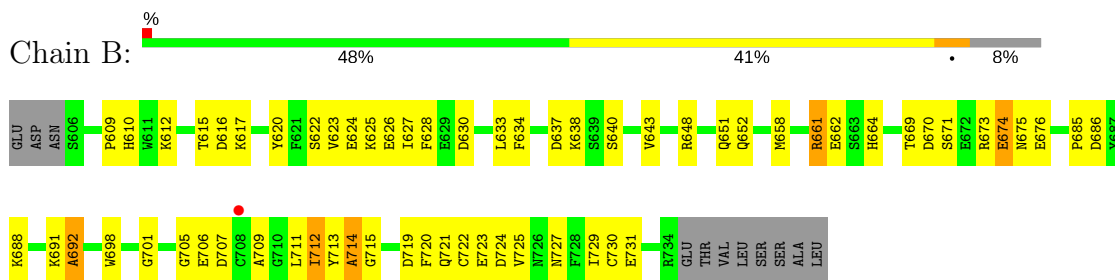
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

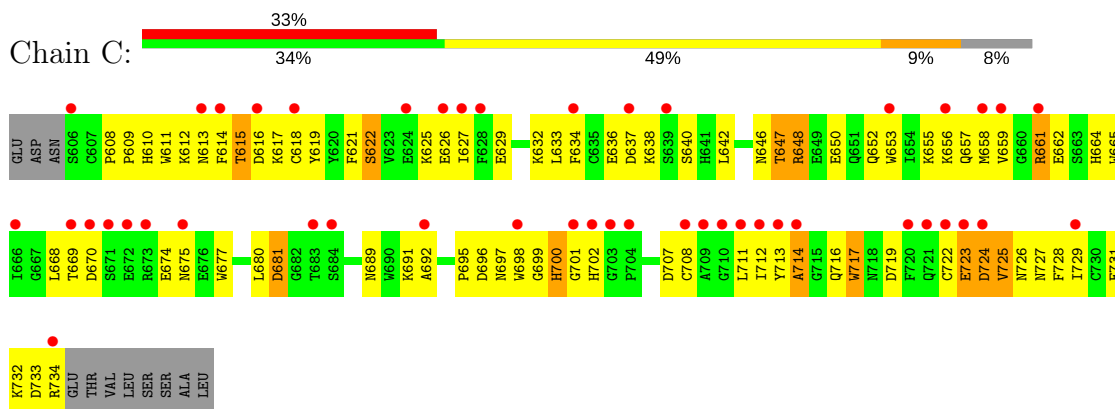
• Molecule 1: Scavenger receptor with C-type lectin type I



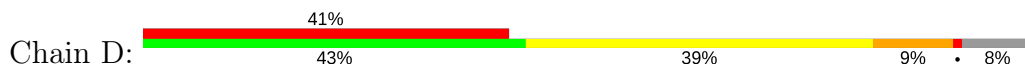
• Molecule 1: Scavenger receptor with C-type lectin type I

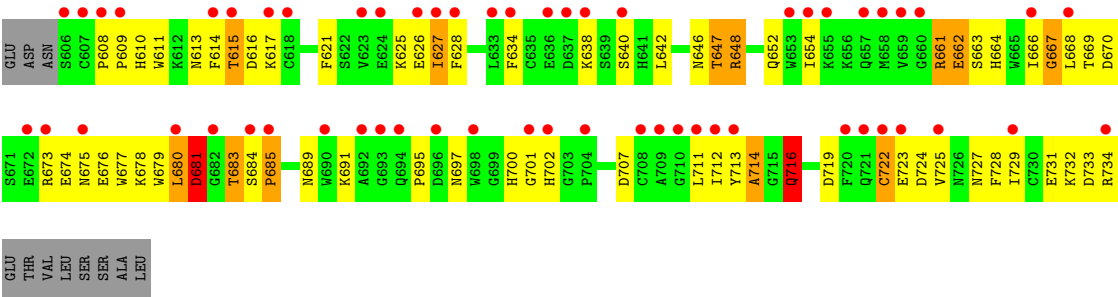


• Molecule 1: Scavenger receptor with C-type lectin type I



• Molecule 1: Scavenger receptor with C-type lectin type I





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	80.42Å 80.42Å 67.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.92 – 2.50 30.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.92-2.50) 98.4 (30.91-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.308 0.236 , 0.309	Depositor DCC
R_{free} test set	840 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.470 for -h,-k,l 0.107 for h,-h-k,-l 0.107 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4379	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 4.66% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, CL

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	0.46	0/1114	0.71	0/1507
1	B	0.45	0/1114	0.68	0/1507
1	C	0.31	0/1114	0.51	0/1507
1	D	0.30	0/1114	0.51	0/1507
All	All	0.39	0/4456	0.61	0/6028

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	1078	0	964	57	0
1	B	1078	0	964	70	0
1	C	1078	0	964	81	0
1	D	1078	0	964	59	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	21	0	0	0	0
5	B	10	0	0	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	4379	0	3856	258	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 31.

All (258) 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:A:615:THR:HG22	1:A:616:ASP:H	1.11	1.15
1:C:615:THR:HG22	1:C:616:ASP:H	1.25	1.01
1:B:669:THR:HG22	1:B:671:SER:H	1.28	0.98
1:C:668:LEU:HD11	1:C:677:TRP:HB3	1.47	0.97
1:A:615:THR:HG22	1:A:616:ASP:N	1.78	0.96
1:B:615:THR:HG22	1:B:616:ASP:H	1.32	0.94
1:A:623:VAL:HG21	1:C:702:HIS:ND1	1.86	0.90
1:B:625:LYS:HB3	1:B:725:VAL:HG12	1.50	0.90
1:A:706:GLU:HA	1:A:721:GLN:HA	1.52	0.89
1:C:627:ILE:HG23	1:C:723:GLU:HA	1.54	0.87
1:B:615:THR:HG22	1:B:616:ASP:N	1.88	0.87
1:C:613:ASN:HD22	1:C:734:ARG:HH12	1.24	0.83
1:D:691:LYS:HB2	1:D:716:GLN:HG3	1.63	0.81
1:C:677:TRP:HE1	1:C:695:PRO:HG3	1.46	0.79
1:C:691:LYS:HG2	1:C:692:ALA:H	1.48	0.79
1:B:623:VAL:HG21	1:D:702:HIS:ND1	1.98	0.78
1:B:661:ARG:HG2	1:B:661:ARG:HH11	1.48	0.78
1:D:668:LEU:HD11	1:D:677:TRP:HB3	1.65	0.77
1:A:625:LYS:HB3	1:A:725:VAL:HG12	1.66	0.77
1:A:661:ARG:HG2	1:A:661:ARG:HH11	1.49	0.76
1:C:615:THR:HG22	1:C:616:ASP:N	2.00	0.75
1:D:625:LYS:O	1:D:626:GLU:HG3	1.87	0.74
1:B:661:ARG:HA	1:B:713:TYR:CD1	2.23	0.74
1:C:661:ARG:HG3	1:C:713:TYR:HD2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:SER:HB2	1:A:731:GLU:O	1.88	0.73
1:C:648:ARG:O	1:C:652:GLN:HG3	1.88	0.73
1:C:625:LYS:HG2	1:C:727:ASN:OD1	1.88	0.72
1:C:627:ILE:CG2	1:C:723:GLU:HA	2.20	0.71
1:B:624:GLU:HG2	1:B:625:LYS:N	2.06	0.71
1:A:615:THR:CG2	1:A:616:ASP:N	2.53	0.70
1:A:721:GLN:O	1:A:724:ASP:HB2	1.90	0.70
1:C:613:ASN:HD22	1:C:734:ARG:NH1	1.90	0.69
1:C:677:TRP:NE1	1:C:695:PRO:HG3	2.07	0.69
1:D:648:ARG:O	1:D:652:GLN:HG3	1.93	0.69
1:A:652:GLN:O	1:A:656:LYS:HG2	1.94	0.68
1:B:648:ARG:O	1:B:652:GLN:HG3	1.94	0.68
1:A:686:ASP:O	1:A:688:LYS:HG3	1.94	0.67
1:A:678:LYS:HD3	1:A:682:GLY:O	1.94	0.67
1:C:613:ASN:HD21	1:C:734:ARG:HH22	1.43	0.67
1:B:721:GLN:HB3	1:B:724:ASP:OD2	1.94	0.67
1:B:706:GLU:HA	1:B:721:GLN:HA	1.77	0.67
1:C:664:HIS:HA	1:C:727:ASN:O	1.94	0.66
1:C:613:ASN:ND2	1:C:734:ARG:HH12	1.93	0.66
1:A:613:ASN:HD22	1:A:734:ARG:HH12	1.44	0.66
1:D:625:LYS:HB3	1:D:725:VAL:HG12	1.78	0.66
1:A:627:ILE:HG12	1:A:723:GLU:HA	1.77	0.66
1:B:686:ASP:O	1:B:688:LYS:HD2	1.95	0.65
1:A:713:TYR:O	1:A:714:ALA:CB	2.44	0.65
1:B:692:ALA:HB1	1:B:698:TRP:CH2	2.32	0.64
1:C:691:LYS:HG2	1:C:692:ALA:N	2.12	0.64
1:B:713:TYR:O	1:B:714:ALA:CB	2.45	0.64
1:B:669:THR:HG23	1:B:707:ASP:O	1.96	0.64
1:B:624:GLU:HG2	1:B:625:LYS:H	1.63	0.63
1:B:669:THR:HG22	1:B:670:ASP:N	2.13	0.63
1:D:634:PHE:O	1:D:638:LYS:HG2	1.98	0.63
1:A:648:ARG:HG3	1:A:649:GLU:OE1	1.98	0.63
1:C:716:GLN:CD	1:C:716:GLN:H	2.03	0.62
1:C:722:CYS:O	1:C:723:GLU:HB2	1.99	0.62
1:B:664:HIS:HA	1:B:727:ASN:O	1.99	0.61
1:A:634:PHE:O	1:A:638:LYS:HG2	2.01	0.61
1:A:689:ASN:ND2	1:A:716:GLN:HA	2.17	0.60
1:A:625:LYS:CB	1:A:725:VAL:HG12	2.31	0.60
1:C:669:THR:HB	1:C:707:ASP:O	2.00	0.60
1:A:670:ASP:HB3	1:A:677:TRP:CE2	2.36	0.59
1:A:711:LEU:HD21	1:A:715:GLY:HA2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:LYS:HB2	1:C:725:VAL:CG1	2.31	0.59
1:D:689:ASN:ND2	1:D:716:GLN:HA	2.17	0.59
1:A:623:VAL:HG21	1:C:702:HIS:CE1	2.36	0.59
1:D:609:PRO:O	1:D:610:HIS:HB2	2.01	0.58
1:D:617:LYS:HG2	1:D:733:ASP:HA	1.84	0.58
1:B:722:CYS:O	1:B:723:GLU:HB2	2.03	0.58
1:D:613:ASN:HD21	1:D:734:ARG:CZ	2.16	0.58
1:B:626:GLU:HB3	1:B:630:ASP:CB	2.33	0.58
1:A:694:GLN:NE2	1:A:718:ASN:OD1	2.37	0.58
1:C:646:ASN:O	1:C:647:THR:HG23	2.03	0.58
1:D:673:ARG:HB2	1:D:676:GLU:OE2	2.04	0.58
1:B:640:SER:HB2	1:B:731:GLU:O	2.03	0.57
1:C:664:HIS:HB3	1:C:729:ILE:HG13	1.85	0.57
1:B:609:PRO:O	1:B:610:HIS:HB2	2.03	0.57
1:C:613:ASN:ND2	1:C:734:ARG:NH1	2.52	0.57
1:B:661:ARG:NH1	1:B:661:ARG:HG2	2.16	0.57
1:A:722:CYS:C	1:A:724:ASP:H	2.08	0.57
1:D:615:THR:HG22	1:D:616:ASP:H	1.68	0.57
1:D:697:ASN:ND2	1:D:700:HIS:HB3	2.19	0.57
1:D:627:ILE:HA	1:D:724:ASP:O	2.05	0.56
1:C:713:TYR:O	1:C:714:ALA:HB2	2.05	0.56
1:D:615:THR:HG22	1:D:616:ASP:N	2.21	0.56
1:D:669:THR:HB	1:D:707:ASP:O	2.05	0.56
1:C:609:PRO:O	1:C:610:HIS:HB2	2.06	0.56
1:D:627:ILE:HG22	1:D:628:PHE:N	2.21	0.56
1:D:679:TRP:HE1	1:D:685:PRO:HA	1.71	0.56
1:D:722:CYS:O	1:D:723:GLU:HB2	2.06	0.56
1:B:658:MET:SD	1:B:711:LEU:HD12	2.46	0.56
1:C:661:ARG:HD2	1:C:661:ARG:N	2.21	0.55
1:A:698:TRP:CE3	1:B:615:THR:HG23	2.40	0.55
1:D:608:PRO:O	1:D:611:TRP:HB2	2.06	0.55
1:C:634:PHE:CZ	1:C:638:LYS:HE2	2.41	0.55
1:A:620:TYR:HB3	1:A:730:CYS:HB2	1.89	0.54
1:C:608:PRO:O	1:C:611:TRP:HB2	2.07	0.54
1:D:713:TYR:O	1:D:714:ALA:HB2	2.07	0.54
1:D:666:ILE:O	1:D:668:LEU:N	2.39	0.54
1:C:661:ARG:HH11	1:C:661:ARG:HG2	1.72	0.54
1:A:625:LYS:HE2	1:C:698:TRP:CE2	2.43	0.54
1:B:722:CYS:C	1:B:724:ASP:H	2.11	0.54
1:A:661:ARG:NH1	1:A:661:ARG:HG2	2.21	0.54
1:B:615:THR:CG2	1:B:616:ASP:N	2.62	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:SER:CB	1:C:732:LYS:HB3	2.37	0.54
1:D:722:CYS:C	1:D:724:ASP:H	2.10	0.54
1:B:673:ARG:HD2	1:B:676:GLU:CD	2.28	0.54
1:A:670:ASP:OD1	1:A:707:ASP:HB3	2.08	0.53
1:B:633:LEU:O	1:B:637:ASP:OD2	2.26	0.53
1:D:664:HIS:HB3	1:D:728:PHE:HA	1.89	0.53
1:D:664:HIS:ND1	1:D:729:ILE:HG13	2.23	0.53
1:A:628:PHE:CD1	1:A:708:CYS:HB3	2.44	0.53
1:D:670:ASP:OD1	1:D:707:ASP:HA	2.09	0.53
1:A:613:ASN:ND2	1:A:734:ARG:HH12	2.04	0.53
1:A:625:LYS:O	1:A:626:GLU:CG	2.56	0.53
1:C:622:SER:HB3	1:C:728:PHE:CE1	2.44	0.53
1:B:626:GLU:HB3	1:B:630:ASP:HB3	1.89	0.53
1:D:642:LEU:HD12	1:D:680:LEU:HD11	1.91	0.53
1:C:615:THR:HG22	1:C:616:ASP:OD1	2.10	0.52
1:B:661:ARG:HG3	1:B:713:TYR:CG	2.44	0.52
1:A:713:TYR:O	1:A:714:ALA:HB3	2.10	0.52
1:A:613:ASN:HD21	1:A:734:ARG:HH22	1.56	0.52
1:A:705:GLY:C	1:A:721:GLN:HG3	2.30	0.52
1:B:625:LYS:CB	1:B:725:VAL:HG12	2.33	0.52
1:D:661:ARG:N	1:D:661:ARG:HD2	2.25	0.51
1:D:674:GLU:O	1:D:675:ASN:HB2	2.09	0.51
1:D:691:LYS:CB	1:D:716:GLN:HG3	2.38	0.51
1:A:720:PHE:N	1:A:720:PHE:CD1	2.78	0.51
1:B:669:THR:CG2	1:B:670:ASP:N	2.73	0.51
1:C:661:ARG:HG3	1:C:713:TYR:CD2	2.39	0.51
1:B:634:PHE:O	1:B:638:LYS:HE2	2.09	0.51
1:B:709:ALA:HA	1:B:719:ASP:HA	1.91	0.51
1:C:722:CYS:O	1:C:723:GLU:CB	2.57	0.51
1:D:615:THR:HG22	1:D:616:ASP:OD1	2.11	0.51
1:C:711:LEU:HD23	1:C:712:ILE:O	2.10	0.51
1:B:623:VAL:HG21	1:D:702:HIS:CE1	2.45	0.50
1:D:663:SER:HB3	1:D:712:ILE:HG22	1.93	0.50
1:C:640:SER:HB2	1:C:731:GLU:O	2.12	0.50
1:B:720:PHE:N	1:B:720:PHE:CD1	2.80	0.50
1:C:724:ASP:O	1:C:725:VAL:C	2.50	0.50
1:B:670:ASP:O	1:B:674:GLU:HA	2.12	0.50
1:C:689:ASN:ND2	1:C:716:GLN:HA	2.26	0.49
1:B:692:ALA:HB1	1:B:698:TRP:CZ2	2.47	0.49
1:D:613:ASN:ND2	1:D:734:ARG:CZ	2.75	0.49
1:A:698:TRP:CD2	1:B:615:THR:HG23	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:LYS:HG2	1:B:692:ALA:H	1.78	0.49
1:D:676:GLU:OE1	1:D:678:LYS:HE3	2.13	0.49
1:B:705:GLY:O	1:B:721:GLN:HA	2.13	0.49
1:C:632:LYS:O	1:C:636:GLU:HG3	2.13	0.48
1:B:617:LYS:HD3	1:B:731:GLU:OE1	2.14	0.48
1:B:721:GLN:HG2	1:B:722:CYS:O	2.14	0.48
1:A:698:TRP:CD1	1:B:616:ASP:HB3	2.48	0.48
1:C:640:SER:HB3	1:C:732:LYS:HD3	1.96	0.48
1:D:663:SER:HA	1:D:711:LEU:O	2.14	0.48
1:C:664:HIS:CE1	1:C:727:ASN:HB3	2.49	0.48
1:B:620:TYR:HB3	1:B:730:CYS:HB2	1.96	0.48
1:B:627:ILE:HG23	1:B:723:GLU:H	1.78	0.48
1:C:653:TRP:O	1:C:657:GLN:HG2	2.14	0.47
1:C:717:TRP:CD1	1:C:717:TRP:N	2.82	0.47
1:D:680:LEU:O	1:D:681:ASP:HB3	2.14	0.47
1:C:711:LEU:HD23	1:C:711:LEU:C	2.35	0.47
1:D:695:PRO:HA	1:D:719:ASP:OD1	2.13	0.47
1:A:733:ASP:OD1	1:A:734:ARG:O	2.33	0.47
1:B:721:GLN:HE21	1:B:723:GLU:HB2	1.79	0.47
1:D:646:ASN:O	1:D:647:THR:HG23	2.14	0.47
1:A:683:THR:HG22	1:A:684:SER:N	2.29	0.47
1:D:683:THR:HG22	1:D:684:SER:N	2.29	0.47
1:B:627:ILE:O	1:B:628:PHE:C	2.52	0.47
1:C:689:ASN:O	1:C:716:GLN:HA	2.14	0.47
1:C:699:GLY:C	1:C:701:GLY:H	2.17	0.47
1:C:619:TYR:CD1	1:C:619:TYR:N	2.83	0.47
1:C:712:ILE:HG12	1:C:716:GLN:O	2.14	0.47
1:C:626:GLU:HB2	1:C:728:PHE:HE2	1.79	0.47
1:C:634:PHE:O	1:C:638:LYS:HG2	2.14	0.47
1:C:697:ASN:ND2	1:C:700:HIS:HB3	2.29	0.47
1:B:713:TYR:O	1:B:714:ALA:HB3	2.14	0.46
1:C:677:TRP:CH2	1:C:719:ASP:HB3	2.51	0.46
1:C:622:SER:HB3	1:C:728:PHE:CD1	2.51	0.46
1:D:662:GLU:OE2	1:D:664:HIS:NE2	2.44	0.46
1:C:655:LYS:HD3	1:C:656:LYS:NZ	2.31	0.46
1:B:721:GLN:C	1:B:722:CYS:O	2.52	0.46
1:B:626:GLU:HB3	1:B:630:ASP:HB2	1.96	0.46
1:B:711:LEU:HD11	1:B:715:GLY:HA2	1.98	0.46
1:D:616:ASP:OD2	1:D:733:ASP:OD2	2.34	0.46
1:B:674:GLU:O	1:B:675:ASN:CB	2.64	0.46
1:B:691:LYS:HG2	1:B:692:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:ILE:CD1	1:B:720:PHE:HZ	2.28	0.46
1:B:722:CYS:O	1:B:723:GLU:CB	2.64	0.46
1:C:617:LYS:HD3	1:C:731:GLU:OE2	2.15	0.46
1:C:647:THR:O	1:C:650:GLU:HB3	2.15	0.46
1:C:629:GLU:O	1:C:633:LEU:HG	2.16	0.45
1:A:673:ARG:HD2	1:A:676:GLU:OE2	2.16	0.45
1:A:625:LYS:O	1:A:626:GLU:HG3	2.17	0.45
1:A:648:ARG:O	1:A:652:GLN:HG3	2.16	0.45
1:B:651:GLN:HE22	1:B:711:LEU:HD21	1.82	0.45
1:B:685:PRO:O	1:B:688:LYS:HE3	2.16	0.45
1:A:664:HIS:HA	1:A:727:ASN:O	2.16	0.45
1:B:673:ARG:NH1	1:B:676:GLU:OE1	2.49	0.45
1:D:664:HIS:HA	1:D:727:ASN:O	2.16	0.45
1:A:614:PHE:O	1:A:615:THR:HB	2.17	0.45
1:B:705:GLY:HA3	1:B:721:GLN:HG3	1.98	0.45
1:C:648:ARG:HH11	1:C:648:ARG:HG2	1.82	0.45
1:D:640:SER:HB2	1:D:731:GLU:O	2.17	0.44
1:D:697:ASN:HD21	1:D:700:HIS:HB3	1.81	0.44
1:B:721:GLN:O	1:B:724:ASP:HB2	2.18	0.44
1:C:716:GLN:CD	1:C:716:GLN:N	2.70	0.44
1:D:667:GLY:O	1:D:679:TRP:HA	2.17	0.44
1:C:674:GLU:O	1:C:675:ASN:HB2	2.17	0.44
1:C:725:VAL:O	1:C:726:ASN:OD1	2.36	0.44
1:B:712:ILE:HD13	1:B:720:PHE:HZ	1.82	0.43
1:C:680:LEU:O	1:C:681:ASP:HB3	2.18	0.43
1:A:681:ASP:C	1:A:681:ASP:OD1	2.56	0.43
1:A:623:VAL:HG11	1:C:702:HIS:HB2	2.01	0.43
1:B:643:VAL:HB	1:B:729:ILE:HG22	2.01	0.43
1:A:667:GLY:O	1:A:679:TRP:HA	2.19	0.43
1:C:658:MET:SD	1:C:711:LEU:HD22	2.59	0.43
1:A:679:TRP:NE1	1:A:685:PRO:HB3	2.34	0.43
1:C:613:ASN:ND2	1:C:734:ARG:HH22	2.14	0.43
1:A:661:ARG:NH1	1:A:661:ARG:CG	2.82	0.43
1:A:720:PHE:H	1:A:720:PHE:HD1	1.67	0.43
1:D:613:ASN:ND2	1:D:734:ARG:NH1	2.68	0.42
1:B:674:GLU:O	1:B:675:ASN:HB3	2.18	0.42
1:C:612:LYS:O	1:C:618:CYS:HA	2.18	0.42
1:C:614:PHE:O	1:C:615:THR:HB	2.20	0.42
1:A:722:CYS:C	1:A:724:ASP:N	2.72	0.42
1:D:646:ASN:OD1	1:D:679:TRP:NE1	2.52	0.42
1:D:673:ARG:O	1:D:676:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:TYR:CE2	1:B:622:SER:HA	2.54	0.42
1:D:668:LEU:HG	1:D:677:TRP:HE3	1.84	0.42
1:C:713:TYR:O	1:C:714:ALA:CB	2.68	0.42
1:D:670:ASP:HA	1:D:676:GLU:O	2.20	0.42
1:C:616:ASP:OD2	1:C:733:ASP:OD2	2.38	0.42
1:D:614:PHE:O	1:D:615:THR:HB	2.20	0.42
1:D:674:GLU:OE2	1:D:707:ASP:OD1	2.38	0.42
1:C:613:ASN:HD21	1:C:734:ARG:NH2	2.11	0.42
1:C:696:ASP:OD2	1:C:698:TRP:HB2	2.20	0.42
1:A:683:THR:CG2	1:A:684:SER:N	2.83	0.41
1:B:661:ARG:HG3	1:B:713:TYR:CD2	2.55	0.41
1:A:722:CYS:O	1:A:723:GLU:HB2	2.19	0.41
1:C:670:ASP:OD1	1:C:707:ASP:HA	2.21	0.41
1:D:731:GLU:HG2	1:D:732:LYS:N	2.35	0.41
1:C:613:ASN:ND2	1:C:734:ARG:NH2	2.68	0.41
1:A:667:GLY:O	1:A:679:TRP:HE3	2.04	0.41
1:C:642:LEU:HD12	1:C:680:LEU:HD11	2.01	0.41
1:B:712:ILE:HG23	1:B:713:TYR:O	2.21	0.41
1:C:655:LYS:HD3	1:C:656:LYS:HZ2	1.86	0.41
1:A:620:TYR:O	1:A:729:ILE:HA	2.21	0.41
1:C:665:TRP:HZ3	1:C:708:CYS:O	2.04	0.41
1:B:612:LYS:HE2	5:B:746:HOH:O	2.22	0.40
1:D:627:ILE:CG2	1:D:628:PHE:N	2.85	0.40
1:D:661:ARG:N	1:D:661:ARG:CD	2.84	0.40
1:A:668:LEU:HG	1:A:677:TRP:HE3	1.86	0.40
1:D:677:TRP:CH2	1:D:719:ASP:HB3	2.56	0.40
1:B:673:ARG:CZ	1:B:676:GLU:OE1	2.70	0.40
1:C:612:LYS:HE2	1:C:621:PHE:CD1	2.57	0.40
1:D:621:PHE:CZ	1:D:654:ILE:HG23	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/140 (91%)	114 (90%)	9 (7%)	4 (3%)	5	6
1	B	127/140 (91%)	111 (87%)	12 (9%)	4 (3%)	5	6
1	C	127/140 (91%)	98 (77%)	21 (16%)	8 (6%)	1	1
1	D	127/140 (91%)	102 (80%)	14 (11%)	11 (9%)	1	1
All	All	508/560 (91%)	425 (84%)	56 (11%)	27 (5%)	2	2

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	692	ALA
1	C	622	SER
1	C	681	ASP
1	C	714	ALA
1	C	723	GLU
1	D	627	ILE
1	D	681	ASP
1	D	714	ALA
1	A	714	ALA
1	B	714	ALA
1	C	725	VAL
1	D	667	GLY
1	D	683	THR
1	D	716	GLN
1	A	686	ASP
1	D	615	THR
1	B	674	GLU
1	C	615	THR
1	D	722	CYS
1	A	680	LEU
1	D	680	LEU
1	A	701	GLY
1	C	700	HIS
1	D	701	GLY
1	B	701	GLY
1	C	659	VAL
1	D	685	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/125 (92%)	107 (93%)	8 (7%)	18	33
1	B	115/125 (92%)	112 (97%)	3 (3%)	51	78
1	C	115/125 (92%)	108 (94%)	7 (6%)	22	40
1	D	115/125 (92%)	109 (95%)	6 (5%)	27	49
All	All	460/500 (92%)	436 (95%)	24 (5%)	27	49

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	639	SER
1	A	661	ARG
1	A	662	GLU
1	A	696	ASP
1	A	711	LEU
1	A	716	GLN
1	A	720	PHE
1	A	724	ASP
1	B	661	ARG
1	B	662	GLU
1	B	712	ILE
1	C	637	ASP
1	C	647	THR
1	C	648	ARG
1	C	661	ARG
1	C	662	GLU
1	C	717	TRP
1	C	724	ASP
1	D	647	THR
1	D	648	ARG
1	D	661	ARG
1	D	662	GLU
1	D	681	ASP
1	D	716	GLN

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

Mol	Chain	Res	Type
1	A	613	ASN
1	A	689	ASN
1	A	716	GLN
1	B	675	ASN
1	B	721	GLN
1	C	613	ASN
1	C	646	ASN
1	C	689	ASN
1	C	694	GLN
1	C	716	GLN
1	C	726	ASN
1	D	613	ASN
1	D	646	ASN
1	D	689	ASN
1	D	694	GLN
1	D	697	ASN
1	D	716	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 34 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	129/140 (92%)	-0.41	1 (0%) 86 86	9, 29, 47, 58	0
1	B	129/140 (92%)	-0.32	1 (0%) 86 86	12, 30, 49, 56	0
1	C	129/140 (92%)	1.83	46 (35%) 0 0	17, 33, 44, 48	129 (100%)
1	D	129/140 (92%)	2.07	57 (44%) 0 0	20, 35, 44, 48	129 (100%)
All	All	516/560 (92%)	0.79	105 (20%) 1 1	9, 33, 47, 58	258 (50%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	702	HIS	14.4
1	C	627	ILE	8.3
1	D	704	PRO	8.3
1	C	722	CYS	7.4
1	C	606	SER	7.1
1	C	671	SER	6.2
1	D	684	SER	6.2
1	D	614	PHE	6.1
1	D	685	PRO	6.0
1	D	658	MET	5.9
1	C	701	GLY	5.8
1	D	607	CYS	5.6
1	C	659	VAL	5.4
1	D	638	LYS	5.4
1	C	637	ASP	5.4
1	C	626	GLU	5.3
1	D	627	ILE	5.3
1	D	721	GLN	5.2
1	C	628	PHE	5.2
1	C	683	THR	5.2
1	D	636	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	640	SER	4.9
1	D	693	GLY	4.8
1	D	722	CYS	4.8
1	C	704	PRO	4.7
1	D	708	CYS	4.6
1	D	725	VAL	4.5
1	D	615	THR	4.4
1	D	712	ILE	4.4
1	D	668	LEU	4.3
1	D	626	GLU	4.3
1	C	720	PHE	4.3
1	D	637	ASP	4.2
1	C	729	ILE	4.0
1	D	690	TRP	4.0
1	D	618	CYS	4.0
1	D	672	GLU	3.9
1	D	734	ARG	3.9
1	C	684	SER	3.8
1	C	721	GLN	3.8
1	C	723	GLU	3.8
1	D	609	PRO	3.7
1	D	608	PRO	3.7
1	C	614	PHE	3.6
1	C	673	ARG	3.5
1	C	708	CYS	3.5
1	D	702	HIS	3.5
1	D	659	VAL	3.5
1	D	606	SER	3.5
1	C	624	GLU	3.5
1	D	680	LEU	3.4
1	C	711	LEU	3.3
1	D	628	PHE	3.3
1	D	624	GLU	3.3
1	B	708	CYS	3.2
1	D	698	TRP	3.2
1	C	703	GLY	3.2
1	A	701	GLY	3.1
1	D	720	PHE	3.1
1	D	713	TYR	3.0
1	C	675	ASN	2.9
1	D	634	PHE	2.9
1	D	675	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	653	TRP	2.9
1	C	713	TYR	2.9
1	D	660	GLY	2.8
1	C	724	ASP	2.8
1	C	712	ILE	2.8
1	C	639	SER	2.7
1	C	698	TRP	2.7
1	D	711	LEU	2.6
1	D	701	GLY	2.6
1	C	656	LYS	2.6
1	D	729	ILE	2.6
1	D	710	GLY	2.5
1	C	666	ILE	2.5
1	D	653	TRP	2.5
1	C	714	ALA	2.5
1	C	658	MET	2.5
1	D	723	GLU	2.4
1	D	709	ALA	2.4
1	D	696	ASP	2.4
1	D	657	GLN	2.4
1	D	633	LEU	2.4
1	D	623	VAL	2.4
1	C	613	ASN	2.4
1	C	672	GLU	2.4
1	D	692	ALA	2.3
1	C	661	ARG	2.3
1	C	634	PHE	2.3
1	C	710	GLY	2.2
1	D	654	ILE	2.2
1	C	669	THR	2.2
1	D	694	GLN	2.1
1	D	617	LYS	2.1
1	C	692	ALA	2.1
1	C	709	ALA	2.1
1	D	655	LYS	2.1
1	C	734	ARG	2.1
1	D	666	ILE	2.1
1	C	670	ASP	2.1
1	C	618	CYS	2.1
1	D	682	GLY	2.0
1	D	673	ARG	2.0
1	C	616	ASP	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	CL	A	8	1/1	1.00	0.10	-0.42	37,37,37,37	0
2	ZN	B	1	1/1	1.00	0.10	-0.46	15,15,15,15	0
2	ZN	B	3	1/1	1.00	0.10	-0.47	27,27,27,27	0
2	ZN	A	3	1/1	0.99	0.08	-0.54	32,32,32,32	0
2	ZN	A	1	1/1	0.99	0.09	-0.89	19,19,19,19	0
3	CL	C	3	1/1	0.95	0.17	-0.94	43,43,43,43	1
3	CL	D	4	1/1	1.00	0.13	-0.99	44,44,44,44	1
4	CA	C	8	1/1	0.97	0.20	-1.02	37,37,37,37	1
2	ZN	D	1	1/1	0.99	0.10	-1.50	31,31,31,31	1
2	ZN	A	2	1/1	0.99	0.07	-1.64	22,22,22,22	0
3	CL	D	5	1/1	0.99	0.05	-1.91	23,23,23,23	1
3	CL	B	8	1/1	1.00	0.07	-1.97	34,34,34,34	0
3	CL	D	3	1/1	0.80	0.11	-2.00	62,62,62,62	1
4	CA	D	6	1/1	0.93	0.12	-2.08	33,33,33,33	1
2	ZN	A	5	1/1	0.99	0.05	-2.14	34,34,34,34	0
2	ZN	C	1	1/1	0.99	0.08	-2.16	39,39,39,39	1
2	ZN	D	2	1/1	0.98	0.05	-2.25	35,35,35,35	1
3	CL	A	7	1/1	0.99	0.06	-2.26	18,18,18,18	0
3	CL	C	4	1/1	0.98	0.06	-2.31	47,47,47,47	1
3	CL	C	5	1/1	0.98	0.06	-2.67	25,25,25,25	1
2	ZN	B	2	1/1	1.00	0.07	-2.77	25,25,25,25	0
4	CA	C	7	1/1	0.76	0.13	-2.90	48,48,48,48	1
2	ZN	C	2	1/1	0.98	0.06	-3.00	36,36,36,36	1
3	CL	B	7	1/1	0.99	0.05	-3.00	14,14,14,14	0
2	ZN	B	4	1/1	1.00	0.05	-3.01	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	C	6	1/1	0.93	0.10	-3.12	26,26,26,26	1
2	ZN	A	4	1/1	1.00	0.04	-4.63	34,34,34,34	0
4	CA	D	7	1/1	0.93	0.10	-6.50	28,28,28,28	1
2	ZN	D	9	1/1	0.97	0.08	-	42,42,42,42	1
4	CA	D	8	1/1	0.97	0.19	-	30,30,30,30	1
3	CL	A	6	1/1	1.00	0.10	-	39,39,39,39	0
2	ZN	C	9	1/1	0.97	0.10	-	35,35,35,35	1
3	CL	B	6	1/1	0.96	0.23	-	22,22,22,22	0
2	ZN	B	5	1/1	0.97	0.06	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.